



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 04:54 am BST

PDB ID : 8PEG / pdb_00008peg
EMDB ID : EMD-17631
Title : Escherichia coli paused disome complex (queueing 70S non-rotated closed PRE state)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-06-13
Resolution : 3.30 Å(reported)
Based on initial model : 7N1P

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

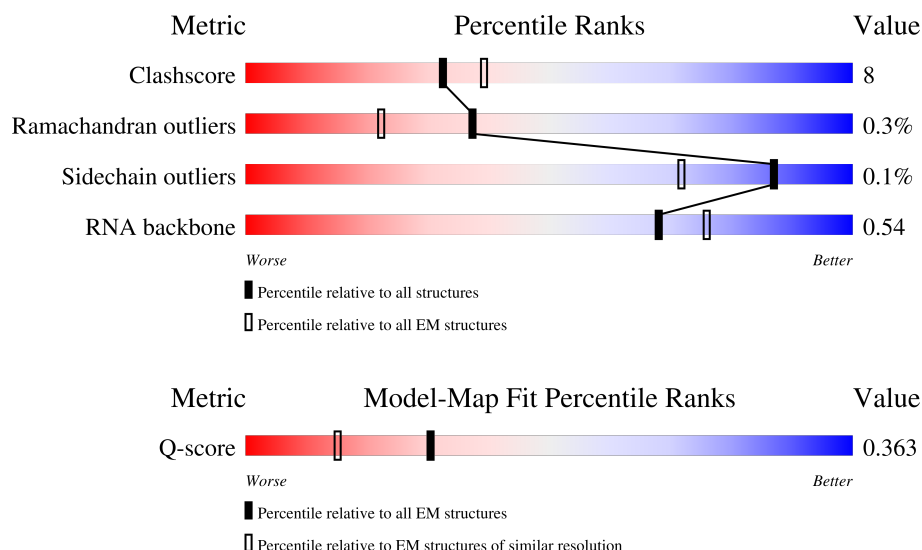
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	38	
2	1	78	
3	2	63	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	59	
5	4	70	
6	5	57	
7	6	65	
8	7	2903	
9	8	120	
10	A	1542	
11	B	241	
12	C	233	
13	D	206	
14	E	167	
15	F	135	
16	G	179	
17	H	130	
18	I	130	
19	J	103	
20	K	129	
21	L	124	
22	M	118	
23	N	101	
24	O	89	
25	P	82	
26	Q	84	
27	R	75	
28	S	92	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	T	87	
30	U	71	
31	V	30	
32	W	76	
33	X	78	
34	Y	76	
35	Z	557	
36	a	234	
37	b	273	
38	c	209	
39	d	201	
40	e	179	
41	f	177	
42	g	55	
43	h	136	
44	i	149	
45	j	165	
46	k	142	
47	l	46	
48	m	142	
49	n	123	
50	o	144	
51	p	18	
52	q	127	
53	r	117	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	s	115	
55	t	118	
56	u	103	
57	v	110	
58	w	100	
59	x	104	
60	y	94	
61	z	85	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153284 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 2 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 4 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 6 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	2903	Total	C	N	O	P	0	0
			62335	27815	11467	20150	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		

- Molecule 11 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	224	Total	C	N	O	S	0	0
			1751	1108	314	321	8		

- Molecule 12 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 15 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 16 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 20 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 21 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 22 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 24 is a protein called 30S ribosomal protein S15.

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

- Molecule 25 is a protein called 30S ribosomal protein S16.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 27 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	74	Total	C	N	O	S	0	0
			624	395	122	105	2		

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 29 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	30	Total	C	N	O	P	0	0
			648	290	124	204	30		

- Molecule 32 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
32	W	76	Total	C	N	O	P	S	0	0
			1632	731	289	534	76	2		

- Molecule 33 is a RNA chain called tRNA-Ser (E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	X	78	Total	C	N	O	P	S	0	0
			1683	750	304	548	78	3		

- Molecule 34 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Y	76	Total	C	N	O	P	S	0	0
			1631	728	292	534	76	1		

- Molecule 35 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Z	170	Total	C	N	O		
			1319	830	228	261	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	a	134	Total	C	N	O	S	
			1026	645	186	193	2	0

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	b	271	Total	C	N	O	S	
			2082	1288	423	364	7	0

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	e	178	Total	C	N	O	S	
			1420	905	251	258	6	0

- Molecule 41 is a protein called 50S ribosomal protein L6.

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

- Molecule 42 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	g	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 43 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 44 is a protein called 50S ribosomal protein L9.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 46 is a protein called 50S ribosomal protein L11.

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

- Molecule 47 is a protein called 50S ribosomal protein L34.

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

- Molecule 48 is a protein called 50S ribosomal protein L13.

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

- Molecule 49 is a protein called 50S ribosomal protein L14.

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

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

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

- Molecule 51 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	p	18	Total	C	N	O	0	0
			101	63	18	20		

- Molecule 52 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	q	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 53 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	r	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 54 is a protein called 50S ribosomal protein L19.

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

- Molecule 55 is a protein called 50S ribosomal protein L20.

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

- Molecule 56 is a protein called 50S ribosomal protein L21.

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

- Molecule 57 is a protein called 50S ribosomal protein L22.

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

- Molecule 58 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 59 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	x	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 60 is a protein called 50S ribosomal protein L25.

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

- Molecule 61 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	z	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

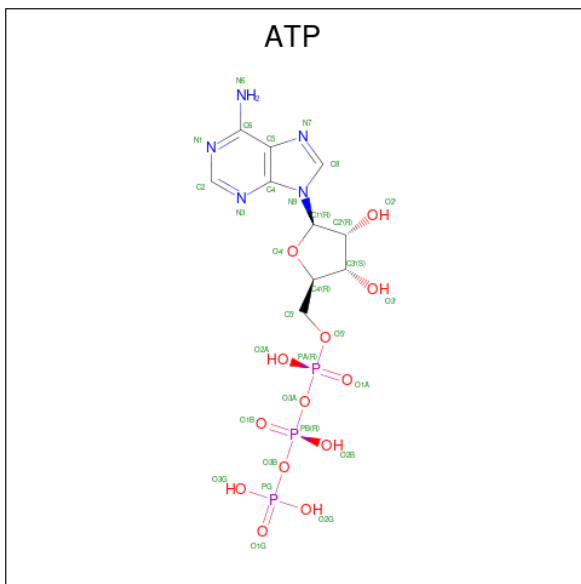
- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	0	1	Total	Zn	0
			1	1	
62	4	1	Total	Zn	0
			1	1	

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
63	7	193	Total Mg 193 193	0
63	A	63	Total Mg 63 63	0
63	X	1	Total Mg 1 1	0
63	Y	1	Total Mg 1 1	0
63	b	1	Total Mg 1 1	0
63	o	1	Total Mg 1 1	0

- Molecule 64 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

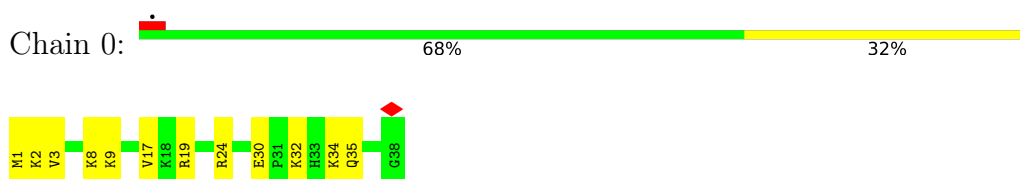


Mol	Chain	Residues	Atoms					AltConf
64	7	1	Total 31	C 10	N 5	O 13	P 3	0
64	7	1	Total 31	C 10	N 5	O 13	P 3	0

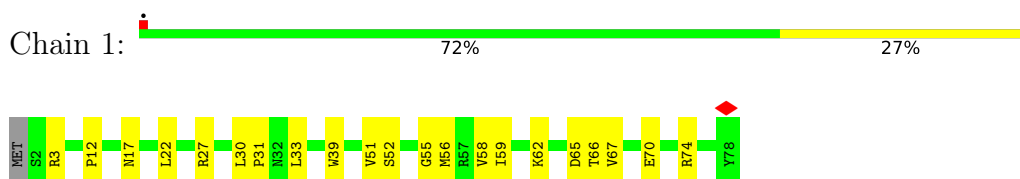
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

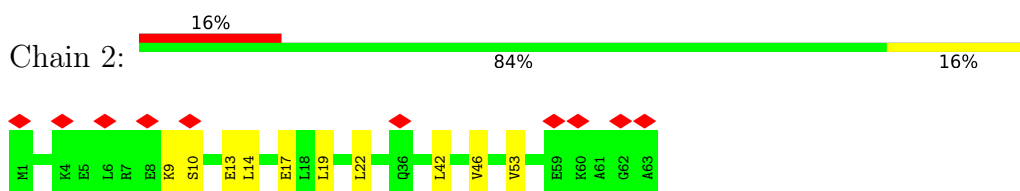
- Molecule 1: 50S ribosomal protein L36



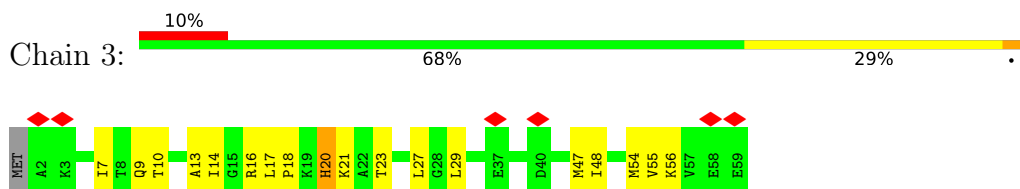
- Molecule 2: 50S ribosomal protein L28



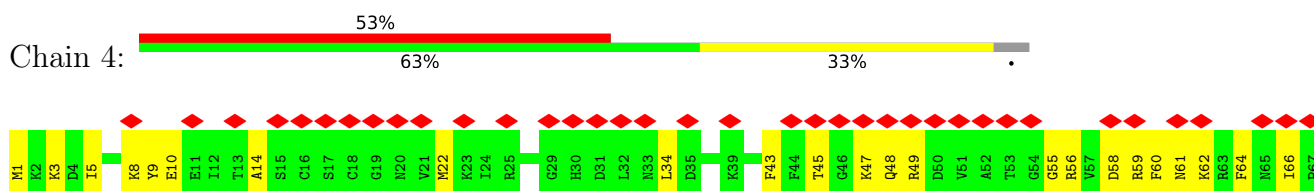
- Molecule 3: 50S ribosomal protein L29



- Molecule 4: 50S ribosomal protein L30

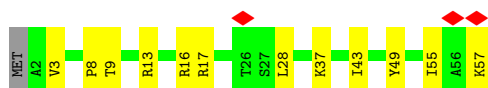
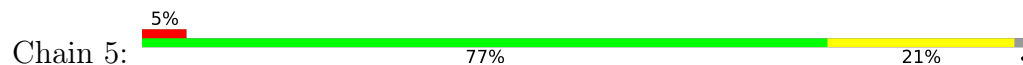


- Molecule 5: Large ribosomal subunit protein bL31A

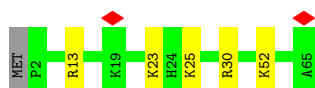
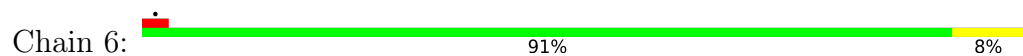


GLY
SER
LYS

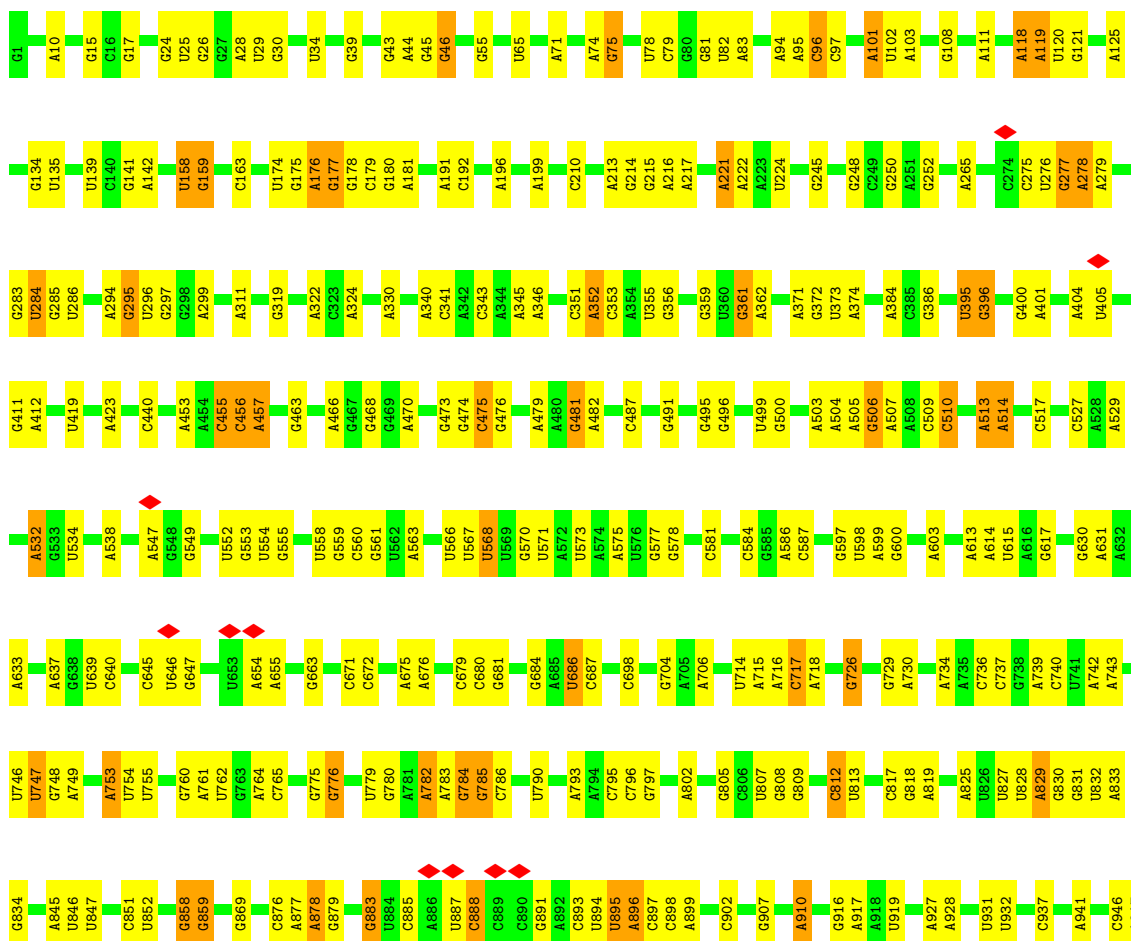
• Molecule 6: 50S ribosomal protein L32



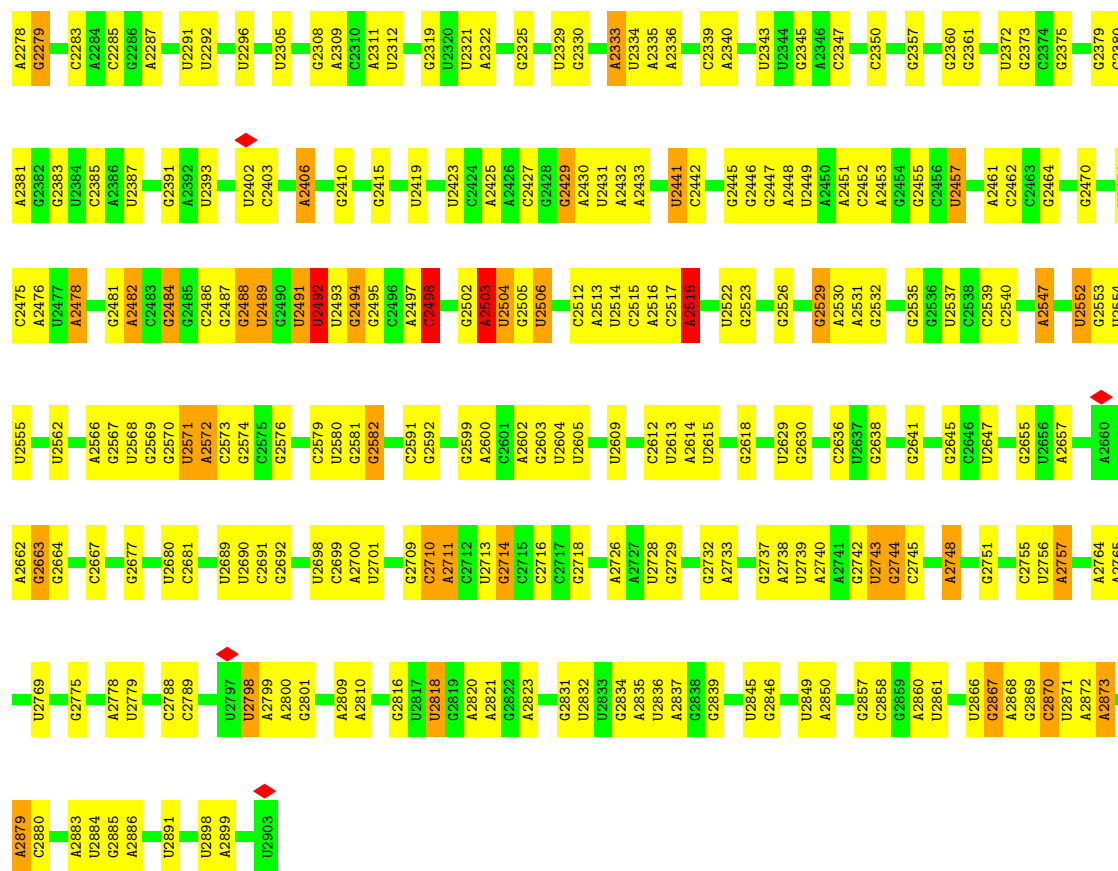
• Molecule 7: 50S ribosomal protein L35



• Molecule 8: 23S ribosomal RNA



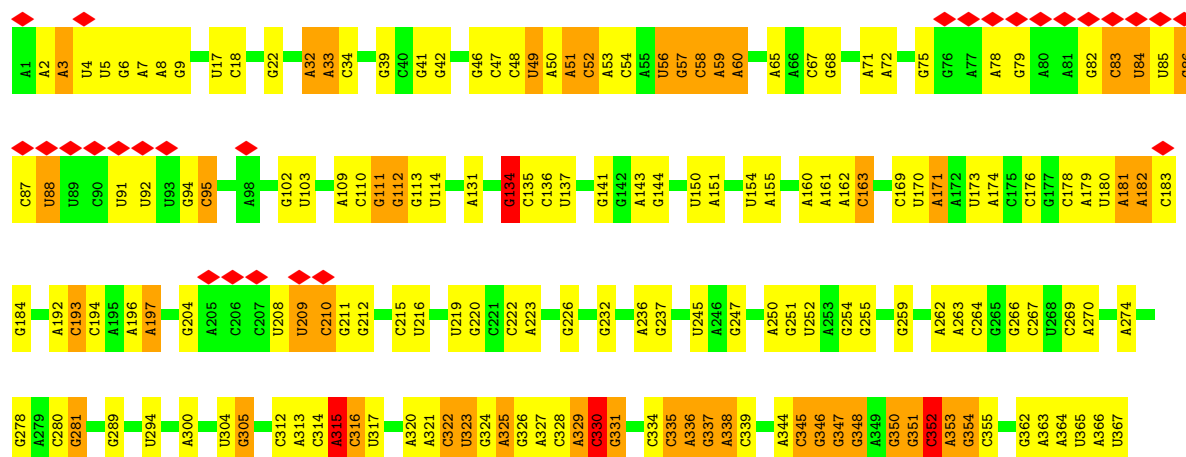
C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2185	G2186	A2188	A2189	A2190	A2198	C2200	G2201	G2204	G2209	U2210	A2211	A2212	U2213	C2214	A2225	U2233	G2234	G2237	G2238	C2239	U2240	A2241	G2242	U2243	G2246	A2247	C2248	G2251	C2258	U2262	C2263	C2264	A2267	A2268	C2269	A2270	G2271	U2272	A2273													
U2118	A2119	G2120	G2121	G2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	A2142	C2143	G2144	C2145	C2146	A2147	G2148	U2149	C2150	U2151	G2152	C2153	A2154	U2155	G2156	A2157	A2158	G2159	C2160	C2161	G2162	A2163	C2164	G2165	U2166	U2167	G2168	A2169	A2170	U2171	U2172	A2173	C2174	C2175	A2176	C2177
A2020	C2021	U2022	C2023	C2024	C2025	U2026	G2027	A2030	A2031	G2032	A2033	U2034	G2035	U2039	G2040	U2041	A2042	C2043	C2047	A2052	C2055	G2056	A2059	A2060	G2061	A2062	G2069	A2070	A2071	C1986	U1991	G1992	U1993	C1996	C1997	A1998	C1999	C2000	C2008	A2009	G2010	U2011	G2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019									
3TD1915	A1916	U1917	G1929	G1930	A1936	U1939	U1940	U1943	A1952	A1953	G1954	U1955	U1956	A1960	A1966	C1967	A1970	U1971	G1972	G1975	A1978	U1982	U1983	C1986	U1991	G1992	U1993	C1996	C1997	A1998	C1999	C2000	C2008	A2009	G2010	U2011	G2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019															
A1789	C1790	A1791	A1794	C1795	U1796	U1797	U1798	C1800	A1801	G1807	A1808	A1809	A1810	G1811	C1816	G1817	U1818	A1819	U1820	G1824	U1825	G1826	U1827	G1828	C1833	U1834	G1835	C1836	A1847	A1848	U1852	C1870	A1871	G1872	G1873	U1880	C1881	G2009	G2010	U2011	G2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019											
G1645	C1646	U1647	G1648	G1649	G1653	G1659	A1664	G1674	C1675	A1676	G1697	G1703	C1704	A1713	U1714	G1715	U1716	A1717	C1727	G1728	U1729	C1730	G1731	G1738	U1742	G1743	A1744	U1751	C1752	G1753	A1754	U1755	G1756	A1759	C1764	A1773	U1779	A1783	A1784	A1785	A1786																		
G1527	A1528	A1532	A1535	C1536	G1537	U1538	U1539	U1542	G1543	A1544	C1556	C1557	A1566	A1569	A1570	A1571	U1578	A1579	C1581	G1582	A1583	U1584	G1585	A1586	G1587	U1594	C1595	A1596	A1597	U1598	U1599	C1600	G1601	U1602	A1603	C1604	C1607	A1608	A1609	A1610	C1615	A1616	C1617	A1618	G1622	C1638													
G1416	C1417	G1418	A1419	A1420	A1427	C1428	A1431	A1432	A1433	A1434	C1447	G1452	A1453	C1454	G1455	C1461	A1469	A1470	G1475	U1476	A1477	G1478	G1482	U1486	U1487	C1488	C1489	A1490	G1491	G1492	C1493	A1494	U1497	A1503	A1504	A1505	U1506	C1507	A1508	A1509	U1513	G1514	A1515	G1524															
U1183	U1184	U1185	G1186	U1187	U1188	A1189	G1190	A1194	U1198	U1199	C1200	U1201	G1202	U1203	A1204	A1205	A1213	A1214	G1215	G1223	A1226	U1230	U1231	U1234	G1235	G1236	A1237	G1238	G1239	C1243	A1244	G1245	A1246	G1247	U1249	G1250	A1253	G1256	A1262	U1263	A1264	G1265	U1267	C1270	G1271														
C1102	A1103	C1104	U1105	G1106	U1107	U1108	G1109	G1110	A1111	G1112	G1115	G1122	G1123	A1126	G1128	A1129	U1130	G1131	A1133	A1134	C1135	G1136	G1137	G1138	G1139	U1141	A1142	A1143	A1144	G1149	C1153	G1154	C1161	G1167	G1168	A1169	G1171	U1173	U1174	A1175	U1176	G1177	C1178	U1180	U1181	G1182													
G1034	U1035	A1040	C1043	C1044	C1045	A1046	G1047	C1053	A1054	G1055	G1056	A1057	U1058	G1059	U1060	U1061	A1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	U1073	G1074	C1075	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	C1089	A1090	G1091	G1092	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101				
C948		U955	U958	A959	A960	C961	A962	U967	C968			G971	A972	A973	G974	A979	A980	A981	C982	A983	A984	C987	A988	G989	A990	C995	A996	G997	C998	U999	A1000	C1005	C1006	U1012	C1013	U1019	A1020	A1021	G1022	U1023	G1024	G1025	G1026	A1027	A1028	U1029	C1030	G1031	U1033										

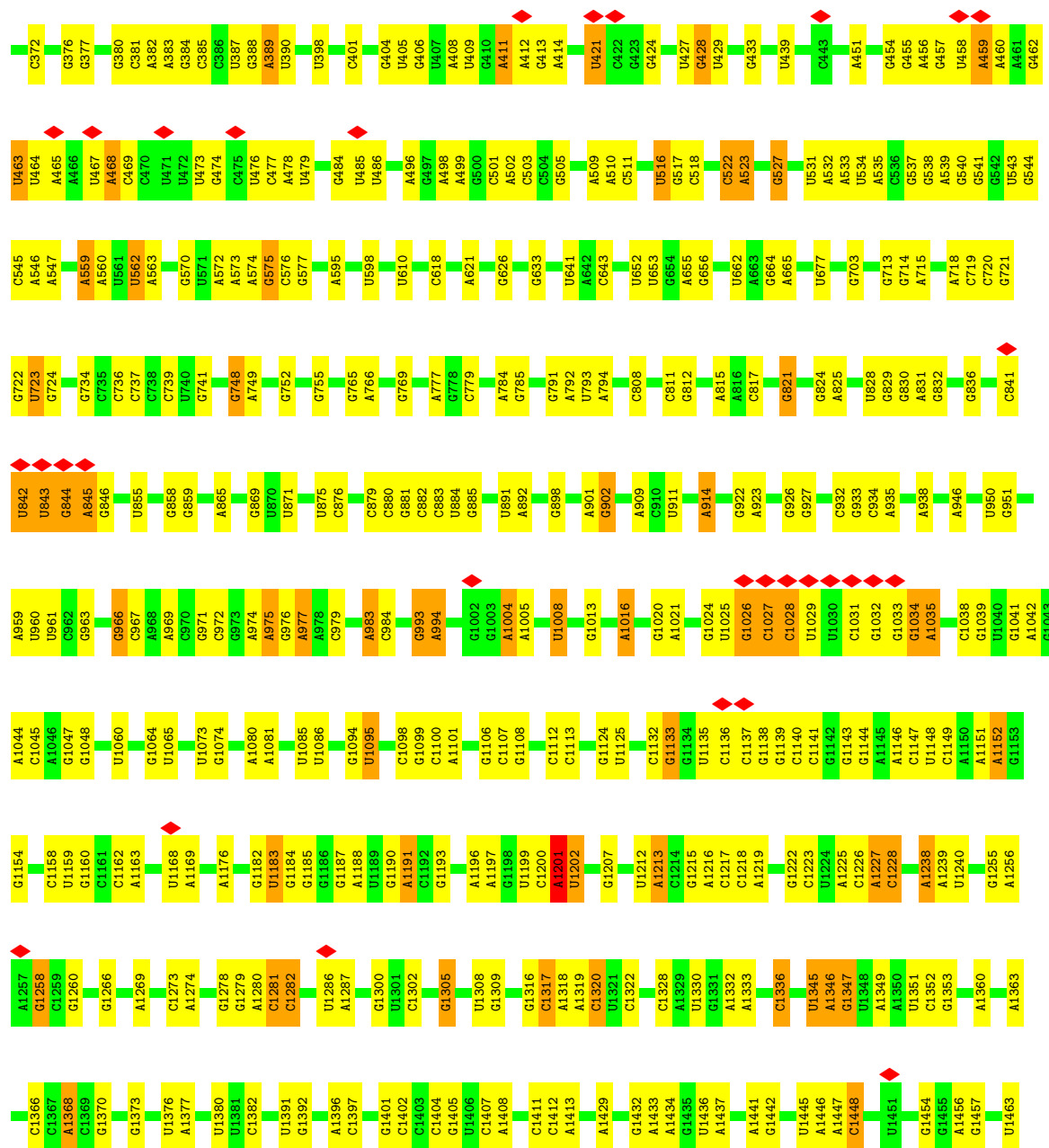


• Molecule 9: 5S ribosomal RNA

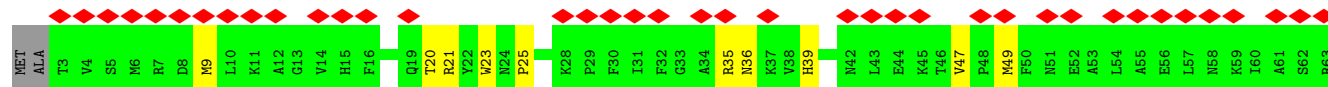


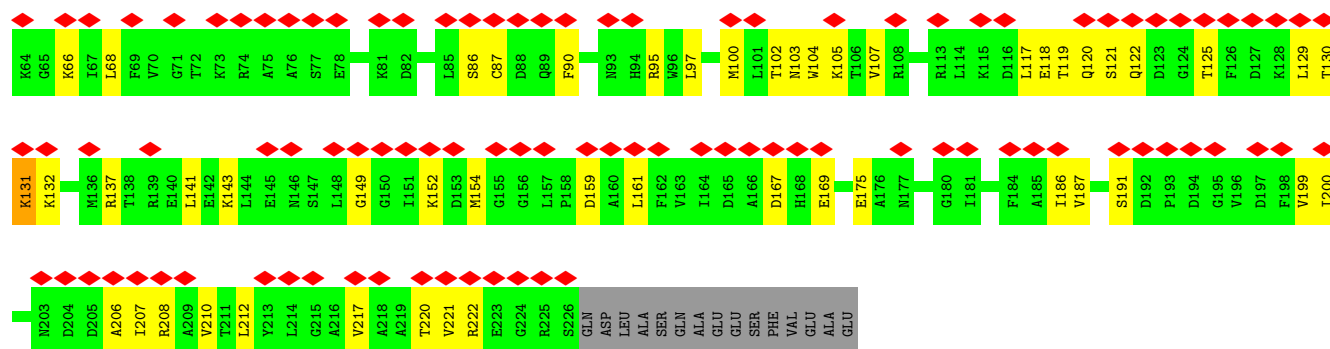
• Molecule 10: 16S ribosomal RNA



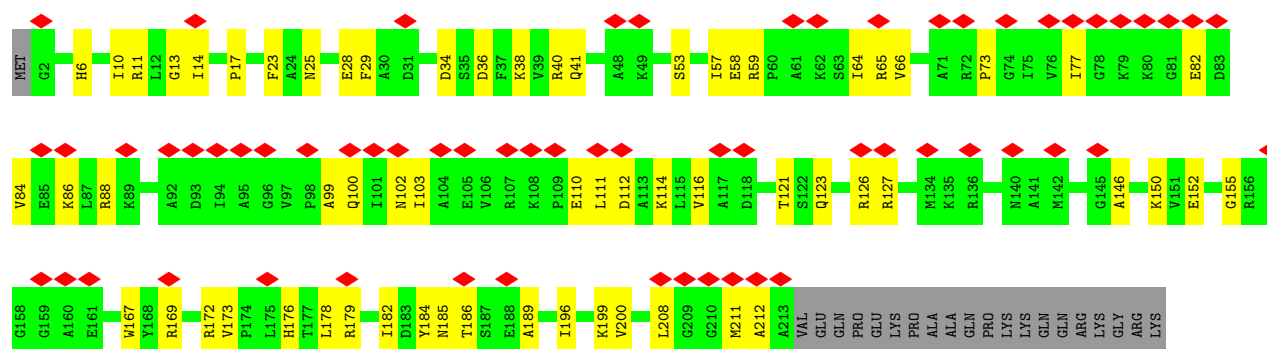


• Molecule 11: Small ribosomal subunit protein uS2

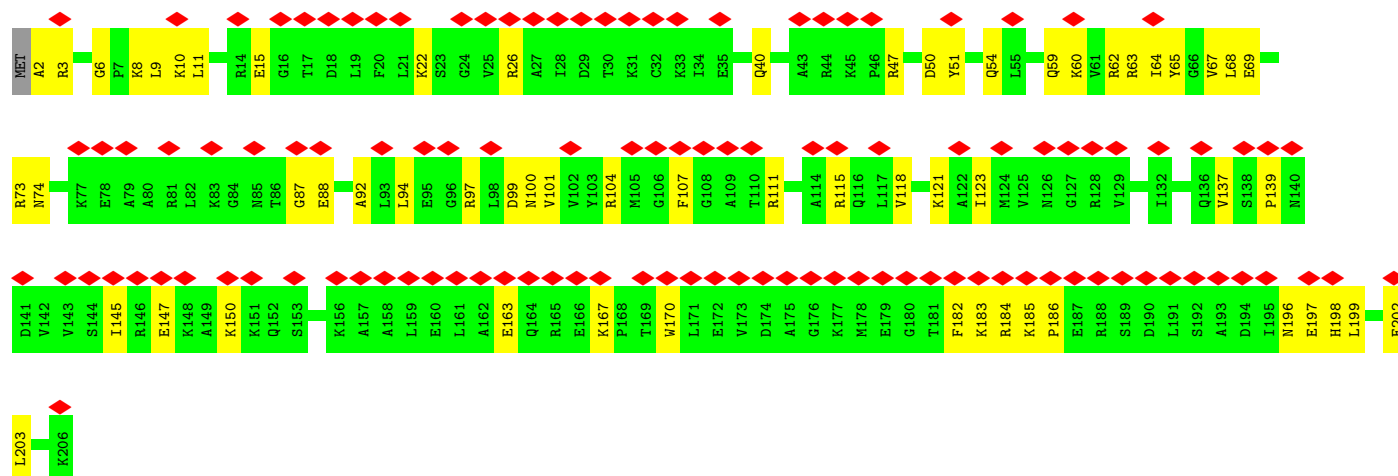
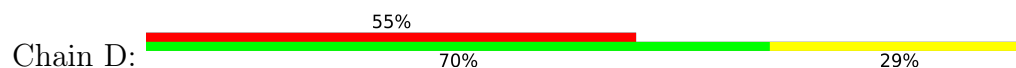




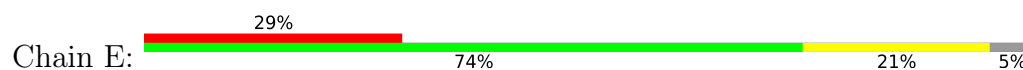
• Molecule 12: Small ribosomal subunit protein uS3

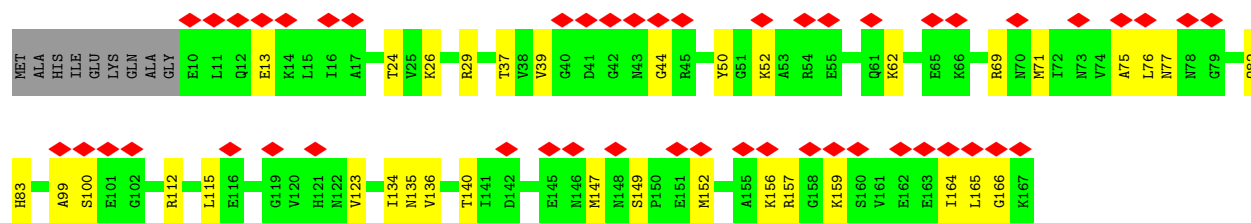


• Molecule 13: Small ribosomal subunit protein uS4

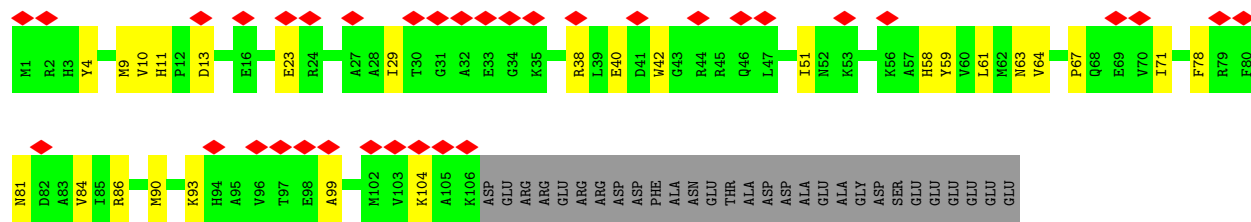


• Molecule 14: Small ribosomal subunit protein uS5

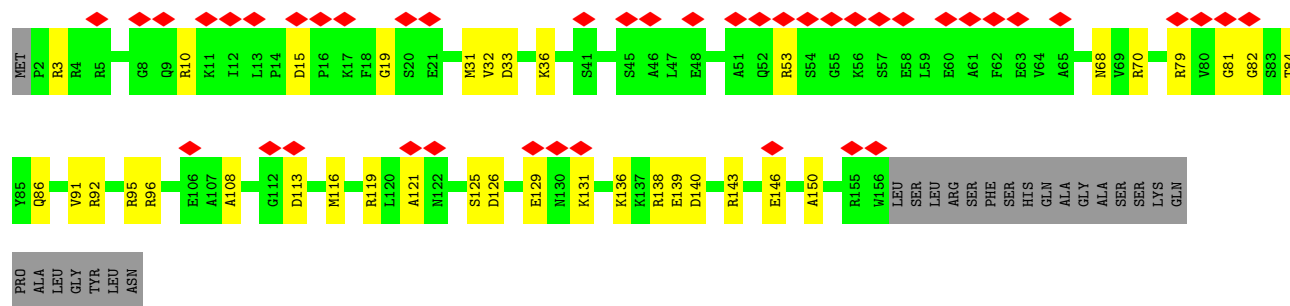




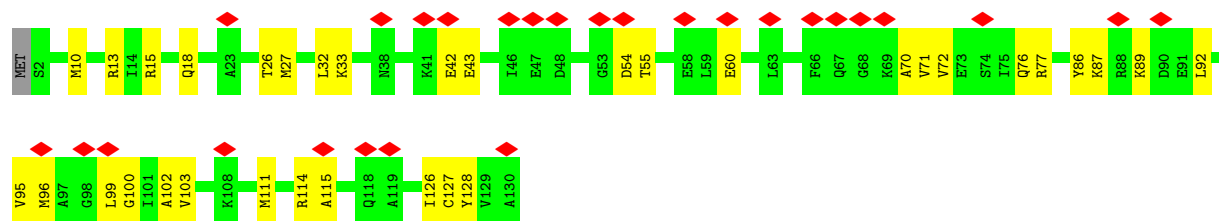
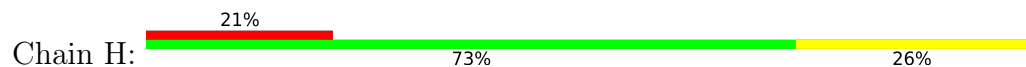
• Molecule 15: 30S ribosomal protein S6



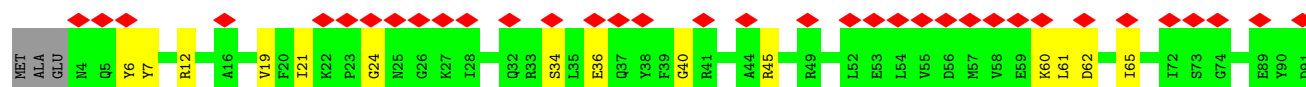
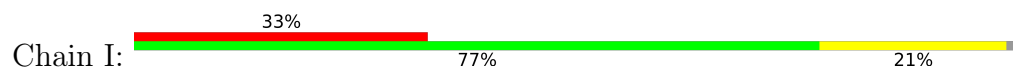
• Molecule 16: 30S ribosomal protein S7

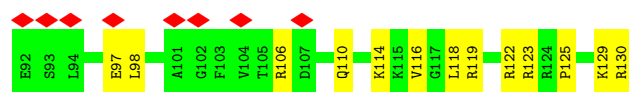


• Molecule 17: Small ribosomal subunit protein uS8

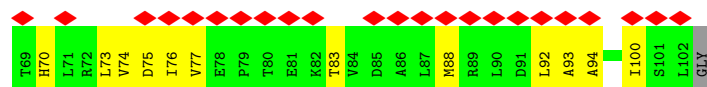
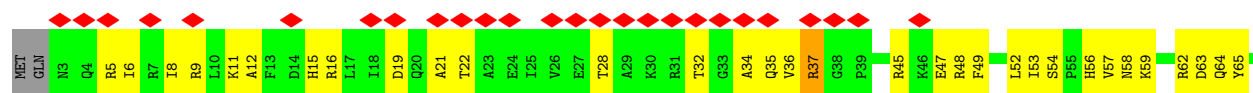


• Molecule 18: Small ribosomal subunit protein uS9

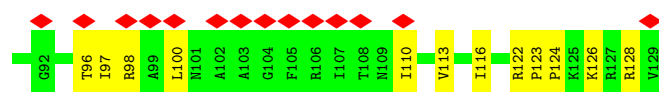
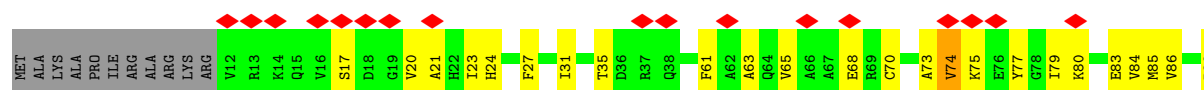




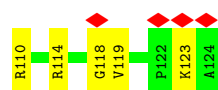
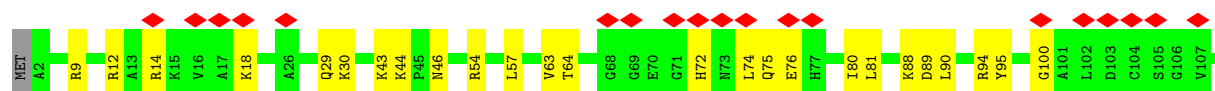
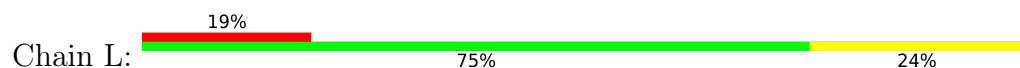
- Molecule 19: 30S ribosomal protein S10



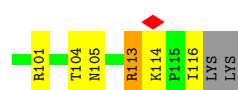
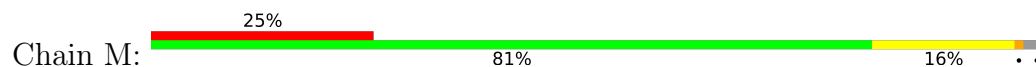
- Molecule 20: Small ribosomal subunit protein uS11



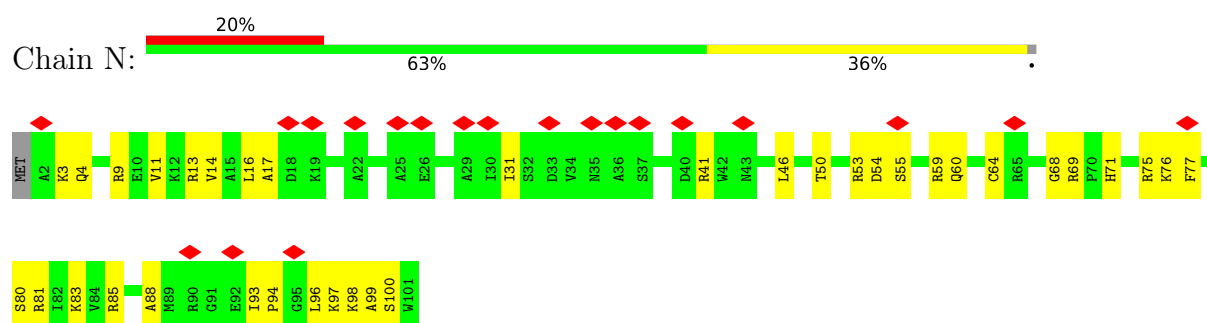
- Molecule 21: Small ribosomal subunit protein uS12



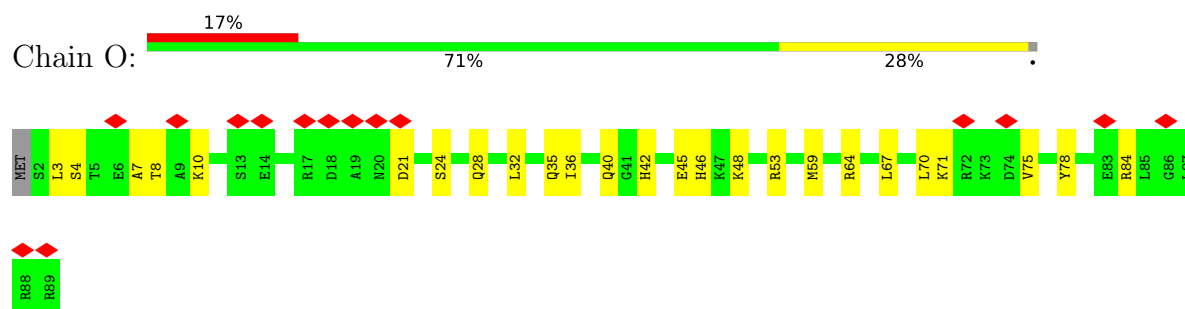
- Molecule 22: Small ribosomal subunit protein uS13



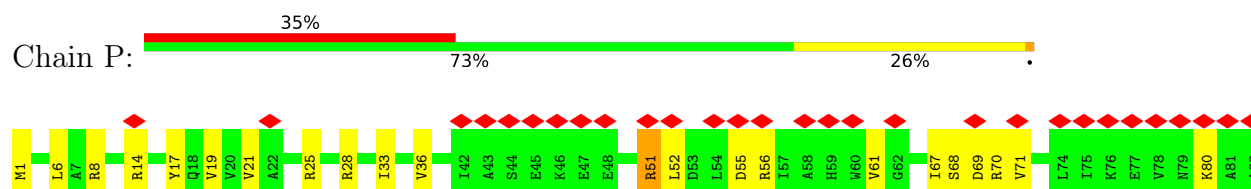
- Molecule 23: Small ribosomal subunit protein uS14



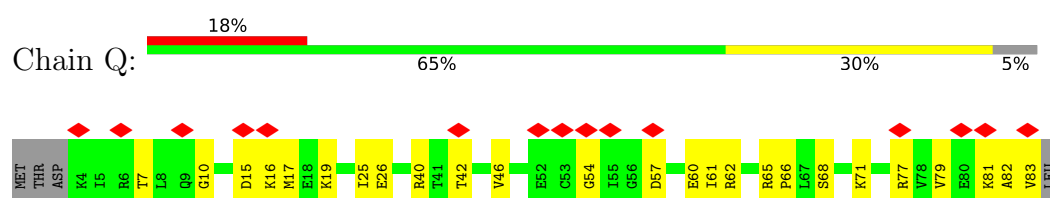
- Molecule 24: 30S ribosomal protein S15



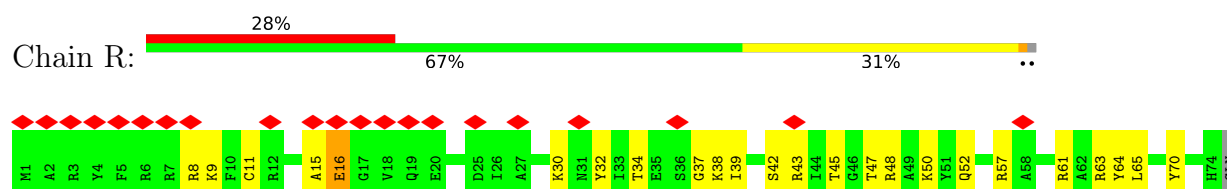
- Molecule 25: 30S ribosomal protein S16



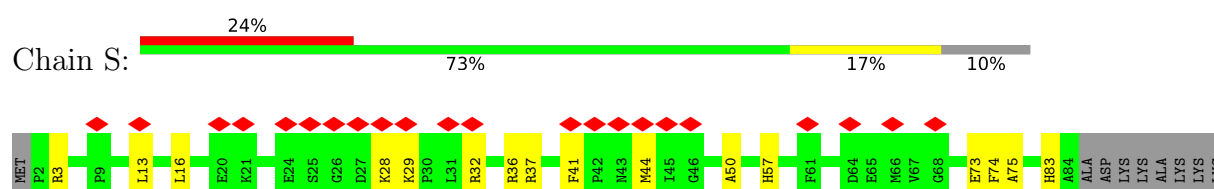
- Molecule 26: Small ribosomal subunit protein uS17



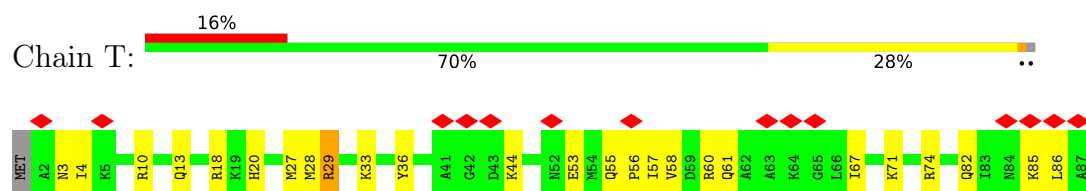
- Molecule 27: Small ribosomal subunit protein bS18



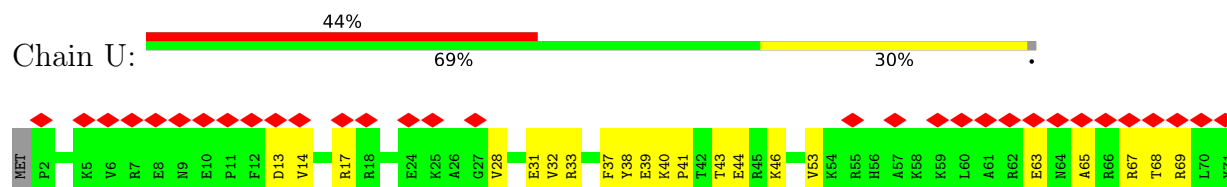
- Molecule 28: Small ribosomal subunit protein uS19



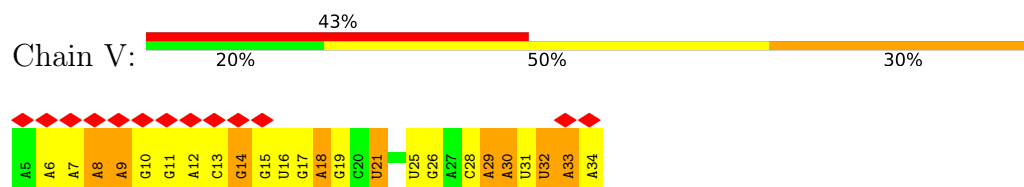
- Molecule 29: Small ribosomal subunit protein bS20



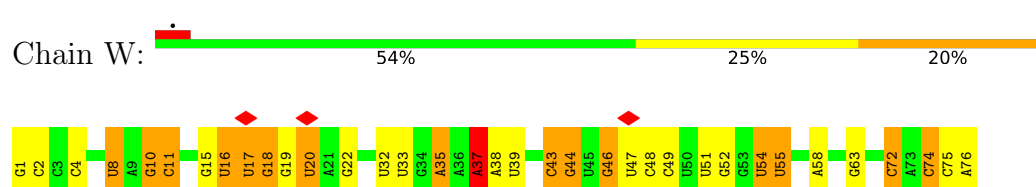
- Molecule 30: 30S ribosomal protein S21



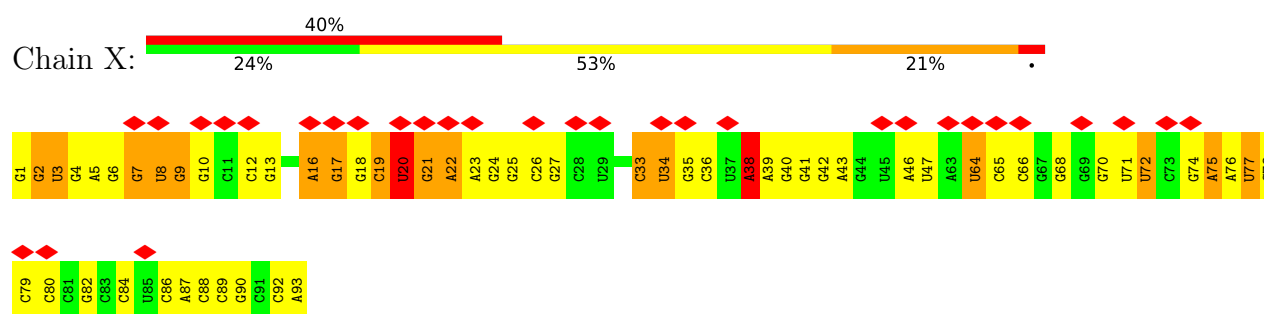
- Molecule 31: mRNA



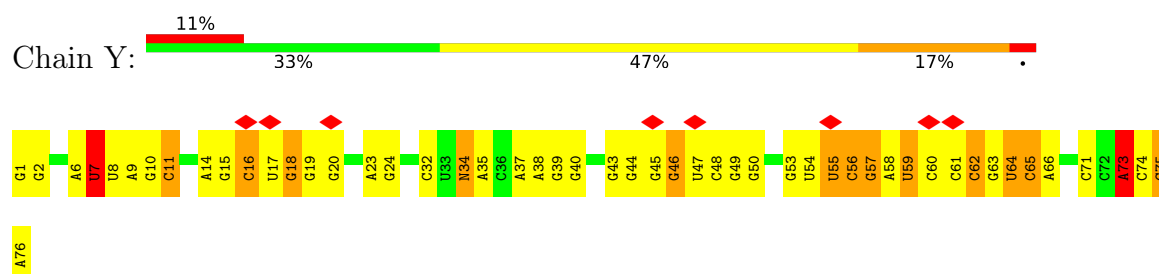
- Molecule 32: tRNA-Phe (P-site)



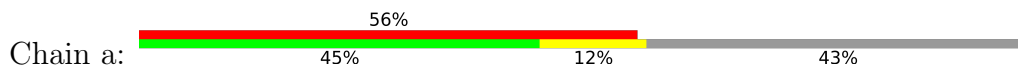
- Molecule 33: tRNA-Ser (E-site)



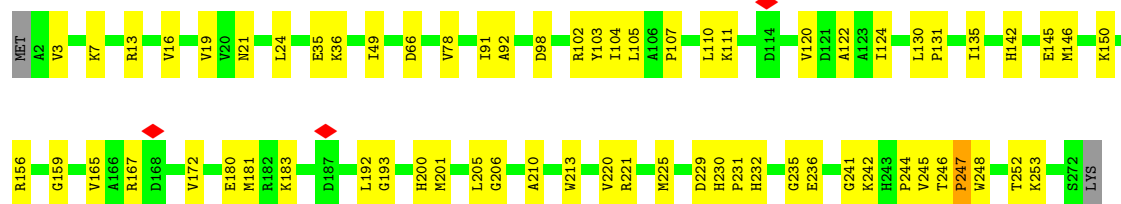
- Molecule 34: tRNA-Val (A-site)



Chain Z:

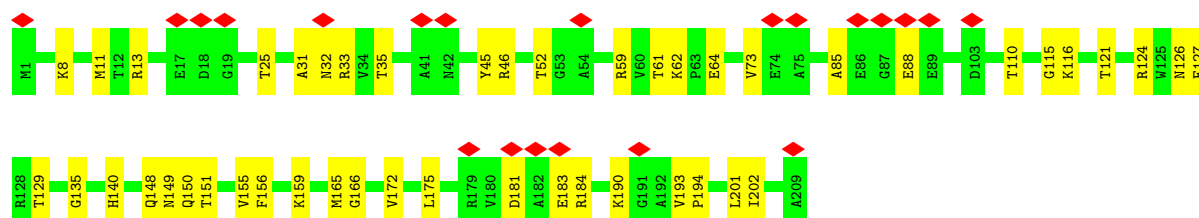


Chain b: 



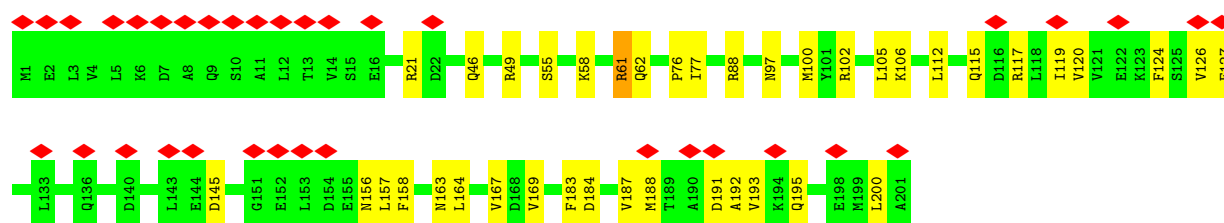
• Molecule 38: 50S ribosomal protein L3

Chain c: 



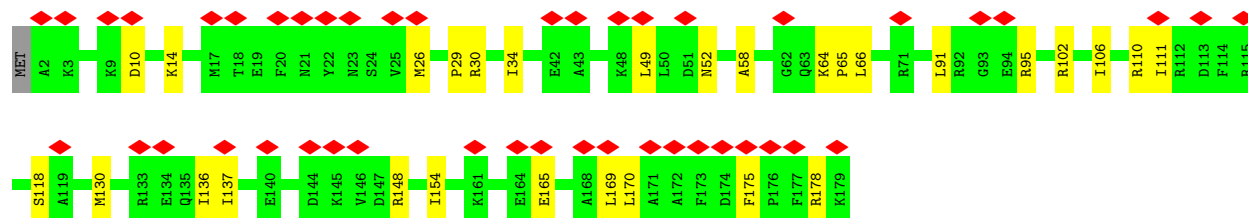
• Molecule 39: 50S ribosomal protein L4

Chain d: 

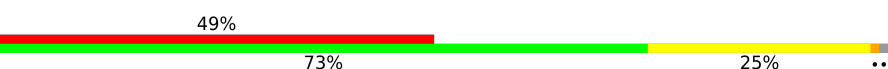


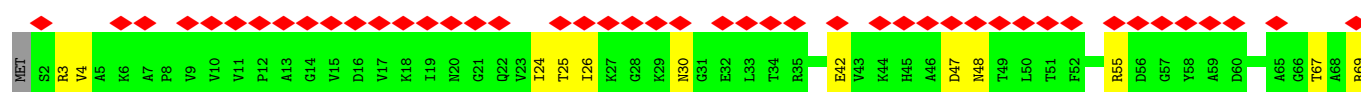
• Molecule 40: 50S ribosomal protein L5

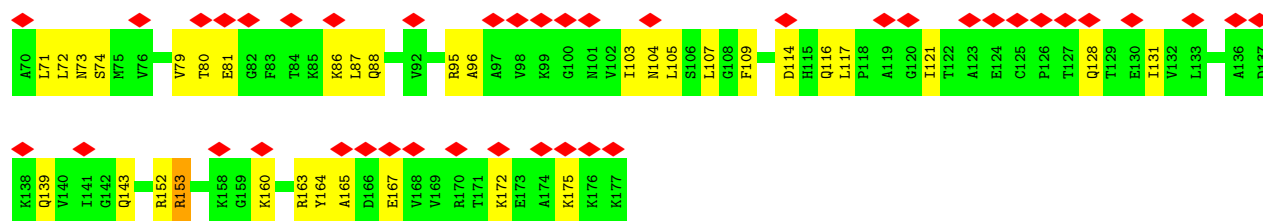
Chain e: 



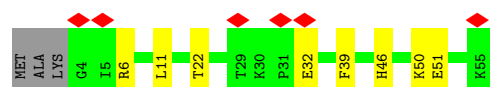
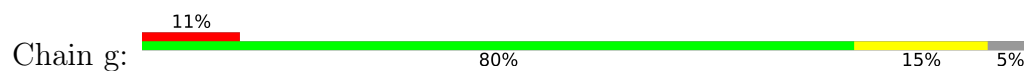
• Molecule 41: 50S ribosomal protein L6

Chain f: 

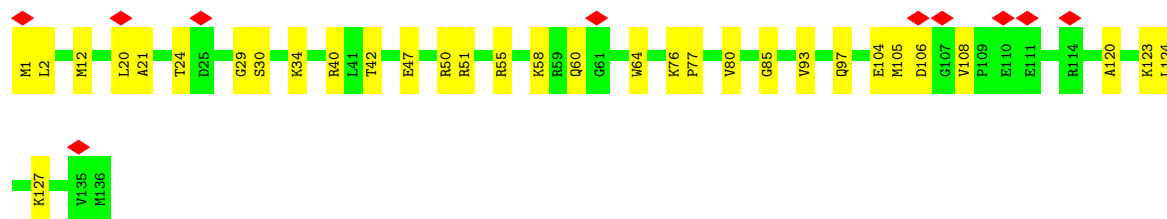
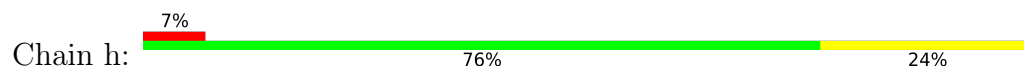




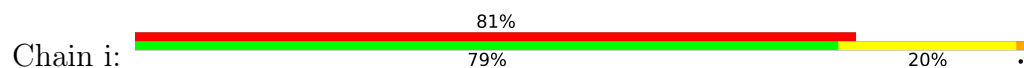
• Molecule 42: 50S ribosomal protein L33



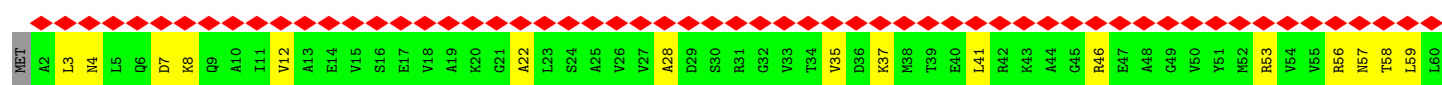
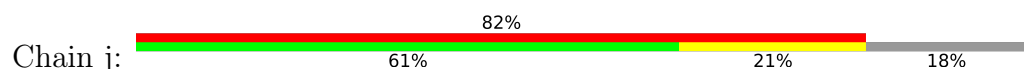
• Molecule 43: 50S ribosomal protein L16

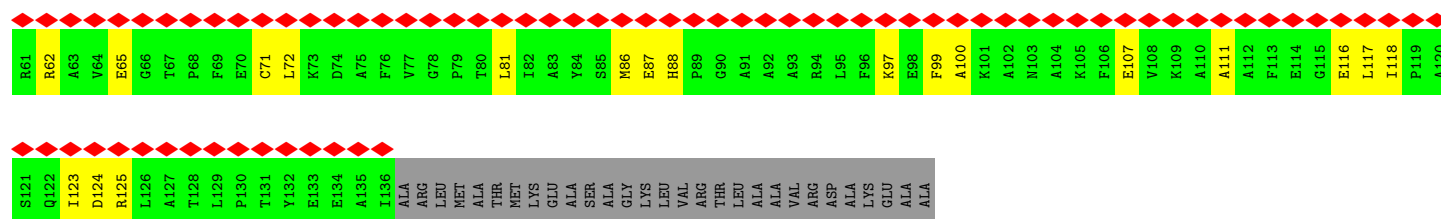


• Molecule 44: 50S ribosomal protein L9

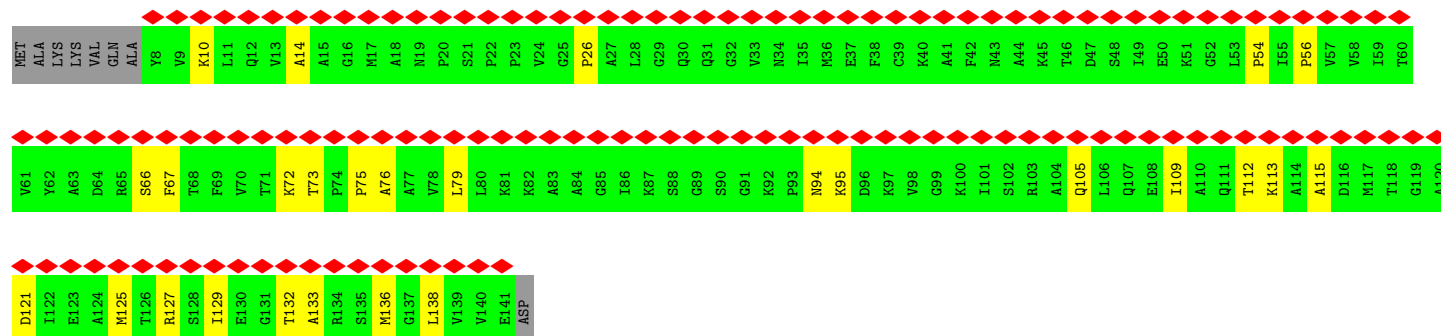
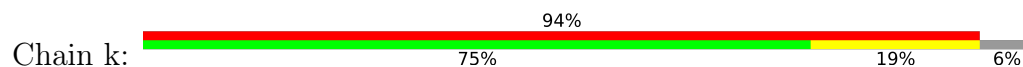


• Molecule 45: Large ribosomal subunit protein uL10





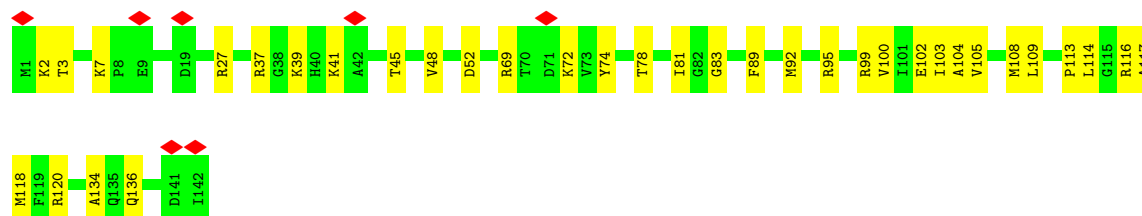
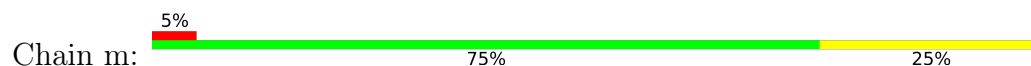
• Molecule 46: 50S ribosomal protein L11



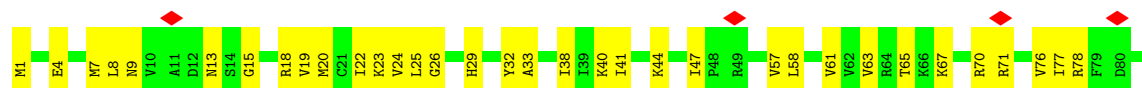
• Molecule 47: 50S ribosomal protein L34

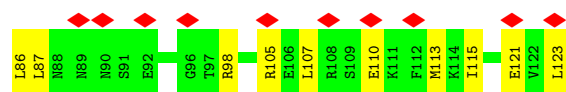


• Molecule 48: 50S ribosomal protein L13

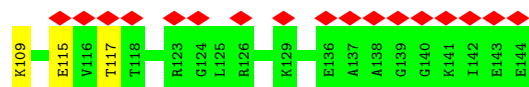
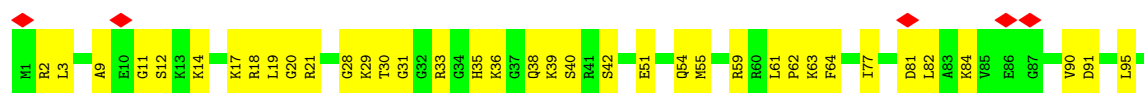


• Molecule 49: 50S ribosomal protein L14





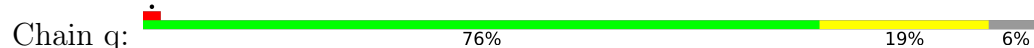
- Molecule 50: 50S ribosomal protein L15



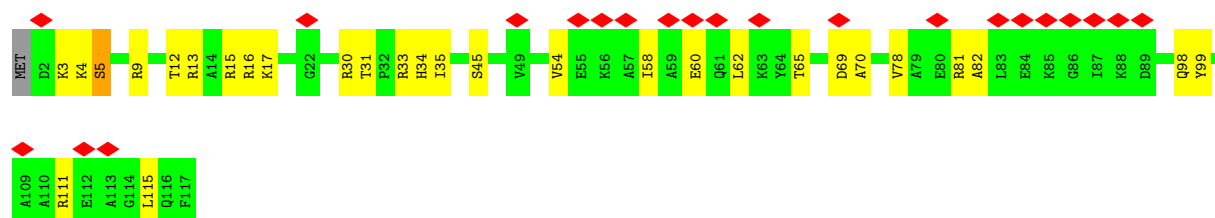
- Molecule 51: Nascent chain



- Molecule 52: 50S ribosomal protein L17



- Molecule 53: 50S ribosomal protein L18

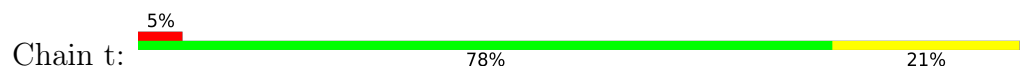


- Molecule 54: 50S ribosomal protein L19

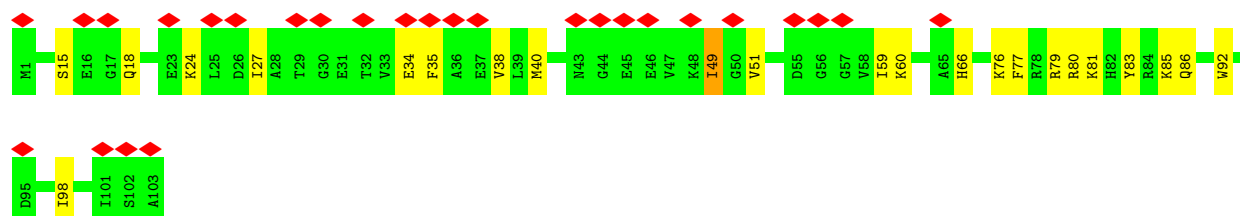
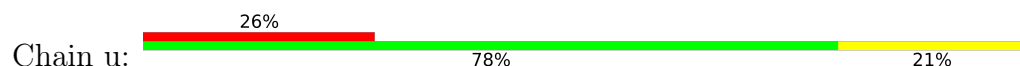




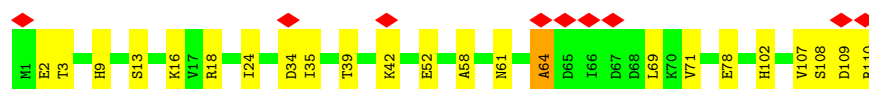
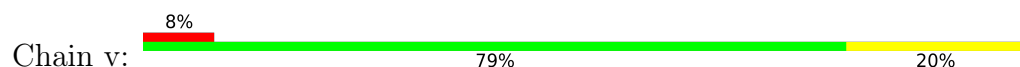
- Molecule 55: 50S ribosomal protein L20



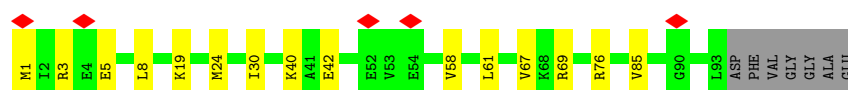
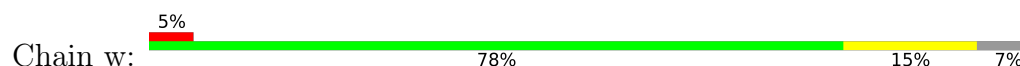
- Molecule 56: 50S ribosomal protein L21



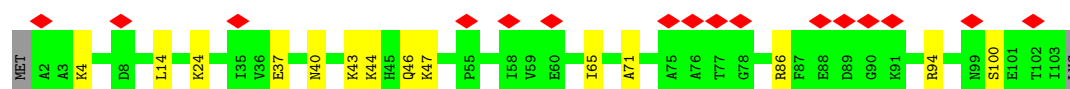
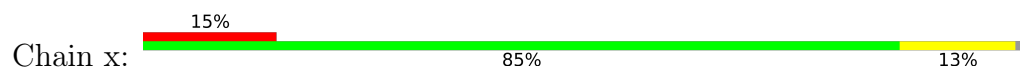
- Molecule 57: 50S ribosomal protein L22



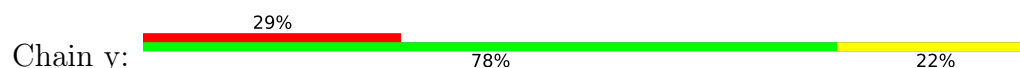
- Molecule 58: 50S ribosomal protein L23

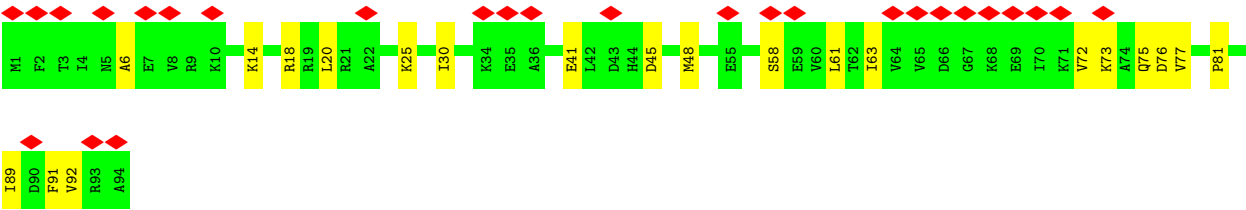


- Molecule 59: 50S ribosomal protein L24

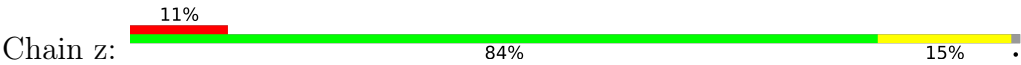


- Molecule 60: 50S ribosomal protein L25





• Molecule 61: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32334	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	24.520	Depositor
Minimum map value	-6.989	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	744.11993, 744.11993, 744.11993	wwPDB
Map dimensions	702, 702, 702	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, H2U, MG, 2MG, 7MG, 4OC, ATP, RSP, 12A, OMG, 1MG, 5MC, CM0, 2MA, PSU, ZN, 6MZ, 5MU, G7M, OMU, 4SU, OMC, UR3, MIA, 3TD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.11	0/303	0.36	0/397
2	1	0.13	0/635	0.38	0/848
3	2	0.12	0/510	0.40	0/677
4	3	0.14	0/453	0.41	0/605
5	4	0.14	0/539	0.46	0/721
6	5	0.12	0/450	0.33	0/599
7	6	0.11	0/513	0.35	0/676
8	7	0.17	2/69284 (0.0%)	0.34	48/108082 (0.0%)
9	8	0.18	0/2872	0.36	4/4478 (0.1%)
10	A	0.18	2/36772 (0.0%)	0.35	41/57358 (0.1%)
11	B	0.15	0/1782	0.42	0/2401
12	C	0.12	0/1685	0.39	0/2270
13	D	0.13	0/1665	0.37	0/2227
14	E	0.14	0/1179	0.41	0/1584
15	F	0.12	0/881	0.36	0/1189
16	G	0.14	0/1246	0.40	0/1672
17	H	0.12	0/989	0.39	0/1326
18	I	0.12	0/1034	0.35	0/1375
19	J	0.21	0/813	0.57	1/1100 (0.1%)
20	K	0.13	0/900	0.40	0/1215
21	L	0.13	0/969	0.42	0/1300
22	M	0.33	0/900	0.58	0/1204
23	N	0.14	0/817	0.46	0/1088
24	O	0.13	0/722	0.44	0/964
25	P	0.14	0/659	0.35	0/884
26	Q	0.14	0/657	0.45	0/881
27	R	0.30	0/635	0.56	0/849
28	S	0.13	0/680	0.38	0/915
29	T	0.15	0/676	0.46	0/895
30	U	0.20	0/592	0.46	0/785
31	V	0.16	0/727	0.41	0/1132

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	W	0.29	0/1585	0.45	3/2467 (0.1%)
33	X	0.26	0/1728	0.58	0/2686
34	Y	0.37	1/1672 (0.1%)	0.67	4/2599 (0.2%)
35	Z	0.11	0/1334	0.32	0/1799
36	a	0.10	0/1033	0.30	0/1387
37	b	0.14	0/2121	0.41	0/2852
38	c	0.13	0/1586	0.37	0/2134
39	d	0.14	0/1571	0.34	0/2113
40	e	0.10	0/1444	0.34	0/1937
41	f	0.10	0/1343	0.34	0/1816
42	g	0.11	0/434	0.40	0/576
43	h	0.21	0/1104	0.43	0/1474
44	i	0.13	0/1121	0.43	0/1515
45	j	0.17	0/1037	0.42	0/1400
46	k	0.16	0/993	0.50	0/1341
47	l	0.30	0/380	0.47	0/498
48	m	0.12	0/1152	0.34	0/1551
49	n	0.15	0/955	0.41	0/1279
50	o	0.12	0/1062	0.39	0/1413
51	p	1.09	0/36	1.72	1/48 (2.1%)
52	q	0.16	0/973	0.40	0/1301
53	r	0.12	0/901	0.42	0/1209
54	s	0.12	0/929	0.34	0/1242
55	t	0.11	0/960	0.35	0/1278
56	u	0.12	0/829	0.38	0/1107
57	v	0.11	0/864	0.43	0/1156
58	w	0.10	0/744	0.35	0/994
59	x	0.10	0/787	0.34	0/1051
60	y	0.11	0/766	0.35	0/1025
61	z	0.10	0/642	0.38	0/848
All	All	0.17	5/164625 (0.0%)	0.37	102/245793 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	D	0	1
19	J	0	1
20	K	0	1
24	O	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
25	P	0	1
29	T	0	2
39	d	0	1
41	f	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	527	G7M	O3'-P	5.67	1.61	1.56
8	7	2069	G7M	O3'-P	5.65	1.61	1.56
8	7	2552	OMU	O3'-P	5.36	1.61	1.56
34	Y	7	4SU	O3'-P	5.25	1.61	1.56
10	A	1498	UR3	O3'-P	5.21	1.61	1.56

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	1129	A	P-O3'-C3'	-10.36	104.65	120.20
8	7	2605	PSU	P-O3'-C3'	-9.26	106.32	120.20
10	A	1407	5MC	P-O3'-C3'	-9.12	106.51	120.20
8	7	2453	A	P-O3'-C3'	-8.95	106.78	120.20
10	A	1408	A	P-O3'-C3'	-8.89	106.86	120.20
10	A	389	A	P-O3'-C3'	-8.38	107.64	120.20
9	8	89	U	P-O3'-C3'	-8.16	107.95	120.20
10	A	1404	C	P-O3'-C3'	-8.07	108.10	120.20
8	7	2570	G	P-O3'-C3'	-8.01	108.19	120.20
8	7	955	PSU	P-O3'-C3'	-7.93	108.31	120.20
9	8	88	C	P-O3'-C3'	-7.92	108.32	120.20
10	A	335	C	P-O3'-C3'	-7.81	108.48	120.20
10	A	56	U	P-O3'-C3'	-7.80	108.50	120.20
8	7	2462	C	P-O3'-C3'	-7.74	108.60	120.20
8	7	2442	C	P-O3'-C3'	-7.70	108.64	120.20
10	A	1516	2MG	P-O3'-C3'	-7.68	108.69	120.20
10	A	338	A	P-O3'-C3'	-7.66	108.71	120.20
10	A	387	U	P-O3'-C3'	-7.59	108.81	120.20
10	A	112	G	P-O3'-C3'	-7.57	108.85	120.20
8	7	2504	PSU	P-O3'-C3'	-7.52	108.92	120.20
8	7	1905	C	P-O3'-C3'	-7.50	108.95	120.20
10	A	315	A	P-O3'-C3'	-7.49	108.96	120.20
8	7	1836	C	P-O3'-C3'	-7.47	109.00	120.20
8	7	2451	A	P-O3'-C3'	-7.46	109.02	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	516	PSU	P-O3'-C3'	-7.44	109.04	120.20
8	7	2495	G	P-O3'-C3'	-7.41	109.08	120.20
8	7	1647	U	P-O3'-C3'	-7.35	109.17	120.20
10	A	111	G	P-O3'-C3'	-7.33	109.21	120.20
32	W	74	C	P-O3'-C3'	-7.30	109.24	120.20
8	7	1939	5MU	P-O3'-C3'	-7.30	109.25	120.20
10	A	1207	2MG	P-O3'-C3'	-7.29	109.27	120.20
10	A	353	A	P-O3'-C3'	-7.26	109.31	120.20
8	7	2568	U	P-O3'-C3'	-7.20	109.40	120.20
8	7	2487	G	P-O3'-C3'	-7.18	109.43	120.20
8	7	1127	A	P-O3'-C3'	-7.16	109.45	120.20
8	7	2446	G	P-O3'-C3'	-7.16	109.46	120.20
8	7	2498	OMC	P-O3'-C3'	-7.16	109.46	120.20
8	7	2488	G	P-O3'-C3'	-7.15	109.48	120.20
10	A	1500	A	P-O3'-C3'	-7.13	109.50	120.20
10	A	316	C	P-O3'-C3'	-7.12	109.53	120.20
8	7	786	C	P-O3'-C3'	-7.02	109.67	120.20
34	Y	32	C	P-O3'-C3'	-6.98	109.73	120.20
8	7	2441	U	P-O3'-C3'	-6.97	109.75	120.20
8	7	2494	G	P-O3'-C3'	-6.96	109.76	120.20
10	A	336	A	P-O3'-C3'	-6.95	109.78	120.20
10	A	330	C	P-O3'-C3'	-6.93	109.81	120.20
10	A	1504	G	P-O3'-C3'	-6.90	109.84	120.20
8	7	1904	G	P-O3'-C3'	-6.88	109.88	120.20
8	7	2489	U	P-O3'-C3'	-6.86	109.92	120.20
8	7	753	A	P-O3'-C3'	-6.85	109.93	120.20
8	7	567	U	P-O3'-C3'	-6.84	109.94	120.20
10	A	350	G	P-O3'-C3'	-6.81	109.98	120.20
8	7	2517	C	P-O3'-C3'	-6.78	110.03	120.20
34	Y	1	G	P-O3'-C3'	-6.76	110.06	120.20
10	A	355	C	P-O3'-C3'	-6.70	110.15	120.20
8	7	2176	A	C2'-C3'-O3'	6.67	123.71	113.70
8	7	1835	2MG	P-O3'-C3'	-6.67	110.19	120.20
8	7	2062	A	P-O3'-C3'	-6.66	110.21	120.20
34	Y	35	A	P-O3'-C3'	-6.61	110.28	120.20
8	7	2461	A	P-O3'-C3'	-6.60	110.29	120.20
8	7	790	U	P-O3'-C3'	-6.56	110.36	120.20
8	7	2455	G	P-O3'-C3'	-6.54	110.39	120.20
9	8	87	U	P-O3'-C3'	-6.53	110.41	120.20
10	A	57	G	P-O3'-C3'	-6.51	110.43	120.20
8	7	2569	G	P-O3'-C3'	-6.42	110.56	120.20
10	A	52	C	P-O3'-C3'	-6.38	110.62	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	337	G	P-O3'-C3'	-6.36	110.66	120.20
10	A	314	C	P-O3'-C3'	-6.30	110.74	120.20
10	A	317	U	P-O3'-C3'	-6.30	110.74	120.20
32	W	72	C	P-O3'-C3'	-6.30	110.75	120.20
9	8	86	G	P-O3'-C3'	-6.26	110.80	120.20
8	7	2580	PSU	P-O3'-C3'	-6.24	110.85	120.20
10	A	134	G	P-O3'-C3'	-6.20	110.89	120.20
10	A	1405	G	P-O3'-C3'	-6.13	111.01	120.20
8	7	2452	C	P-O3'-C3'	-6.13	111.01	120.20
10	A	53	A	P-O3'-C3'	-6.11	111.03	120.20
10	A	354	G	P-O3'-C3'	-6.08	111.08	120.20
8	7	2518	A	P-O3'-C3'	-6.06	111.11	120.20
32	W	75	C	P-O3'-C3'	-6.05	111.12	120.20
8	7	1128	G	P-O3'-C3'	-6.00	111.20	120.20
8	7	2457	PSU	P-O3'-C3'	-5.96	111.26	120.20
10	A	58	C	P-O3'-C3'	-5.96	111.26	120.20
10	A	388	G	P-O3'-C3'	-5.91	111.34	120.20
8	7	2492	U	P-O3'-C3'	-5.88	111.37	120.20
34	Y	73	A	P-O3'-C3'	-5.81	111.49	120.20
10	A	1499	A	P-O3'-C3'	-5.80	111.50	120.20
19	J	37	ARG	N-CA-C	-5.76	99.79	108.96
10	A	1201	A	P-O3'-C3'	5.75	128.82	120.20
8	7	1833	C	P-O3'-C3'	-5.67	111.70	120.20
8	7	1271	G	P-O3'-C3'	-5.66	111.70	120.20
10	A	113	G	P-O3'-C3'	-5.66	111.72	120.20
8	7	568	U	P-O3'-C3'	-5.60	111.80	120.20
51	p	18	VAL	CA-C-O	-5.58	111.31	120.80
10	A	329	A	P-O3'-C3'	-5.54	111.90	120.20
8	7	2445	2MG	P-O3'-C3'	-5.53	111.90	120.20
8	7	2571	U	P-O3'-C3'	-5.41	112.09	120.20
10	A	59	A	P-O3'-C3'	-5.36	112.16	120.20
10	A	346	G	O3'-P-O5'	5.27	111.90	104.00
10	A	1503	A	P-O3'-C3'	-5.26	112.31	120.20
8	7	1270	C	P-O3'-C3'	-5.23	112.35	120.20
8	7	1130	U	C4'-C3'-O3'	-5.12	105.32	113.00
10	A	352	C	P-O3'-C3'	-5.07	112.59	120.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	D	104	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
19	J	48	ARG	Sidechain
20	K	98	ARG	Sidechain
24	O	84	ARG	Sidechain
25	P	51	ARG	Sidechain
29	T	29	ARG	Sidechain
29	T	60	ARG	Sidechain
39	d	61	ARG	Sidechain
41	f	153	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	302	0	340	12	0
2	1	625	0	652	15	0
3	2	509	0	543	6	0
4	3	449	0	488	13	0
5	4	529	0	527	18	0
6	5	444	0	458	12	0
7	6	504	0	572	9	0
8	7	62335	0	31374	602	0
9	8	2569	0	1301	20	0
10	A	33092	0	16676	379	0
11	B	1751	0	1779	47	0
12	C	1658	0	1732	61	0
13	D	1643	0	1707	45	0
14	E	1166	0	1212	32	0
15	F	862	0	864	18	0
16	G	1228	0	1277	31	0
17	H	979	0	1031	29	0
18	I	1022	0	1070	22	0
19	J	803	0	842	40	0
20	K	884	0	896	26	0
21	L	955	0	1016	25	0
22	M	891	0	952	14	0
23	N	805	0	844	40	0
24	O	714	0	734	16	0
25	P	649	0	666	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Q	648	0	691	21	0
27	R	624	0	652	16	0
28	S	663	0	688	15	0
29	T	670	0	719	19	0
30	U	584	0	618	24	0
31	V	648	0	325	22	0
32	W	1632	0	842	12	0
33	X	1683	0	859	44	0
34	Y	1631	0	831	25	0
35	Z	1319	0	1338	21	0
36	a	1026	0	1092	20	0
37	b	2082	0	2154	56	0
38	c	1565	0	1616	44	0
39	d	1552	0	1619	30	0
40	e	1420	0	1457	21	0
41	f	1323	0	1371	34	0
42	g	427	0	464	6	0
43	h	1085	0	1169	22	0
44	i	1110	0	1148	19	0
45	j	1023	0	1050	26	0
46	k	979	0	1028	24	0
47	l	377	0	418	13	0
48	m	1129	0	1162	33	0
49	n	946	0	1023	40	0
50	o	1053	0	1129	37	0
51	p	101	0	55	0	0
52	q	960	0	1000	17	0
53	r	891	0	923	25	0
54	s	917	0	962	37	0
55	t	947	0	1019	28	0
56	u	816	0	839	19	0
57	v	857	0	922	20	0
58	w	738	0	807	10	0
59	x	779	0	831	8	0
60	y	753	0	780	16	0
61	z	634	0	653	15	0
62	0	1	0	0	0	0
62	4	1	0	0	0	0
63	7	193	0	0	0	0
63	A	63	0	0	0	0
63	X	1	0	0	0	0
63	Y	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	b	1	0	0	0	0
63	o	1	0	0	0	0
64	7	62	0	24	2	0
All	All	153284	0	103831	1948	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1948) 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)
31:V:26:G:N2	34:Y:34:CM0:H3	1.62	0.98
8:7:568:U:H1'	8:7:2030:6MZ:H9C1	1.56	0.88
4:3:9:GLN:HB3	4:3:29:LEU:HD23	1.58	0.84
33:X:1:G:H2'	33:X:2:G:H4'	1.60	0.84
11:B:131:LYS:HE3	11:B:132:LYS:HG3	1.61	0.82
23:N:93:ILE:HG21	23:N:96:LEU:HD12	1.58	0.82
5:4:8:LYS:HD3	5:4:10:GLU:HG2	1.60	0.82
13:D:62:ARG:HH21	13:D:68:LEU:HA	1.42	0.81
10:A:836:G:OP1	27:R:50:LYS:NZ	2.13	0.81
8:7:1800:C:HO2'	8:7:1818:U:H3	1.26	0.81
10:A:830:G:O2'	11:B:21:ARG:NH1	2.14	0.81
8:7:1936:A:H2	8:7:1943:U:H3	1.27	0.81
10:A:1537:U:O2'	10:A:1538:C:OP2	1.97	0.80
54:s:60:THR:HG22	54:s:73:VAL:HG12	1.64	0.79
10:A:1349:A:H5''	18:I:123:ARG:HG2	1.66	0.78
8:7:78:U:H3	8:7:108:G:H1	1.31	0.78
10:A:1538:C:O2'	30:U:17:ARG:NH2	2.17	0.78
8:7:496:G:H1'	57:v:61:ASN:HD22	1.50	0.77
41:f:104:ASN:ND2	41:f:114:ASP:OD1	2.18	0.77
13:D:15:GLU:OE2	13:D:63:ARG:NH2	2.19	0.76
8:7:2137:U:H2'	8:7:2138:G:H8	1.50	0.76
31:V:26:G:H22	34:Y:34:CM0:H3	0.82	0.76
10:A:254:G:H1'	26:Q:17:MET:HE2	1.67	0.76
8:7:1190:G:OP1	50:o:30:THR:OG1	2.03	0.76
12:C:10:ILE:HG23	12:C:11:ARG:HD3	1.68	0.76
33:X:38:12A:H2M2	33:X:39:A:H1'	1.68	0.75
38:c:13:ARG:HH21	54:s:56:HIS:HA	1.51	0.75
32:W:51:U:H3	32:W:63:G:H1	1.33	0.75
8:7:1427:A:N6	8:7:1571:A:OP2	2.16	0.75
8:7:1478:G:H1	8:7:1513:U:H3	1.32	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:2681:C:H4'	38:c:11:MET:HE1	1.68	0.75
12:C:65:ARG:HH21	19:J:94:ALA:HB2	1.52	0.75
10:A:1034:G:H2'	10:A:1035:A:H5'	1.68	0.75
13:D:54:GLN:HA	13:D:199:LEU:HD21	1.67	0.74
39:d:46:GLN:O	39:d:88:ARG:NH2	2.20	0.74
10:A:1073:U:OP2	14:E:62:LYS:NZ	2.21	0.74
10:A:963:G:H21	19:J:57:VAL:HG11	1.53	0.74
19:J:65:TYR:HB3	23:N:96:LEU:HD22	1.70	0.74
8:7:2530:A:N7	41:f:172:LYS:NZ	2.36	0.73
37:b:21:ASN:HB3	37:b:24:LEU:HD23	1.69	0.73
8:7:1203:U:H4'	50:o:3:LEU:HD21	1.70	0.72
8:7:600:G:H1'	39:d:100:MET:HE1	1.70	0.72
10:A:1064:G:N2	10:A:1191:A:OP1	2.22	0.72
5:4:61:ASN:HB3	5:4:62:LYS:HZ2	1.54	0.72
10:A:315:A:H1'	10:A:353:A:H2	1.55	0.72
10:A:1086:U:H3	10:A:1099:G:H22	1.36	0.72
10:A:58:C:H2'	10:A:59:A:H8	1.55	0.72
37:b:3:VAL:HG12	37:b:19:VAL:HG12	1.72	0.72
5:4:47:LYS:HA	5:4:49:ARG:HH21	1.53	0.72
10:A:1539:C:H2'	10:A:1540:U:C6	2.25	0.72
17:H:13:ARG:NH1	17:H:26:THR:O	2.22	0.72
27:R:9:LYS:NZ	27:R:43:ARG:O	2.22	0.72
8:7:2330:G:O3'	61:z:44:LYS:NZ	2.23	0.72
5:4:43:PHE:HA	5:4:48:GLN:HB2	1.72	0.71
8:7:1335:C:OP1	58:w:69:ARG:NH1	2.23	0.71
12:C:59:ARG:HG2	12:C:64:ILE:HG22	1.71	0.71
38:c:8:LYS:HB2	38:c:201:LEU:HD11	1.73	0.71
39:d:119:ILE:HB	39:d:187:VAL:HG22	1.72	0.70
47:l:18:PHE:HB2	47:l:43:THR:HG21	1.73	0.70
8:7:896:A:O2'	34:Y:56:C:O2	2.06	0.70
15:F:40:GLU:HB2	15:F:61:LEU:HB3	1.73	0.70
15:F:81:ASN:HB3	15:F:84:VAL:HG12	1.73	0.70
10:A:911:U:OP2	21:L:94:ARG:NH2	2.25	0.70
5:4:9:TYR:OH	40:e:102:ARG:NH1	2.25	0.70
21:L:46:ASN:ND2	21:L:89:ASP:OD2	2.24	0.70
10:A:259:G:OP1	29:T:36:TYR:OH	2.10	0.69
12:C:36:ASP:OD1	12:C:59:ARG:NH2	2.24	0.69
10:A:1316:G:N1	10:A:1319:A:OP2	2.23	0.69
49:n:70:ARG:HG2	49:n:76:VAL:HG12	1.73	0.69
8:7:825:A:O2'	50:o:54:GLN:OE1	2.08	0.69
41:f:69:ARG:HH12	41:f:73:ASN:HB2	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:1044:C:O2'	8:7:1111:A:N1	2.24	0.69
10:A:719:C:H1'	27:R:38:LYS:HG2	1.74	0.69
10:A:808:C:OP2	24:O:48:LYS:NZ	2.23	0.69
8:7:973:A:OP2	56:u:81:LYS:NZ	2.23	0.69
8:7:2100:G:H1	8:7:2189:U:H3	1.37	0.69
10:A:346:G:OP1	54:s:41:GLN:NE2	2.25	0.69
10:A:538:G:OP2	21:L:110:ARG:NH2	2.26	0.69
48:m:72:LYS:HE3	48:m:74:TYR:HE1	1.58	0.69
8:7:534:U:O2'	55:t:49:ASP:OD2	2.09	0.68
9:8:93:C:OP2	60:y:18:ARG:NH1	2.27	0.68
10:A:664:G:H22	10:A:741:G:H1	1.42	0.68
7:6:13:ARG:NH2	8:7:250:G:OP2	2.27	0.68
8:7:1416:G:O2'	8:7:1417:C:OP2	2.11	0.68
55:t:112:LYS:HD2	56:u:49:ILE:HD12	1.75	0.68
38:c:172:VAL:HG12	38:c:175:LEU:HD21	1.75	0.68
46:k:14:ALA:H	46:k:54:PRO:HA	1.59	0.68
8:7:2816:G:O3'	52:q:99:LYS:NZ	2.27	0.67
10:A:1081:A:N7	14:E:52:LYS:NZ	2.42	0.67
8:7:1537:G:OP2	8:7:1537:G:N2	2.26	0.67
10:A:363:A:H1'	21:L:29:GLN:HE21	1.59	0.67
10:A:859:G:OP2	10:A:869:G:N1	2.21	0.67
40:e:10:ASP:O	40:e:14:LYS:NZ	2.26	0.67
10:A:1216:A:O3'	23:N:9:ARG:NH2	2.28	0.67
8:7:1952:A:OP1	49:n:44:LYS:NZ	2.27	0.67
12:C:100:GLN:NE2	12:C:102:ASN:OD1	2.28	0.67
39:d:49:ARG:HD2	39:d:76:PRO:HD3	1.77	0.67
49:n:1:MET:HB2	49:n:32:TYR:HB3	1.76	0.66
10:A:211:G:H2'	10:A:212:G:O4'	1.95	0.66
9:8:3:C:O2'	9:8:4:C:OP1	2.11	0.66
12:C:53:SER:O	12:C:114:LYS:HG3	1.95	0.66
13:D:97:ARG:NH2	13:D:99:ASP:OD2	2.28	0.66
9:8:30:C:H1'	9:8:57:A:H61	1.60	0.66
10:A:505:G:H5'	10:A:534:U:H2'	1.77	0.66
14:E:159:LYS:NZ	17:H:42:GLU:O	2.28	0.66
10:A:1281:C:O2'	10:A:1282:C:OP1	2.11	0.66
15:F:99:ALA:O	15:F:104:LYS:NZ	2.27	0.66
39:d:97:ASN:HB2	39:d:100:MET:HG2	1.78	0.66
47:l:24:THR:HG23	47:l:27:GLY:H	1.61	0.66
61:z:75:LYS:HB2	61:z:77:ARG:HG3	1.77	0.66
8:7:858:G:O2'	8:7:859:G:O4'	2.11	0.66
41:f:163:ARG:NH2	41:f:167:GLU:O	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:55:GLY:HA2	5:4:58:ASP:HB3	1.78	0.66
9:8:29:A:O2'	9:8:58:A:N1	2.27	0.66
31:V:33:A:H4'	31:V:34:A:H5'	1.77	0.66
10:A:898:G:N2	10:A:901:A:OP2	2.28	0.65
38:c:88:GLU:OE1	38:c:88:GLU:N	2.29	0.65
8:7:1112:G:O2'	41:f:3:ARG:NH2	2.29	0.65
10:A:454:G:H1	10:A:478:A:H61	1.44	0.65
10:A:1279:G:H4'	10:A:1281:C:H41	1.60	0.65
44:i:104:THR:HG22	44:i:109:GLU:HG2	1.76	0.65
8:7:1138:G:H2'	8:7:1139:G:O4'	1.97	0.65
11:B:35:ARG:NH1	11:B:36:ASN:OD1	2.30	0.65
10:A:182:A:N1	10:A:223:A:O2'	2.28	0.65
8:7:1278:C:H5'	52:q:24:MET:HE1	1.78	0.65
12:C:88:ARG:NH1	12:C:99:ALA:O	2.30	0.65
49:n:24:VAL:HG23	49:n:33:ALA:HB2	1.78	0.65
12:C:57:ILE:HG12	12:C:66:VAL:HG22	1.78	0.65
8:7:587:C:C5	50:o:19:LEU:HD11	2.31	0.64
8:7:858:G:N2	8:7:2269:G:OP2	2.28	0.64
8:7:2898:U:O2'	48:m:136:GLN:NE2	2.20	0.64
10:A:263:A:OP2	29:T:74:ARG:NH1	2.30	0.64
10:A:722:G:H5'	10:A:723:U:OP2	1.97	0.64
23:N:16:LEU:HD23	23:N:54:ASP:HB2	1.79	0.64
46:k:72:LYS:HG3	46:k:73:THR:H	1.62	0.64
8:7:1108:U:OP2	45:j:56:ARG:NH2	2.29	0.64
10:A:522:C:O2'	10:A:523:A:OP1	2.13	0.64
10:A:1346:A:N7	16:G:10:ARG:NH1	2.44	0.64
55:t:88:VAL:HG22	56:u:51:VAL:HG12	1.78	0.64
8:7:2263:C:N4	61:z:15:ASP:OD1	2.27	0.64
13:D:185:LYS:HD2	13:D:186:PRO:HD2	1.80	0.64
33:X:42:G:H2'	33:X:43:A:H8	1.63	0.64
41:f:107:LEU:O	41:f:152:ARG:NH2	2.30	0.64
8:7:1952:A:C4	49:n:22:ILE:HD11	2.32	0.64
8:7:2710:C:H2'	8:7:2711:A:C8	2.32	0.64
10:A:1073:U:O2'	11:B:103:ASN:OD1	2.14	0.64
44:i:97:ARG:O	44:i:112:LYS:NZ	2.31	0.64
23:N:31:ILE:O	23:N:41:ARG:NH1	2.31	0.64
44:i:26:ALA:HA	44:i:30:LEU:HB2	1.80	0.64
8:7:1475:G:O2'	8:7:1476:U:O5'	2.13	0.64
43:h:76:LYS:NZ	43:h:85:GLY:O	2.27	0.64
5:4:34:LEU:HD22	40:e:106:ILE:HD12	1.80	0.64
8:7:2393:U:H5''	50:o:62:PRO:HB3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:2845:U:H2'	8:7:2846:G:H8	1.63	0.64
8:7:2112:G:H5''	8:7:2113:U:H5	1.62	0.64
8:7:2165:C:OP2	8:7:2170:A:N6	2.26	0.64
8:7:747:5MU:H72	8:7:2612:C:H4'	1.79	0.64
10:A:1188:A:O3'	23:N:98:LYS:HE2	1.98	0.64
24:O:70:LEU:HD22	24:O:78:TYR:HB2	1.79	0.64
55:t:49:ASP:HA	55:t:52:GLN:HB2	1.79	0.64
1:0:3:VAL:HG21	8:7:2539:C:H5'	1.81	0.63
8:7:2134:A:H1'	8:7:2159:G:H1'	1.78	0.63
10:A:411:A:OP1	13:D:26:ARG:NH1	2.32	0.63
10:A:1317:C:N3	28:S:37:ARG:NH1	2.42	0.63
10:A:1320:C:H1'	28:S:73:GLU:HG3	1.81	0.63
12:C:82:GLU:O	12:C:86:LYS:NZ	2.32	0.63
13:D:47:ARG:HH21	31:V:34:A:H8	1.46	0.63
14:E:157:ARG:NH1	17:H:99:LEU:O	2.31	0.63
19:J:52:LEU:HD11	23:N:81:ARG:HD2	1.80	0.63
54:s:97:LEU:HB3	54:s:100:LEU:HD23	1.81	0.63
10:A:335:C:H2'	10:A:336:A:C8	2.33	0.63
39:d:158:PHE:HA	39:d:169:VAL:HG11	1.80	0.63
19:J:53:ILE:HD13	19:J:63:ASP:HB2	1.81	0.63
45:j:87:GLU:O	45:j:88:HIS:C	2.41	0.63
59:x:86:ARG:NH1	59:x:100:SER:OG	2.31	0.63
17:H:96:MET:HB3	17:H:100:GLY:H	1.64	0.63
20:K:74:VAL:HG23	20:K:75:LYS:H	1.64	0.63
25:P:6:LEU:HD13	25:P:71:VAL:HG12	1.79	0.63
13:D:65:TYR:O	13:D:97:ARG:NH1	2.23	0.63
16:G:53:ARG:HH12	16:G:121:ALA:HB1	1.62	0.63
37:b:107:PRO:HD2	37:b:110:LEU:HD22	1.80	0.63
8:7:1800:C:O2'	8:7:1818:U:N3	2.24	0.63
10:A:408:A:H2'	10:A:409:U:C6	2.34	0.63
8:7:2052:A:O2'	38:c:148:GLN:O	2.12	0.63
10:A:891:U:H2'	10:A:892:A:H8	1.63	0.63
12:C:212:ALA:H	19:J:16:ARG:HH12	1.45	0.63
8:7:1194:A:OP2	50:o:14:LYS:NZ	2.29	0.62
59:x:46:GLN:NE2	59:x:47:LYS:O	2.32	0.62
60:y:76:ASP:OD1	60:y:77:VAL:N	2.32	0.62
8:7:1580:A:O2'	8:7:1581:G:OP1	2.15	0.62
8:7:1752:C:H2'	8:7:1753:G:C8	2.34	0.62
10:A:49:U:H3	10:A:362:G:H1'	1.64	0.62
10:A:401:C:O2'	10:A:621:A:N3	2.31	0.62
33:X:16:A:H2	33:X:76:A:H62	1.47	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:43:ASP:OD1	36:a:44:VAL:N	2.32	0.62
8:7:2237:G:O2'	8:7:2239:G:N7	2.30	0.62
8:7:2552:OMU:H6	8:7:2552:OMU:O5'	1.99	0.62
10:A:216:U:H4'	10:A:464:U:H4'	1.80	0.62
7:6:30:ARG:HH21	50:o:62:PRO:HB2	1.62	0.62
8:7:571:U:H3'	56:u:80:ARG:HH12	1.62	0.62
10:A:315:A:H1'	10:A:353:A:C2	2.33	0.62
10:A:1352:C:H2'	10:A:1353:G:C8	2.34	0.62
38:c:46:ARG:NH1	38:c:85:ALA:O	2.33	0.62
58:w:24:MET:HE1	58:w:30:ILE:HG22	1.82	0.62
8:7:296:U:H2'	8:7:297:G:C8	2.34	0.62
8:7:1818:U:OP2	37:b:156:ARG:NE	2.29	0.62
11:B:9:MET:HE1	11:B:47:VAL:HG22	1.81	0.62
23:N:64:CYS:HB2	23:N:80:SER:HB3	1.81	0.62
33:X:72:PSU:H2'	33:X:74:G:N7	2.14	0.62
7:6:13:ARG:HG2	50:o:63:LYS:HA	1.80	0.62
10:A:1027:C:O2'	10:A:1028:C:OP1	2.14	0.62
10:A:451:A:OP2	25:P:70:ARG:NH2	2.29	0.62
29:T:28:MET:HG2	29:T:58:VAL:HG12	1.80	0.62
8:7:584:C:P	55:t:6:ARG:HH21	2.23	0.62
16:G:68:ASN:O	16:G:138:ARG:NH2	2.33	0.62
35:Z:156:VAL:HA	35:Z:168:VAL:HG12	1.81	0.62
8:7:793:A:OP2	8:7:2071:A:O2'	2.17	0.62
10:A:337:G:H2'	10:A:338:A:C8	2.35	0.62
58:w:67:VAL:HG22	58:w:76:ARG:HG2	1.80	0.62
22:M:75:MET:HA	22:M:78:LYS:HE3	1.81	0.61
25:P:6:LEU:CD1	25:P:19:VAL:HG22	2.30	0.61
30:U:33:ARG:NH1	31:V:14:G:OP2	2.32	0.61
8:7:1030:C:OP2	43:h:127:LYS:NZ	2.33	0.61
8:7:1537:G:H3'	8:7:1538:G:O4'	2.00	0.61
49:n:77:ILE:HD11	54:s:72:ARG:HD2	1.82	0.61
8:7:558:U:H2'	8:7:559:G:H8	1.63	0.61
10:A:56:U:H2'	10:A:57:G:C8	2.35	0.61
49:n:4:GLU:HG2	49:n:23:LYS:HA	1.82	0.61
41:f:69:ARG:NH1	41:f:73:ASN:HB2	2.16	0.61
55:t:45:TYR:HD1	55:t:48:ARG:HH12	1.48	0.61
10:A:346:G:H2'	10:A:347:G:O4'	2.00	0.61
10:A:353:A:H2'	10:A:353:A:N3	2.13	0.61
10:A:408:A:H2'	10:A:409:U:H6	1.63	0.61
8:7:1779:U:OP2	8:7:1784:A:N6	2.33	0.61
19:J:64:GLN:O	23:N:99:ALA:N	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:522:C:HO2'	10:A:523:A:P	2.23	0.61
10:A:562:U:O2'	21:L:14:ARG:NH2	2.34	0.61
10:A:966:2MG:HM21	18:I:129:LYS:HE2	1.81	0.61
23:N:13:ARG:NH1	23:N:54:ASP:OD2	2.33	0.61
54:s:25:THR:HB	54:s:88:ARG:HB3	1.83	0.61
60:y:58:SER:O	60:y:73:LYS:NZ	2.34	0.61
53:r:31:THR:HG22	53:r:33:ARG:H	1.66	0.61
60:y:20:LEU:HG	60:y:25:LYS:HB2	1.82	0.61
8:7:2279:G:N7	61:z:14:ARG:NH2	2.47	0.61
33:X:22:A:H2	33:X:23:A:H62	1.47	0.61
38:c:110:THR:HB	38:c:202:ILE:HB	1.83	0.61
8:7:1607:C:N4	8:7:1622:G:OP2	2.26	0.61
8:7:1820:U:H1'	37:b:200:HIS:HD2	1.66	0.61
12:C:186:THR:HG22	12:C:199:LYS:HG2	1.82	0.61
25:P:55:ASP:OD1	25:P:56:ARG:N	2.34	0.61
27:R:63:ARG:HB3	27:R:70:TYR:CE1	2.36	0.61
8:7:1230:A:H2'	8:7:1231:U:C6	2.36	0.60
10:A:6:G:O6	14:E:100:SER:N	2.32	0.60
10:A:501:C:H2'	10:A:502:A:C8	2.35	0.60
21:L:72:HIS:HB2	21:L:74:LEU:HD23	1.84	0.60
1:0:24:ARG:NH2	8:7:2742:G:OP2	2.33	0.60
30:U:13:ASP:OD1	30:U:14:VAL:N	2.34	0.60
10:A:570:G:O6	10:A:865:A:N6	2.34	0.60
44:i:15:LEU:HD13	44:i:58:LEU:HD11	1.82	0.60
8:7:684:G:OP1	47:l:21:ARG:NH1	2.30	0.60
9:8:75:G:H2'	9:8:76:G:H8	1.66	0.60
10:A:1530:G:N7	30:U:46:LYS:NZ	2.48	0.60
8:7:1249:U:H4'	55:t:4:VAL:HG21	1.81	0.60
8:7:1594:U:H2'	8:7:1595:C:C6	2.36	0.60
8:7:1800:C:H3'	37:b:146:MET:HE1	1.83	0.60
10:A:1255:G:O2'	10:A:1258:G:N3	2.28	0.60
19:J:54:SER:HB3	19:J:58:ASN:HB3	1.83	0.60
23:N:50:THR:HG22	28:S:13:LEU:HD22	1.81	0.60
54:s:90:GLY:O	54:s:113:ARG:NH1	2.32	0.60
57:v:3:THR:HG21	57:v:58:ALA:HB2	1.83	0.60
8:7:577:G:H2'	8:7:578:G:C8	2.37	0.60
8:7:2839:G:O2'	52:q:49:GLU:OE1	2.12	0.60
13:D:6:GLY:O	13:D:8:LYS:NZ	2.32	0.60
49:n:15:GLY:O	49:n:47:ILE:HD12	2.02	0.60
8:7:1600:C:H2'	8:7:1601:G:H8	1.67	0.60
8:7:2618:G:H21	38:c:155:VAL:HG21	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:65:ARG:HG2	12:C:100:GLN:HB3	1.84	0.60
22:M:81:MET:HE2	22:M:91:HIS:HB3	1.84	0.60
10:A:459:A:H61	10:A:473:U:H3	1.49	0.60
21:L:100:GLY:HA3	21:L:118:GLY:HA3	1.84	0.60
49:n:1:MET:HG2	49:n:67:LYS:HD2	1.83	0.60
8:7:2112:G:N1	8:7:2168:G:OP1	2.34	0.59
10:A:902:G:H4'	10:A:902:G:OP1	2.02	0.59
8:7:2512:C:H5''	38:c:127:PHE:CD1	2.37	0.59
26:Q:68:SER:HB3	26:Q:71:LYS:HB2	1.84	0.59
44:i:133:GLN:NE2	44:i:138:VAL:O	2.35	0.59
11:B:9:MET:HG2	11:B:212:LEU:HD21	1.84	0.59
31:V:29:A:H1'	31:V:30:A:H5'	1.84	0.59
35:Z:16:ILE:O	35:Z:25:ARG:NH2	2.35	0.59
35:Z:42:LEU:HD12	35:Z:75:VAL:HG13	1.84	0.59
41:f:86:LYS:NZ	41:f:87:LEU:O	2.35	0.59
8:7:1791:A:N6	8:7:1828:G:O2'	2.35	0.59
14:E:157:ARG:HH21	17:H:43:GLU:HB3	1.68	0.59
19:J:9:ARG:HG3	19:J:73:LEU:HD13	1.83	0.59
30:U:40:LYS:HB2	30:U:43:THR:HG22	1.85	0.59
45:j:71:CYS:HB2	45:j:117:LEU:HB3	1.84	0.59
8:7:487:C:O2'	57:v:52:GLU:OE1	2.20	0.59
8:7:776:G:O2'	8:7:2241:A:OP1	2.20	0.59
8:7:2497:A:H1'	8:7:2498:OMC:H5	1.67	0.59
10:A:562:U:H1'	21:L:12:ARG:HD2	1.83	0.59
52:q:95:THR:HB	52:q:113:ILE:HD11	1.85	0.59
8:7:858:G:N3	8:7:2268:A:H2'	2.18	0.59
9:8:47:C:O2'	53:r:98:GLN:NE2	2.36	0.59
10:A:350:G:H2'	10:A:351:G:C8	2.38	0.59
10:A:1380:U:O2'	16:G:3:ARG:NH1	2.35	0.59
20:K:27:PHE:HE1	20:K:89:PRO:HG2	1.66	0.59
8:7:495:G:H21	57:v:61:ASN:HD21	1.49	0.59
8:7:2109:U:H2'	8:7:2110:G:C8	2.38	0.59
8:7:65:U:O2'	8:7:456:C:N3	2.36	0.59
10:A:501:C:OP1	21:L:114:ARG:NH2	2.36	0.59
10:A:335:C:H2'	10:A:336:A:H8	1.68	0.59
10:A:1266:G:N2	10:A:1269:A:OP2	2.32	0.59
43:h:1:MET:HG2	43:h:2:LEU:H	1.67	0.59
8:7:675:A:OP1	39:d:58:LYS:NZ	2.33	0.59
8:7:1043:C:H5''	45:j:3:LEU:HD13	1.85	0.59
10:A:1536:C:H42	31:V:14:G:H1	1.50	0.59
33:X:1:G:C4	33:X:2:G:H1'	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:475:C:H4'	8:7:510:C:H5'	1.85	0.58
10:A:180:U:O2	10:A:196:A:N6	2.36	0.58
23:N:46:LEU:HD21	28:S:16:LEU:HD23	1.85	0.58
39:d:61:ARG:HH11	39:d:61:ARG:HG2	1.68	0.58
46:k:94:ASN:OD1	46:k:95:LYS:HD3	2.02	0.58
8:7:971:G:O2'	8:7:983:A:N3	2.35	0.58
8:7:1715:G:O2'	8:7:1743:G:O6	2.19	0.58
8:7:2691:C:H2'	8:7:2692:G:H8	1.68	0.58
8:7:45:G:H5'	8:7:46:G:H5'	1.85	0.58
8:7:2137:U:H2'	8:7:2138:G:C8	2.35	0.58
8:7:2470:G:O6	8:7:2481:G:N2	2.37	0.58
8:7:2818:U:OP2	52:q:42:LYS:NZ	2.36	0.58
8:7:2857:G:N2	8:7:2860:A:OP2	2.35	0.58
36:a:49:GLY:H	36:a:210:LYS:HE2	1.68	0.58
8:7:1076:C:O2'	46:k:95:LYS:NZ	2.29	0.58
20:K:20:VAL:HG13	20:K:35:THR:HG23	1.86	0.58
57:v:2:GLU:OE2	57:v:110:ARG:NH1	2.37	0.58
13:D:11:LEU:HD23	13:D:63:ARG:HG2	1.85	0.58
14:E:156:LYS:NZ	17:H:71:VAL:O	2.31	0.58
37:b:205:LEU:HD13	37:b:210:ALA:HB3	1.84	0.58
8:7:706:A:OP1	37:b:7:LYS:NZ	2.37	0.58
8:7:1167:C:H2'	8:7:1168:G:H8	1.68	0.58
28:S:50:ALA:HB1	28:S:57:HIS:HB3	1.84	0.58
8:7:1742:U:H2'	8:7:1743:G:C8	2.39	0.58
33:X:68:G:H1	33:X:80:C:H42	1.51	0.58
8:7:883:G:H1	8:7:893:C:H42	1.52	0.58
10:A:33:A:O2'	21:L:29:GLN:NE2	2.37	0.58
36:a:6:LYS:HA	36:a:9:ARG:HE	1.69	0.58
41:f:164:TYR:HB2	41:f:167:GLU:HB2	1.86	0.58
50:o:90:VAL:HG13	50:o:95:LEU:HD21	1.85	0.58
6:5:16:ARG:HH12	8:7:1265:A:H3'	1.68	0.58
10:A:1238:A:H5'	10:A:1336:C:H41	1.69	0.58
57:v:64:ALA:HB1	57:v:69:LEU:HD21	1.85	0.58
10:A:932:C:H5''	16:G:3:ARG:HG2	1.86	0.57
10:A:979:C:OP1	10:A:1223:C:N4	2.37	0.57
10:A:1347:G:O6	18:I:12:ARG:NH2	2.37	0.57
12:C:34:ASP:OD2	12:C:38:LYS:NZ	2.38	0.57
8:7:2130:U:O2'	8:7:2158:A:N7	2.32	0.57
20:K:84:VAL:HB	20:K:110:ILE:HG22	1.86	0.57
34:Y:62:C:H2'	34:Y:63:G:C8	2.38	0.57
8:7:1167:C:H2'	8:7:1168:G:C8	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:987:C:O2'	8:7:1000:A:N3	2.35	0.57
8:7:1789:A:OP2	37:b:221:ARG:NH1	2.38	0.57
10:A:1305:G:O2'	10:A:1332:A:N6	2.37	0.57
25:P:6:LEU:HD11	25:P:19:VAL:HG22	1.86	0.57
49:n:71:ARG:NH2	49:n:123:LEU:O	2.37	0.57
54:s:6:LYS:O	54:s:10:GLN:NE2	2.37	0.57
2:1:58:VAL:HG12	8:7:372:G:H2'	1.86	0.57
10:A:1360:A:OP2	23:N:75:ARG:NH2	2.35	0.57
10:A:1522:U:OP1	20:K:128:ARG:NH1	2.33	0.57
8:7:958:U:OP1	43:h:40:ARG:NH2	2.38	0.57
8:7:1826:G:O2'	8:7:1971:U:OP2	2.23	0.57
34:Y:56:C:N4	34:Y:57:G:O6	2.37	0.57
56:u:15:SER:N	56:u:18:GLN:OE1	2.33	0.57
22:M:75:MET:HG3	22:M:78:LYS:HE3	1.87	0.57
8:7:1744:A:H3'	8:7:1745:A:H8	1.70	0.57
9:8:75:G:H2'	9:8:76:G:C8	2.39	0.57
45:j:41:LEU:HD21	45:j:99:PHE:HB2	1.87	0.57
46:k:72:LYS:HE2	46:k:115:ALA:HB3	1.86	0.57
8:7:715:A:H61	24:O:53:ARG:NH2	2.03	0.57
8:7:1056:G:N1	8:7:1102:C:OP2	2.38	0.57
8:7:2529:G:H4'	41:f:175:LYS:HE2	1.87	0.57
18:I:119:ARG:HH12	18:I:125:PRO:HA	1.70	0.57
8:7:671:C:N4	50:o:40:SER:O	2.24	0.57
8:7:2788:C:O2'	8:7:2809:A:N3	2.34	0.57
10:A:1328:C:OP1	22:M:28:THR:HG21	2.05	0.57
16:G:150:ALA:HA	20:K:61:PHE:HB3	1.87	0.57
23:N:54:ASP:HA	23:N:59:ARG:HG2	1.86	0.57
38:c:116:LYS:HB2	38:c:165:MET:HB2	1.87	0.57
8:7:2531:A:H61	8:7:2662:A:H61	1.52	0.56
10:A:1227:A:H5''	28:S:83:HIS:HD2	1.70	0.56
10:A:1048:G:H5''	23:N:3:LYS:HD2	1.87	0.56
8:7:75:G:H22	8:7:111:A:H2	1.52	0.56
8:7:517:C:O2'	57:v:78:GLU:OE2	2.22	0.56
8:7:686:U:O4	47:l:12:ARG:NH1	2.32	0.56
8:7:2112:G:H5''	8:7:2113:U:C5	2.39	0.56
10:A:543:U:H2'	10:A:544:G:H8	1.70	0.56
10:A:626:G:O3'	25:P:51:ARG:NH2	2.37	0.56
11:B:208:ARG:HH12	35:Z:41:GLY:HA2	1.71	0.56
13:D:147:GLU:HA	13:D:150:LYS:HG2	1.88	0.56
46:k:133:ALA:HB1	46:k:138:LEU:HB2	1.87	0.56
10:A:176:C:OP1	29:T:20:HIS:NE2	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:149:SER:OG	14:E:152:MET:HE3	2.04	0.56
23:N:60:GLN:OE1	23:N:60:GLN:N	2.38	0.56
52:q:28:LEU:HD13	52:q:34:ILE:HG12	1.86	0.56
57:v:69:LEU:HD23	57:v:109:ASP:HB3	1.87	0.56
1:0:1:MET:N	8:7:2526:G:N3	2.53	0.56
5:4:1:MET:SD	40:e:95:ARG:NH1	2.70	0.56
8:7:1006:C:H1'	48:m:108:MET:SD	2.46	0.56
8:7:2016:U:H2'	8:7:2017:U:C6	2.40	0.56
10:A:951:G:OP2	22:M:101:ARG:NH2	2.38	0.56
24:O:24:SER:O	24:O:28:GLN:HG2	2.05	0.56
30:U:67:ARG:HA	35:Z:79:PHE:HE2	1.69	0.56
35:Z:7:GLN:NE2	35:Z:11:GLU:OE2	2.38	0.56
52:q:97:ILE:HG13	52:q:113:ILE:HD13	1.88	0.56
8:7:455:C:H3'	8:7:456:C:H5''	1.88	0.56
16:G:15:ASP:OD1	16:G:19:GLY:N	2.39	0.56
6:5:13:ARG:O	6:5:17:ARG:HG3	2.06	0.56
10:A:938:A:O3'	16:G:95:ARG:NH2	2.39	0.56
10:A:1534:A:H2'	10:A:1535:C:C6	2.41	0.56
21:L:114:ARG:HG2	21:L:119:VAL:HB	1.88	0.56
8:7:517:C:O2'	57:v:18:ARG:NH2	2.37	0.56
41:f:116:GLN:NE2	41:f:117:LEU:O	2.39	0.56
10:A:598:U:H4'	17:H:86:TYR:CD2	2.41	0.56
29:T:82:GLN:HA	29:T:85:LYS:HE3	1.88	0.56
43:h:58:LYS:O	43:h:60:GLN:NE2	2.37	0.56
44:i:3:VAL:HG12	44:i:38:PRO:HA	1.88	0.56
8:7:2177:C:P	36:a:221:GLY:H	2.29	0.55
10:A:278:G:O3'	10:A:281:G:H5'	2.07	0.55
36:a:31:LYS:NZ	36:a:178:VAL:O	2.39	0.55
40:e:110:ARG:NH2	40:e:136:ILE:O	2.39	0.55
44:i:6:LEU:HD11	44:i:37:VAL:HG23	1.88	0.55
8:7:630:G:N2	8:7:633:A:OP2	2.29	0.55
8:7:1215:G:H1	8:7:1234:U:H3	1.53	0.55
8:7:1528:A:N6	8:7:1543:G:O2'	2.39	0.55
12:C:116:VAL:HG21	12:C:200:VAL:HG11	1.88	0.55
23:N:4:GLN:OE1	23:N:4:GLN:N	2.36	0.55
55:t:91:ASP:OD1	55:t:92:ARG:N	2.34	0.55
20:K:73:ALA:HB1	20:K:77:TYR:HD2	1.72	0.55
35:Z:98:LEU:HD23	35:Z:108:VAL:HG11	1.88	0.55
8:7:1653:G:H3'	52:q:2:ARG:HG2	1.88	0.55
8:7:2264:C:N4	61:z:15:ASP:OD2	2.39	0.55
8:7:499:U:H5''	59:x:43:LYS:HD2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:2008:C:H2'	8:7:2009:A:H8	1.72	0.55
11:B:125:THR:HG22	11:B:137:ARG:HH11	1.72	0.55
20:K:116:ILE:HD11	30:U:31:GLU:HG3	1.89	0.55
39:d:184:ASP:HA	50:o:2:ARG:HH12	1.71	0.55
40:e:49:LEU:HD23	40:e:52:ASN:HD21	1.72	0.55
8:7:1675:C:H3'	8:7:1676:A:H8	1.72	0.55
12:C:77:ILE:HD11	12:C:103:ILE:HG13	1.89	0.55
17:H:76:GLN:NE2	17:H:77:ARG:O	2.40	0.55
36:a:51:ASP:O	36:a:57:GLN:NE2	2.40	0.55
39:d:112:LEU:HD23	39:d:115:GLN:HE21	1.71	0.55
45:j:8:LYS:HD3	45:j:59:LEU:HD11	1.88	0.55
52:q:53:THR:HA	52:q:56:LYS:HE3	1.87	0.55
8:7:213:A:H2'	8:7:214:G:C8	2.42	0.55
8:7:558:U:H2'	8:7:559:G:C8	2.41	0.55
8:7:2641:G:H5''	48:m:78:THR:HB	1.89	0.55
8:7:1600:C:H2'	8:7:1601:G:C8	2.42	0.55
8:7:1791:A:H5''	37:b:205:LEU:HD11	1.88	0.55
10:A:1106:G:O2'	12:C:169:ARG:NH2	2.39	0.55
19:J:34:ALA:HB2	19:J:83:THR:HG21	1.89	0.55
49:n:40:LYS:HE3	49:n:57:VAL:HG22	1.89	0.55
8:7:2134:A:P	8:7:2156:G:H22	2.30	0.55
8:7:2645:G:OP2	8:7:2645:G:N2	2.26	0.55
11:B:23:TRP:CD1	11:B:39:HIS:HE2	2.25	0.55
45:j:124:ASP:N	45:j:124:ASP:OD1	2.40	0.55
10:A:136:C:H1'	25:P:1:MET:HE2	1.88	0.54
10:A:421:U:O4	12:C:127:ARG:NH2	2.39	0.54
12:C:212:ALA:HA	19:J:16:ARG:HH22	1.72	0.54
29:T:27:MET:HE2	29:T:27:MET:HA	1.88	0.54
32:W:10:G:O2'	32:W:11:C:OP1	2.22	0.54
57:v:2:GLU:HG3	57:v:108:SER:HB3	1.89	0.54
8:7:910:A:N3	8:7:2264:C:O2'	2.38	0.54
33:X:3:U:H2'	33:X:4:G:C8	2.42	0.54
8:7:779:U:OP1	37:b:49:ILE:HD12	2.07	0.54
44:i:86:ASP:OD1	44:i:87:GLU:N	2.40	0.54
8:7:192:C:O2'	8:7:802:A:N3	2.40	0.54
8:7:859:G:H22	8:7:916:G:H2'	1.72	0.54
10:A:1027:C:HO2'	10:A:1028:C:P	2.29	0.54
13:D:73:ARG:NH2	13:D:74:ASN:OD1	2.34	0.54
8:7:468:G:N7	47:l:39:ARG:NH2	2.54	0.54
8:7:833:A:OP1	50:o:39:LYS:NZ	2.31	0.54
34:Y:2:G:H1	34:Y:71:C:H42	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:34:ALA:HB2	36:a:216:THR:HG21	1.90	0.54
38:c:31:ALA:O	38:c:33:ARG:NH1	2.41	0.54
57:v:71:VAL:HA	57:v:107:VAL:HG12	1.88	0.54
8:7:500:G:N1	8:7:503:A:OP2	2.39	0.54
8:7:1570:A:H2'	8:7:1571:A:C8	2.43	0.54
18:I:6:TYR:HB2	18:I:21:ILE:HB	1.89	0.54
8:7:481:G:O2'	8:7:507:A:N1	2.36	0.54
8:7:1022:G:N2	8:7:1142:A:N1	2.56	0.54
10:A:769:G:H4'	10:A:1513:A:H4'	1.89	0.54
45:j:37:LYS:HG2	45:j:99:PHE:HZ	1.72	0.54
8:7:2129:C:O2'	8:7:2159:G:O6	2.26	0.54
8:7:2680:U:H5'	38:c:194:PRO:HA	1.90	0.54
10:A:1222:G:OP2	10:A:1322:C:N4	2.32	0.54
10:A:1228:C:H5'	22:M:114:LYS:O	2.06	0.54
18:I:130:ARG:HH12	32:W:35:A:P	2.31	0.54
20:K:124:PRO:O	30:U:38:TYR:N	2.40	0.54
44:i:93:SER:HB3	44:i:121:VAL:HB	1.90	0.54
10:A:575:G:O2'	10:A:821:G:H5'	2.08	0.54
13:D:170:TRP:CD2	13:D:186:PRO:HB3	2.43	0.54
14:E:83:HIS:CD2	17:H:96:MET:HE1	2.43	0.54
8:7:675:A:O2'	39:d:62:GLN:OE1	2.25	0.53
8:7:1278:C:H2'	8:7:1279:G:C8	2.43	0.53
10:A:404:G:OP1	13:D:115:ARG:NH1	2.41	0.53
10:A:409:U:H3	10:A:433:G:H1	1.56	0.53
10:A:876:C:P	17:H:15:ARG:HH12	2.31	0.53
13:D:50:ASP:OD1	13:D:51:TYR:N	2.41	0.53
32:W:18:G:H1	32:W:55:PSU:H1'	1.72	0.53
45:j:22:ALA:HA	45:j:86:MET:HA	1.89	0.53
8:7:1105:U:H2'	8:7:1106:G:C8	2.43	0.53
8:7:1716:U:H2'	8:7:1717:A:C8	2.43	0.53
8:7:1952:A:C5	49:n:22:ILE:HD11	2.43	0.53
8:7:2010:G:H5'	57:v:42:LYS:HE2	1.88	0.53
8:7:2108:A:H2	8:7:2181:U:H3	1.56	0.53
50:o:20:GLY:HA2	50:o:28:GLY:HA2	1.89	0.53
8:7:1071:G:N3	8:7:1089:A:O2'	2.39	0.53
8:7:2334:U:N3	53:r:16:ARG:HG3	2.23	0.53
41:f:88:GLN:HE22	41:f:165:ALA:HB2	1.74	0.53
2:1:65:ASP:OD1	2:1:66:THR:N	2.42	0.53
8:7:2144:G:H1'	8:7:2147:A:H61	1.73	0.53
9:8:27:C:OP1	53:r:34:HIS:NE2	2.32	0.53
14:E:136:VAL:O	14:E:140:THR:HG23	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:31:MET:SD	16:G:36:LYS:HG2	2.49	0.53
21:L:54:ARG:HH11	21:L:64:THR:HB	1.72	0.53
30:U:41:PRO:O	30:U:44:GLU:HG3	2.08	0.53
33:X:71:5MU:O2	36:a:167:LYS:NZ	2.39	0.53
37:b:107:PRO:HG2	37:b:110:LEU:HB2	1.90	0.53
8:7:1645:G:H5''	8:7:1646:C:H5'	1.90	0.53
11:B:121:SER:HA	11:B:125:THR:HG23	1.90	0.53
12:C:40:ARG:NH1	12:C:57:ILE:HD12	2.24	0.53
26:Q:81:LYS:NZ	26:Q:82:ALA:O	2.36	0.53
28:S:28:LYS:HA	28:S:28:LYS:HE3	1.89	0.53
56:u:35:PHE:HB2	56:u:59:ILE:HB	1.91	0.53
8:7:1201:U:H2'	8:7:1202:G:C8	2.43	0.53
8:7:1716:U:H2'	8:7:1717:A:H8	1.74	0.53
8:7:2562:U:H1'	49:n:23:LYS:NZ	2.24	0.53
10:A:1382:C:H1'	16:G:79:ARG:CZ	2.39	0.53
10:A:1497:G:H1'	10:A:1518:MA6:H2	1.91	0.53
10:A:1534:A:H2'	10:A:1535:C:H6	1.74	0.53
12:C:121:THR:HG22	12:C:189:ALA:HB2	1.90	0.53
16:G:140:ASP:OD1	16:G:143:ARG:NH2	2.35	0.53
27:R:15:ALA:O	27:R:16:GLU:HB2	2.08	0.53
34:Y:15:G:H2'	34:Y:59:U:H3	1.72	0.53
9:8:98:G:H1	60:y:14:LYS:HB2	1.73	0.53
10:A:474:G:OP1	25:P:80:LYS:NZ	2.32	0.53
15:F:11:HIS:ND1	15:F:13:ASP:OD1	2.42	0.53
35:Z:102:TYR:OH	35:Z:158:LYS:NZ	2.41	0.53
35:Z:122:VAL:HB	35:Z:129:ALA:HB3	1.91	0.53
38:c:156:PHE:HD2	48:m:81:ILE:HG13	1.74	0.53
5:4:14:ALA:HB3	5:4:22:MET:HB2	1.91	0.53
8:7:453:A:N3	8:7:457:A:O2'	2.41	0.53
8:7:1604:C:O2'	8:7:1610:A:N1	2.35	0.53
8:7:2334:U:H3	53:r:16:ARG:HG3	1.73	0.53
11:B:86:SER:O	11:B:222:ARG:NH2	2.41	0.53
43:h:1:MET:HG3	43:h:47:GLU:HG3	1.91	0.53
10:A:322:C:H2'	10:A:323:U:C6	2.44	0.53
10:A:1225:A:H2'	10:A:1225:A:N3	2.24	0.53
16:G:91:VAL:HG13	16:G:96:ARG:HG2	1.90	0.53
19:J:88:MET:HE1	19:J:100:ILE:HD13	1.90	0.53
8:7:1060:U:OP1	46:k:76:ALA:N	2.41	0.53
8:7:2540:C:O2'	8:7:2740:A:N3	2.36	0.53
10:A:477:C:H2'	10:A:478:A:C8	2.44	0.53
31:V:18:A:H2'	31:V:19:G:C8	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:m:114:LEU:O	48:m:118:MET:HG3	2.08	0.53
8:7:717:C:H3'	8:7:718:A:H8	1.74	0.52
8:7:1329:U:H5''	8:7:1330:C:H5	1.74	0.52
8:7:2105:U:H2'	8:7:2106:U:C6	2.44	0.52
8:7:2419:U:H4'	42:g:22:THR:HG21	1.90	0.52
10:A:54:C:H2'	10:A:352:C:H41	1.74	0.52
10:A:1346:A:O2'	10:A:1347:G:H4'	2.09	0.52
13:D:101:VAL:HG21	13:D:137:VAL:HG21	1.91	0.52
30:U:63:GLU:C	30:U:65:ALA:H	2.16	0.52
32:W:37:MIA:H112	32:W:38:A:H1'	1.91	0.52
49:n:1:MET:HG3	49:n:1:MET:O	2.08	0.52
2:1:59:ILE:HD13	2:1:67:VAL:HG11	1.91	0.52
4:3:20:HIS:O	4:3:23:THR:N	2.41	0.52
8:7:813:U:O3'	56:u:86:GLN:NE2	2.42	0.52
8:7:1169:A:H61	8:7:1180:U:H3	1.56	0.52
19:J:45:ARG:NH1	19:J:47:GLU:OE2	2.42	0.52
20:K:74:VAL:HG23	20:K:75:LYS:N	2.24	0.52
22:M:83:LEU:HG	28:S:74:PHE:HE1	1.74	0.52
33:X:42:G:H2'	33:X:43:A:C8	2.43	0.52
39:d:117:ARG:NH2	39:d:183:PHE:O	2.41	0.52
4:3:13:ALA:HA	4:3:16:ARG:HD3	1.89	0.52
4:3:54:MET:HG3	4:3:55:VAL:HG13	1.92	0.52
8:7:859:G:N2	8:7:916:G:H2'	2.24	0.52
8:7:2710:C:H2'	8:7:2711:A:H8	1.74	0.52
9:8:10:G:H3'	9:8:11:C:H6	1.73	0.52
10:A:618:C:O2'	25:P:14:ARG:NH1	2.42	0.52
16:G:82:GLY:H	31:V:16:U:H4'	1.73	0.52
49:n:22:ILE:HG22	49:n:40:LYS:O	2.08	0.52
8:7:1288:G:OP2	8:7:1288:G:N2	2.29	0.52
10:A:160:A:H2'	10:A:161:A:O4'	2.10	0.52
49:n:19:VAL:HG21	49:n:41:ILE:HD12	1.92	0.52
8:7:2512:C:O2'	38:c:159:LYS:NZ	2.43	0.52
8:7:2845:U:H2'	8:7:2846:G:C8	2.44	0.52
10:A:1217:C:H5'	23:N:9:ARG:HH21	1.74	0.52
23:N:83:LYS:HA	23:N:83:LYS:HE3	1.90	0.52
8:7:717:C:H2'	8:7:718:A:O4'	2.09	0.52
8:7:762:U:N3	8:7:1431:A:OP1	2.42	0.52
8:7:832:U:H5'	50:o:38:GLN:HG2	1.91	0.52
8:7:2600:A:N6	37:b:236:GLU:OE1	2.41	0.52
10:A:321:A:H2'	10:A:322:C:C6	2.44	0.52
12:C:152:GLU:HG3	12:C:199:LYS:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:184:TYR:OH	12:C:199:LYS:HD3	2.10	0.52
14:E:39:VAL:HG23	14:E:71:MET:HE1	1.92	0.52
21:L:123:LYS:HA	21:L:123:LYS:HE3	1.92	0.52
41:f:24:ILE:HG21	41:f:72:LEU:HD11	1.92	0.52
54:s:75:GLN:HB2	54:s:78:SER:HB2	1.91	0.52
8:7:1143:A:OP1	48:m:27:ARG:NH1	2.28	0.52
8:7:1213:A:H62	8:7:1236:G:H1'	1.75	0.52
8:7:1580:A:HO2'	8:7:1581:G:P	2.33	0.52
10:A:110:C:O2'	25:P:25:ARG:O	2.23	0.52
12:C:23:PHE:HZ	19:J:11:LYS:HZ3	1.57	0.52
29:T:3:ASN:OD1	29:T:4:ILE:HD12	2.10	0.52
32:W:43:C:H2'	32:W:44:G:C8	2.44	0.52
8:7:191:A:H2'	8:7:192:C:C6	2.45	0.52
9:8:48:U:P	53:r:30:ARG:HH12	2.32	0.52
13:D:60:LYS:O	13:D:64:ILE:HD12	2.09	0.52
22:M:44:LYS:HB2	22:M:47:GLU:OE1	2.10	0.52
23:N:88:ALA:HA	23:N:93:ILE:HB	1.92	0.52
29:T:10:ARG:HA	29:T:13:GLN:NE2	2.24	0.52
49:n:65:THR:HG22	49:n:67:LYS:H	1.73	0.52
8:7:1954:G:N1	8:7:1986:C:OP1	2.30	0.52
10:A:264:C:O2'	26:Q:66:PRO:O	2.23	0.52
45:j:65:GLU:OE1	45:j:65:GLU:N	2.41	0.52
52:q:35:LYS:HG2	52:q:112:TYR:CE1	2.44	0.52
8:7:558:U:OP1	48:m:113:PRO:HD2	2.10	0.52
10:A:67:C:H2'	10:A:68:G:C8	2.45	0.52
10:A:320:A:H2'	10:A:321:A:C8	2.45	0.52
10:A:845:A:H61	27:R:8:ARG:HG3	1.75	0.52
39:d:21:ARG:HD3	39:d:106:LYS:HB3	1.91	0.52
45:j:100:ALA:HB1	45:j:107:GLU:HA	1.91	0.52
4:3:10:THR:HG21	4:3:56:LYS:HG2	1.92	0.51
10:A:923:A:OP1	14:E:26:LYS:NZ	2.35	0.51
16:G:79:ARG:NH2	33:X:35:G:OP1	2.43	0.51
29:T:29:ARG:HB3	29:T:33:LYS:NZ	2.25	0.51
32:W:37:MIA:N1	32:W:37:MIA:H131	2.25	0.51
37:b:252:THR:O	37:b:253:LYS:HB2	2.10	0.51
39:d:192:ALA:HA	39:d:195:GLN:OE1	2.10	0.51
1:0:32:LYS:HZ2	8:7:2478:A:H5'	1.73	0.51
8:7:1024:G:HO2'	8:7:1144:A:HO2'	1.59	0.51
8:7:1077:A:H5'	46:k:95:LYS:HZ2	1.74	0.51
8:7:1954:G:O2'	8:7:1956:U:O4	2.20	0.51
8:7:2111:U:H5''	8:7:2118:U:H1'	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:2432:A:H2'	8:7:2433:A:C8	2.45	0.51
8:7:2484:G:H1'	43:h:123:LYS:HD2	1.92	0.51
24:O:21:ASP:OD1	24:O:24:SER:HB3	2.10	0.51
36:a:8:MET:HA	36:a:11:ILE:HB	1.91	0.51
38:c:183:GLU:OE2	38:c:184:ARG:HG3	2.10	0.51
40:e:49:LEU:HA	40:e:52:ASN:HD21	1.74	0.51
44:i:100:ALA:HB3	44:i:112:LYS:HZ3	1.75	0.51
1:0:32:LYS:NZ	8:7:2478:A:H5'	2.25	0.51
8:7:947:A:H2'	8:7:948:C:C6	2.45	0.51
8:7:2019:A:H2	8:7:2035:G:H22	1.58	0.51
37:b:232:HIS:NE2	37:b:244:PRO:HA	2.25	0.51
54:s:106:LYS:HD3	54:s:109:ARG:HD3	1.92	0.51
8:7:411:G:OP2	8:7:2406:A:O2'	2.28	0.51
8:7:663:G:H5''	50:o:17:LYS:NZ	2.25	0.51
8:7:983:A:N6	8:7:984:A:N1	2.58	0.51
8:7:1028:A:N3	8:7:2486:C:O2'	2.35	0.51
10:A:8:A:N6	13:D:202:GLU:O	2.43	0.51
10:A:1132:C:N4	10:A:1133:G:O6	2.43	0.51
13:D:40:GLN:H	13:D:40:GLN:CD	2.19	0.51
14:E:115:LEU:HD13	14:E:123:VAL:HG11	1.93	0.51
19:J:5:ARG:HG2	19:J:77:VAL:HA	1.92	0.51
47:l:22:MET:HG3	47:l:28:ARG:HG2	1.91	0.51
8:7:2150:C:H2'	8:7:2151:U:C6	2.46	0.51
26:Q:82:ALA:O	26:Q:83:VAL:HG12	2.10	0.51
45:j:37:LYS:HG2	45:j:99:PHE:CZ	2.46	0.51
8:7:2011:U:H2'	8:7:2012:G:O4'	2.11	0.51
10:A:414:A:OP2	10:A:428:G:N2	2.41	0.51
10:A:1008:U:H3	10:A:1021:A:H61	1.59	0.51
37:b:91:ILE:HD12	37:b:103:TYR:CD1	2.46	0.51
37:b:145:GLU:OE2	37:b:150:LYS:N	2.43	0.51
8:7:1791:A:H4'	37:b:205:LEU:HD11	1.91	0.51
8:7:2123:G:H3'	8:7:2124:G:H8	1.75	0.51
8:7:2868:A:H3'	8:7:2869:G:H8	1.75	0.51
9:8:48:U:H5'	53:r:98:GLN:NE2	2.25	0.51
10:A:972:C:O2'	19:J:57:VAL:O	2.29	0.51
33:X:21:G:C8	33:X:21:G:H5''	2.45	0.51
8:7:1852:U:OP1	33:X:88:C:O2'	2.29	0.51
8:7:2008:C:H2'	8:7:2009:A:C8	2.45	0.51
10:A:51:A:N7	10:A:114:U:O2'	2.44	0.51
12:C:6:HIS:CE1	12:C:184:TYR:HD2	2.29	0.51
12:C:212:ALA:N	19:J:16:ARG:HH12	2.08	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:j:4:ASN:HB3	45:j:7:ASP:HB2	1.93	0.51
8:7:1040:A:H61	8:7:1115:G:H1	1.59	0.51
8:7:1046:A:O4'	45:j:62:ARG:NH2	2.44	0.51
10:A:503:C:O2'	10:A:510:A:N1	2.41	0.51
10:A:1240:U:P	16:G:116:MET:HE2	2.50	0.51
14:E:83:HIS:NE2	14:E:147:MET:HG3	2.25	0.51
17:H:54:ASP:OD1	17:H:55:THR:N	2.43	0.51
19:J:92:LEU:HG	19:J:93:ALA:H	1.76	0.51
48:m:41:LYS:NZ	48:m:52:ASP:OD1	2.32	0.51
2:1:17:ASN:OD1	2:1:27:ARG:HD2	2.11	0.51
7:6:23:LYS:NZ	8:7:630:G:OP2	2.38	0.51
8:7:742:A:H2'	8:7:743:A:C8	2.45	0.51
8:7:2182:U:H2'	8:7:2183:A:C8	2.45	0.51
10:A:950:U:H2'	10:A:951:G:H8	1.77	0.51
20:K:27:PHE:CE1	20:K:89:PRO:HG2	2.46	0.51
37:b:16:VAL:HG12	37:b:206:GLY:HA3	1.93	0.51
8:7:753:A:H2'	8:7:754:U:C6	2.47	0.50
8:7:2041:U:H2'	8:7:2042:A:H8	1.76	0.50
8:7:2267:A:H5''	8:7:2268:A:H5'	1.93	0.50
10:A:33:A:H2'	10:A:34:C:C6	2.46	0.50
10:A:330:C:H2'	10:A:331:G:H5'	1.93	0.50
10:A:655:A:H2'	10:A:656:G:H8	1.76	0.50
10:A:880:C:H2'	10:A:881:G:H8	1.77	0.50
10:A:972:C:OP2	19:J:59:LYS:NZ	2.40	0.50
10:A:1256:A:O2'	10:A:1278:G:O6	2.24	0.50
12:C:114:LYS:HA	12:C:185:ASN:HD22	1.74	0.50
16:G:70:ARG:HG2	16:G:96:ARG:HE	1.77	0.50
33:X:35:G:H2'	33:X:36:C:C6	2.46	0.50
49:n:115:ILE:H	49:n:115:ILE:HD12	1.76	0.50
2:1:55:GLY:O	2:1:59:ILE:HG12	2.11	0.50
6:5:13:ARG:NH1	8:7:1263:U:OP1	2.44	0.50
8:7:1019:U:OP1	8:7:1035:U:O2'	2.19	0.50
8:7:1062:G:OP1	8:7:1070:A:H4'	2.11	0.50
8:7:1105:U:H2'	8:7:1106:G:H8	1.76	0.50
8:7:2100:G:H3'	8:7:2101:A:H8	1.77	0.50
10:A:390:U:H4'	25:P:28:ARG:HH21	1.75	0.50
10:A:405:U:OP2	13:D:3:ARG:NE	2.44	0.50
10:A:1095:U:OP1	10:A:1108:G:N2	2.31	0.50
10:A:1498:UR3:H4'	10:A:1519:MA6:H2	1.92	0.50
16:G:79:ARG:HG2	16:G:84:THR:HB	1.93	0.50
8:7:355:U:H2'	8:7:356:G:H8	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:1341:G:O6	58:w:19:LYS:NZ	2.38	0.50
8:7:1447:C:O2'	8:7:1544:A:N3	2.38	0.50
11:B:97:LEU:H	11:B:100:MET:HE1	1.77	0.50
11:B:117:LEU:HD12	11:B:120:GLN:HE21	1.76	0.50
13:D:100:ASN:OD1	13:D:111:ARG:NH1	2.44	0.50
48:m:72:LYS:HE3	48:m:74:TYR:CE1	2.44	0.50
53:r:12:THR:HA	53:r:15:ARG:HH11	1.76	0.50
8:7:276:U:H2'	8:7:277:G:C2	2.47	0.50
8:7:859:G:OP2	8:7:859:G:H8	1.94	0.50
10:A:677:U:H3	10:A:713:G:H22	1.59	0.50
10:A:1413:A:H2	10:A:1487:G:H22	1.60	0.50
16:G:32:VAL:HG22	16:G:33:ASP:OD2	2.12	0.50
32:W:1:G:H1'	61:z:5:LYS:HD2	1.94	0.50
34:Y:55:PSU:OP1	43:h:50:ARG:NH1	2.36	0.50
38:c:181:ASP:OD1	38:c:183:GLU:HG3	2.12	0.50
50:o:81:ASP:HA	50:o:84:LYS:HD2	1.92	0.50
61:z:21:LEU:HD21	61:z:41:ARG:HG2	1.93	0.50
6:5:43:ILE:HG22	6:5:49:TYR:HB2	1.92	0.50
8:7:782:A:C2	37:b:225:MET:HG2	2.46	0.50
8:7:2009:A:O2'	57:v:42:LYS:NZ	2.45	0.50
10:A:950:U:H2'	10:A:951:G:C8	2.46	0.50
16:G:113:ASP:HB2	16:G:119:ARG:CG	2.42	0.50
29:T:53:GLU:O	29:T:56:PRO:HD2	2.10	0.50
34:Y:18:G:O2'	34:Y:57:G:N2	2.44	0.50
37:b:66:ASP:OD2	37:b:102:ARG:NH1	2.41	0.50
37:b:122:ALA:O	37:b:130:LEU:HD21	2.11	0.50
49:n:25:LEU:HD12	49:n:26:GLY:H	1.75	0.50
8:7:1243:C:H2'	8:7:1244:A:H8	1.77	0.50
10:A:455:G:H2'	10:A:456:A:C8	2.47	0.50
10:A:1143:G:H2'	10:A:1144:G:H8	1.76	0.50
11:B:119:THR:O	11:B:122:GLN:HG3	2.11	0.50
25:P:19:VAL:HG12	25:P:36:VAL:HG23	1.93	0.50
40:e:26:MET:O	40:e:30:ARG:NH2	2.39	0.50
48:m:92:MET:HE2	48:m:100:VAL:HG12	1.93	0.50
8:7:468:G:H5''	39:d:55:SER:HB2	1.94	0.50
8:7:2831:G:N7	38:c:59:ARG:NH2	2.60	0.50
10:A:544:G:H2'	10:A:545:C:C6	2.47	0.50
10:A:1073:U:H4'	11:B:105:LYS:NZ	2.27	0.50
44:i:103:VAL:HG21	44:i:110:VAL:HG22	1.94	0.50
55:t:94:ILE:H	55:t:94:ILE:HD12	1.76	0.50
8:7:179:C:H2'	8:7:180:G:C8	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:566:U:H5''	50:o:29:LYS:HE3	1.93	0.50
8:7:2737:G:H2'	8:7:2738:A:C8	2.47	0.50
8:7:2868:A:H3'	8:7:2869:G:C8	2.47	0.50
10:A:655:A:H2'	10:A:656:G:C8	2.47	0.50
10:A:1308:U:H2'	10:A:1309:G:H8	1.77	0.50
12:C:150:LYS:HG3	12:C:169:ARG:HB3	1.92	0.50
33:X:24:G:H2'	33:X:25:G:C8	2.47	0.50
43:h:24:THR:O	43:h:34:LYS:NZ	2.43	0.50
54:s:29:LYS:HE2	54:s:40:LEU:HB3	1.94	0.50
8:7:1368:G:P	47:l:25:LYS:HZ1	2.34	0.50
8:7:2518:A:H2'	8:7:2518:A:N3	2.25	0.50
10:A:766:A:OP2	10:A:812:G:N2	2.45	0.50
10:A:844:G:C8	10:A:845:A:H3'	2.46	0.50
10:A:1541:U:O2'	31:V:7:A:OP2	2.30	0.50
60:y:45:ASP:N	60:y:45:ASP:OD1	2.42	0.50
8:7:118:A:OP2	8:7:119:A:H2'	2.12	0.49
8:7:463:G:N2	8:7:466:A:OP2	2.28	0.49
10:A:455:G:H2'	10:A:456:A:H8	1.77	0.49
10:A:1213:A:O2'	10:A:1215:G:N7	2.43	0.49
15:F:23:GLU:OE1	15:F:23:GLU:N	2.36	0.49
46:k:72:LYS:HG3	46:k:73:THR:N	2.27	0.49
46:k:73:THR:HG21	46:k:112:THR:HG22	1.94	0.49
8:7:481:G:O5'	59:x:44:LYS:NZ	2.44	0.49
8:7:1085:A:H61	45:j:35:VAL:HB	1.78	0.49
8:7:1796:U:H2'	8:7:1797:G:C8	2.47	0.49
10:A:334:C:HO2'	10:A:1434:A:HO2'	1.60	0.49
10:A:1346:A:H62	16:G:10:ARG:NH1	2.10	0.49
12:C:77:ILE:HD13	12:C:84:VAL:HG11	1.93	0.49
13:D:9:LEU:HD21	13:D:22:LYS:HG2	1.93	0.49
14:E:156:LYS:HZ3	17:H:71:VAL:HG13	1.77	0.49
16:G:92:ARG:O	16:G:96:ARG:HG3	2.13	0.49
36:a:42:VAL:HG22	36:a:216:THR:HG22	1.94	0.49
55:t:45:TYR:HA	55:t:48:ARG:HH12	1.75	0.49
8:7:224:U:O4	8:7:419:U:O2'	2.30	0.49
8:7:1198:U:H2'	8:7:1199:U:C6	2.48	0.49
8:7:2506:U:OP2	8:7:2576:G:N1	2.33	0.49
10:A:339:C:H3'	49:n:98:ARG:NH2	2.27	0.49
10:A:477:C:H2'	10:A:478:A:H8	1.76	0.49
11:B:66:LYS:N	11:B:159:ASP:OD2	2.43	0.49
21:L:63:VAL:HG21	21:L:95:TYR:HE2	1.77	0.49
54:s:48:ILE:HB	54:s:97:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:8:PRO:HD2	8:7:1263:U:O2'	2.13	0.49
7:6:13:ARG:NH1	50:o:59:ARG:HA	2.27	0.49
8:7:476:G:H22	8:7:479:A:H5''	1.76	0.49
8:7:558:U:H5'	48:m:114:LEU:HD13	1.94	0.49
8:7:1913:A:C6	34:Y:38:A:H5'	2.47	0.49
13:D:118:VAL:HG22	13:D:123:ILE:HG13	1.94	0.49
13:D:196:ASN:HB2	13:D:198:HIS:CE1	2.47	0.49
21:L:30:LYS:HB3	21:L:57:LEU:HD12	1.94	0.49
39:d:188:MET:HE1	39:d:193:VAL:HG22	1.94	0.49
53:r:30:ARG:HA	53:r:35:ILE:HD12	1.94	0.49
56:u:76:LYS:HB2	56:u:85:LYS:HB2	1.94	0.49
4:3:17:LEU:HB2	4:3:20:HIS:CE1	2.48	0.49
8:7:2869:G:H2'	8:7:2870:C:C6	2.47	0.49
37:b:124:ILE:O	37:b:124:ILE:HG13	2.12	0.49
40:e:49:LEU:HA	40:e:52:ASN:ND2	2.28	0.49
46:k:10:LYS:HD3	46:k:56:PRO:HB3	1.92	0.49
54:s:43:PHE:CZ	54:s:63:LYS:HE3	2.47	0.49
2:1:70:GLU:OE1	2:1:74:ARG:NH2	2.46	0.49
8:7:299:A:O5'	8:7:299:A:H8	1.95	0.49
8:7:466:A:N1	8:7:795:C:O2'	2.40	0.49
8:7:2149:U:H2'	8:7:2150:C:C6	2.47	0.49
10:A:811:C:O2'	10:A:901:A:N1	2.44	0.49
26:Q:77:ARG:HH12	26:Q:79:VAL:HG22	1.77	0.49
48:m:99:ARG:NH1	48:m:102:GLU:OE2	2.45	0.49
48:m:105:VAL:O	48:m:109:LEU:HD13	2.13	0.49
55:t:27:ALA:O	55:t:31:VAL:HG12	2.11	0.49
8:7:1278:C:H2'	8:7:1279:G:H8	1.77	0.49
8:7:2176:A:O3'	36:a:221:GLY:N	2.46	0.49
8:7:2343:U:O2'	8:7:2373:G:O2'	2.19	0.49
10:A:109:A:H5'	10:A:110:C:H5	1.78	0.49
10:A:312:C:H2'	10:A:313:A:H8	1.77	0.49
10:A:559:A:H4'	10:A:560:A:H3'	1.94	0.49
20:K:113:VAL:O	20:K:113:VAL:HG12	2.13	0.49
33:X:20:H2U:H52	33:X:74:G:C2	2.47	0.49
8:7:210:C:OP1	47:l:29:GLN:NE2	2.45	0.49
8:7:1059:G:N2	46:k:132:THR:OG1	2.46	0.49
8:7:2576:G:O2'	8:7:2579:C:OP2	2.30	0.49
10:A:86:G:O2'	10:A:88:U:O4	2.16	0.49
10:A:1041:G:H2'	10:A:1042:A:C8	2.47	0.49
10:A:1193:G:OP1	12:C:167:TRP:NE1	2.42	0.49
23:N:69:ARG:CZ	23:N:81:ARG:HH21	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:X:12:C:H42	33:X:24:G:H1	1.61	0.49
38:c:25:THR:HG21	38:c:193:VAL:HG22	1.95	0.49
46:k:66:SER:OG	46:k:67:PHE:N	2.44	0.49
8:7:17:G:H4'	55:t:25:TYR:HE1	1.78	0.49
8:7:214:G:H1'	8:7:217:A:H5'	1.94	0.49
8:7:743:A:O2'	8:7:1659:G:OP1	2.26	0.49
8:7:833:A:H2'	8:7:834:G:C8	2.48	0.49
8:7:1378:A:O2'	8:7:1380:G:OP2	2.31	0.49
8:7:1597:A:H5''	8:7:1598:A:H5'	1.95	0.49
10:A:595:A:N6	10:A:641:U:O2'	2.43	0.49
40:e:170:LEU:HB3	40:e:175:PHE:CD2	2.48	0.49
56:u:98:ILE:H	56:u:98:ILE:HD12	1.78	0.49
8:7:514:A:N3	8:7:581:C:O2'	2.42	0.49
8:7:817:C:H2'	8:7:818:G:C8	2.48	0.49
8:7:910:A:H62	43:h:12:MET:HA	1.78	0.49
8:7:996:A:O2'	55:t:91:ASP:OD2	2.22	0.49
8:7:2744:G:N2	41:f:143:GLN:OE1	2.43	0.49
9:8:10:G:H3'	9:8:11:C:C6	2.48	0.49
10:A:1080:A:OP1	14:E:50:TYR:OH	2.22	0.49
15:F:38:ARG:HB3	15:F:63:ASN:HB2	1.95	0.49
37:b:35:GLU:OE1	37:b:35:GLU:N	2.46	0.49
37:b:135:ILE:O	37:b:167:ARG:NH2	2.45	0.49
41:f:80:THR:OG1	41:f:81:GLU:OE1	2.26	0.49
60:y:20:LEU:HD21	60:y:41:GLU:HB2	1.94	0.49
8:7:2470:G:OP1	43:h:55:ARG:NH2	2.45	0.48
8:7:2492:U:H2'	8:7:2493:U:C6	2.48	0.48
10:A:1199:U:H4'	19:J:56:HIS:CD2	2.47	0.48
10:A:1530:G:H2'	10:A:1531:A:C8	2.47	0.48
37:b:231:PRO:HB2	37:b:245:VAL:HG21	1.95	0.48
45:j:111:ALA:HB3	45:j:118:ILE:HB	1.95	0.48
56:u:40:MET:HG2	56:u:49:ILE:HA	1.95	0.48
8:7:1141:U:H4'	8:7:1142:A:O4'	2.13	0.48
24:O:36:ILE:HD11	24:O:59:MET:HG3	1.94	0.48
43:h:20:LEU:HD13	60:y:81:PRO:HG3	1.95	0.48
8:7:784:G:H5'	8:7:785:G:OP1	2.14	0.48
8:7:894:U:H2'	8:7:895:U:O4'	2.13	0.48
10:A:1183:U:O2'	10:A:1185:G:OP1	2.31	0.48
11:B:169:GLU:OE1	11:B:169:GLU:N	2.46	0.48
38:c:32:ASN:ND2	38:c:52:THR:HB	2.28	0.48
8:7:1916:A:H2'	8:7:1917:U:O4'	2.14	0.48
10:A:111:G:H2'	10:A:112:G:H8	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:216:U:O2'	10:A:468:A:N6	2.46	0.48
10:A:959:A:O2'	10:A:984:C:O2'	2.28	0.48
31:V:8:A:H4'	31:V:9:A:OP1	2.12	0.48
38:c:124:ARG:HA	38:c:165:MET:SD	2.53	0.48
3:2:22:LEU:HD22	58:w:8:LEU:HD13	1.94	0.48
4:3:47:MET:HE1	8:7:851:C:O4'	2.13	0.48
8:7:760:G:H2'	8:7:761:A:O4'	2.14	0.48
8:7:1020:A:H1'	8:7:1021:A:OP2	2.13	0.48
8:7:2144:G:H1'	8:7:2147:A:N6	2.28	0.48
17:H:89:LYS:O	17:H:92:LEU:HD22	2.12	0.48
3:2:42:LEU:O	3:2:46:VAL:HG12	2.13	0.48
8:7:2899:A:H5'	48:m:136:GLN:HE21	1.78	0.48
10:A:380:G:N2	10:A:383:A:OP2	2.47	0.48
10:A:1108:G:H5'	12:C:176:HIS:ND1	2.28	0.48
10:A:1225:A:H5''	10:A:1226:C:OP2	2.13	0.48
33:X:26:C:H2'	33:X:27:G:C8	2.49	0.48
52:q:29:VAL:HG21	52:q:75:ILE:HG23	1.95	0.48
53:r:82:ALA:HB3	53:r:115:LEU:HD21	1.95	0.48
8:7:2258:C:O2'	8:7:2427:C:OP2	2.25	0.48
8:7:2655:G:O2'	8:7:2664:G:O6	2.22	0.48
11:B:20:THR:O	11:B:23:TRP:CD1	2.67	0.48
24:O:3:LEU:HD23	24:O:8:THR:HG22	1.96	0.48
5:4:56:ARG:HA	5:4:56:ARG:HH11	1.78	0.48
8:7:1664:A:H61	8:7:1996:C:H42	1.61	0.48
10:A:1396:A:H2	14:E:24:THR:HG21	1.79	0.48
14:E:82:GLN:HG3	14:E:147:MET:HE3	1.96	0.48
20:K:96:THR:O	20:K:100:LEU:HD23	2.14	0.48
26:Q:10:GLY:HA3	26:Q:25:ILE:HD13	1.96	0.48
43:h:47:GLU:OE2	43:h:51:ARG:HD2	2.13	0.48
49:n:71:ARG:NH2	49:n:105:ARG:H	2.11	0.48
49:n:110:GLU:HA	49:n:113:MET:HG2	1.96	0.48
52:q:87:PHE:CE2	52:q:115:LEU:HD23	2.48	0.48
8:7:26:G:H8	8:7:26:G:O5'	1.96	0.48
8:7:1199:U:H1'	55:t:4:VAL:HG12	1.94	0.48
8:7:2124:G:H2'	8:7:2125:G:C8	2.48	0.48
10:A:280:C:H6	10:A:280:C:O5'	1.97	0.48
10:A:304:U:H2'	10:A:305:G:C8	2.49	0.48
10:A:1412:C:H2'	10:A:1413:A:C8	2.49	0.48
10:A:1540:U:O2'	10:A:1541:U:H2'	2.13	0.48
17:H:18:GLN:HB3	17:H:70:ALA:HB1	1.95	0.48
8:7:1490:A:O2'	8:7:1491:G:OP1	2.22	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:1653:G:O6	52:q:11:ASN:ND2	2.47	0.48
13:D:87:GLY:HA3	13:D:197:GLU:OE1	2.14	0.48
18:I:129:LYS:NZ	32:W:33:U:OP1	2.46	0.48
37:b:13:ARG:O	37:b:16:VAL:HG22	2.14	0.48
45:j:72:LEU:HD23	45:j:72:LEU:H	1.78	0.48
5:4:61:ASN:HA	5:4:66:ILE:HD11	1.96	0.47
8:7:440:C:O2'	64:7:3193:ATP:O2'	2.31	0.47
8:7:1311:G:H21	8:7:1603:A:H62	1.59	0.47
10:A:779:C:H1'	20:K:122:ARG:HD3	1.95	0.47
11:B:87:CYS:SG	11:B:222:ARG:HG3	2.54	0.47
14:E:75:ALA:O	14:E:82:GLN:NE2	2.29	0.47
18:I:106:ARG:HH12	18:I:110:GLN:HE22	1.60	0.47
40:e:148:ARG:NH1	40:e:148:ARG:HB2	2.28	0.47
8:7:973:A:H5'	8:7:1188:U:H1'	1.95	0.47
8:7:1056:G:H4'	8:7:1086:A:H8	1.78	0.47
8:7:2013:A:H3'	8:7:2014:A:H8	1.78	0.47
8:7:2357:G:N2	8:7:2360:G:OP2	2.41	0.47
8:7:2553:G:H1'	8:7:2582:G:H21	1.79	0.47
10:A:643:C:H5''	17:H:32:LEU:HD11	1.95	0.47
10:A:975:A:N1	10:A:1366:C:O2'	2.38	0.47
10:A:993:G:O2'	10:A:994:A:N7	2.47	0.47
10:A:1060:U:P	23:N:85:ARG:HH22	2.37	0.47
24:O:45:GLU:OE1	24:O:46:HIS:CD2	2.68	0.47
27:R:30:LYS:C	27:R:32:TYR:H	2.22	0.47
38:c:46:ARG:NH2	38:c:88:GLU:O	2.45	0.47
39:d:145:ASP:HB3	39:d:184:ASP:HB2	1.95	0.47
8:7:979:A:H2'	8:7:982:C:H42	1.79	0.47
8:7:2788:C:H2'	8:7:2789:C:C6	2.50	0.47
9:8:98:G:N1	60:y:14:LYS:HB2	2.30	0.47
10:A:32:A:H2'	10:A:33:A:C8	2.49	0.47
10:A:736:C:H5''	15:F:90:MET:HE1	1.97	0.47
10:A:1345:U:H5''	18:I:122:ARG:HH11	1.79	0.47
11:B:97:LEU:HB2	11:B:100:MET:SD	2.54	0.47
37:b:247:PRO:HG2	37:b:248:TRP:CZ3	2.49	0.47
57:v:9:HIS:H	57:v:102:HIS:CE1	2.33	0.47
1:0:19:ARG:HH21	8:7:2755:C:H3'	1.79	0.47
8:7:1006:C:O3'	48:m:37:ARG:NH2	2.47	0.47
8:7:1818:U:H5	37:b:156:ARG:HH22	1.63	0.47
8:7:2429:G:C8	50:o:55:MET:HE3	2.49	0.47
10:A:875:U:O3'	17:H:15:ARG:NH1	2.46	0.47
16:G:136:LYS:HA	16:G:139:GLU:OE1	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:36:VAL:HG12	19:J:76:ILE:HG13	1.96	0.47
21:L:75:GLN:NE2	21:L:76:GLU:O	2.48	0.47
35:Z:87:GLU:OE1	35:Z:87:GLU:N	2.39	0.47
38:c:183:GLU:CD	38:c:184:ARG:HG3	2.39	0.47
45:j:56:ARG:HG3	45:j:58:THR:H	1.78	0.47
49:n:76:VAL:HG22	54:s:73:VAL:HG21	1.96	0.47
58:w:3:ARG:HG3	58:w:5:GLU:H	1.79	0.47
8:7:1697:G:H4'	8:7:1978:A:H5''	1.97	0.47
8:7:2677:G:P	38:c:126:ASN:HD21	2.36	0.47
10:A:652:U:O4	10:A:752:G:O2'	2.25	0.47
10:A:1376:U:H2'	10:A:1377:A:C8	2.50	0.47
13:D:139:PRO:HA	13:D:182:PHE:HD2	1.78	0.47
15:F:9:MET:HE2	15:F:86:ARG:HB3	1.96	0.47
22:M:15:ALA:O	22:M:19:LEU:HD23	2.13	0.47
44:i:57:LYS:O	44:i:60:GLU:HG3	2.15	0.47
45:j:56:ARG:HE	45:j:57:ASN:H	1.63	0.47
8:7:39:G:H21	64:7:3193:ATP:H2	1.62	0.47
8:7:1820:U:C2	37:b:201:MET:SD	3.07	0.47
10:A:337:G:H2'	10:A:338:A:H8	1.79	0.47
11:B:49:MET:HE3	11:B:199:VAL:O	2.14	0.47
13:D:107:PHE:CG	13:D:145:ILE:HD11	2.49	0.47
20:K:17:SER:HA	20:K:79:ILE:HA	1.96	0.47
21:L:30:LYS:HA	21:L:30:LYS:HD3	1.67	0.47
56:u:34:GLU:OE1	56:u:60:LYS:HE2	2.15	0.47
8:7:1223:G:N2	8:7:1226:A:OP2	2.43	0.47
8:7:1311:G:N2	8:7:1603:A:H62	2.12	0.47
8:7:1315:C:O2'	8:7:1392:A:N3	2.44	0.47
9:8:78:A:OP2	60:y:14:LYS:NZ	2.47	0.47
10:A:721:G:H4'	10:A:722:G:O4'	2.13	0.47
10:A:1004:A:H2'	10:A:1005:A:O4'	2.14	0.47
10:A:1038:C:H2'	10:A:1039:G:H8	1.79	0.47
12:C:17:PRO:HA	12:C:211:MET:HE1	1.96	0.47
19:J:6:ILE:HG23	19:J:76:ILE:HB	1.96	0.47
36:a:46:VAL:HG22	36:a:212:VAL:HG13	1.95	0.47
37:b:220:VAL:HG13	37:b:225:MET:HE3	1.96	0.47
38:c:35:THR:HG22	38:c:73:VAL:HG21	1.95	0.47
46:k:125:MET:O	46:k:129:ILE:HG12	2.15	0.47
49:n:25:LEU:HB3	49:n:38:ILE:O	2.15	0.47
55:t:65:ILE:HD11	55:t:79:PHE:HE2	1.80	0.47
60:y:61:LEU:N	60:y:72:VAL:O	2.45	0.47
8:7:299:A:N3	8:7:319:G:O2'	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:1182:G:H2'	8:7:1183:U:O4'	2.15	0.47
9:8:9:G:O2'	53:r:45:SER:OG	2.31	0.47
10:A:232:G:H1'	10:A:262:A:N1	2.30	0.47
10:A:1113:C:O4'	12:C:178:LEU:HD11	2.14	0.47
10:A:1187:G:N3	23:N:100:SER:OG	2.39	0.47
11:B:206:ALA:HB2	35:Z:43:LYS:O	2.15	0.47
18:I:60:LYS:HG3	18:I:61:LEU:HD12	1.96	0.47
26:Q:46:VAL:HG11	26:Q:61:ILE:HD12	1.95	0.47
28:S:36:ARG:NH2	28:S:75:ALA:O	2.48	0.47
35:Z:107:THR:HG22	35:Z:155:LYS:HE3	1.96	0.47
36:a:60:ARG:HH22	36:a:162:ARG:HD2	1.79	0.47
2:1:22:LEU:HD23	33:X:92:C:N4	2.30	0.47
2:1:62:LYS:NZ	8:7:372:G:OP2	2.26	0.47
8:7:2246:G:H2'	8:7:2247:A:H8	1.80	0.47
8:7:2285:C:OP2	42:g:6:ARG:NH2	2.48	0.47
10:A:60:A:OP1	10:A:331:G:N1	2.46	0.47
10:A:501:C:H2'	10:A:502:A:H8	1.78	0.47
10:A:1380:U:C5	16:G:3:ARG:HA	2.50	0.47
10:A:1536:C:N4	31:V:14:G:H1	2.13	0.47
33:X:40:G:H2'	33:X:41:G:C8	2.50	0.47
33:X:75:A:O2'	33:X:77:U:OP2	2.32	0.47
38:c:175:LEU:HD12	38:c:190:LYS:O	2.14	0.47
54:s:99:TYR:O	54:s:102:GLU:HG3	2.15	0.47
8:7:278:A:OP2	8:7:361:G:N1	2.48	0.47
8:7:1341:G:H5'	58:w:61:LEU:HB3	1.96	0.47
8:7:2011:U:OP2	57:v:16:LYS:NZ	2.40	0.47
8:7:2209:G:H3'	8:7:2210:U:H2'	1.95	0.47
8:7:2547:A:H4'	49:n:29:HIS:NE2	2.30	0.47
12:C:167:TRP:HZ3	12:C:169:ARG:HG2	1.80	0.47
23:N:64:CYS:HB3	23:N:68:GLY:H	1.79	0.47
48:m:45:THR:HB	48:m:48:VAL:HB	1.97	0.47
2:1:55:GLY:O	2:1:58:VAL:HG22	2.15	0.46
6:5:17:ARG:NE	8:7:1266:G:OP2	2.34	0.46
8:7:1416:G:HO2'	8:7:1417:C:P	2.35	0.46
8:7:2032:G:N2	38:c:151:THR:OG1	2.49	0.46
10:A:364:A:H2'	10:A:365:U:C5	2.51	0.46
10:A:880:C:H2'	10:A:881:G:C8	2.51	0.46
10:A:1218:C:H2'	10:A:1219:A:C8	2.50	0.46
10:A:1533:C:H5''	10:A:1534:A:C8	2.49	0.46
13:D:88:GLU:H	13:D:88:GLU:CD	2.22	0.46
27:R:42:SER:HB3	27:R:52:GLN:OE1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:X:80:C:H4'	36:a:54:LYS:HE3	1.96	0.46
5:4:3:LYS:N	5:4:3:LYS:HD2	2.31	0.46
8:7:807:U:H2'	8:7:808:G:C8	2.50	0.46
8:7:1187:G:H5''	56:u:83:TYR:CE1	2.50	0.46
10:A:222:C:H2'	10:A:223:A:H8	1.79	0.46
10:A:363:A:H2'	10:A:364:A:O4'	2.15	0.46
15:F:90:MET:HA	15:F:90:MET:HE3	1.97	0.46
17:H:10:MET:HA	17:H:27:MET:HE1	1.96	0.46
50:o:91:ASP:N	50:o:91:ASP:OD1	2.48	0.46
53:r:69:ASP:OD1	53:r:70:ALA:N	2.48	0.46
1:0:30:GLU:HG3	1:0:32:LYS:HB2	1.96	0.46
8:7:1914:C:H2'	8:7:1915:3TD:H6	1.96	0.46
10:A:543:U:H2'	10:A:544:G:C8	2.48	0.46
10:A:879:C:H2'	10:A:880:C:H6	1.80	0.46
11:B:187:VAL:HG21	11:B:199:VAL:HG13	1.97	0.46
12:C:25:ASN:O	12:C:29:PHE:HB2	2.15	0.46
17:H:10:MET:HE1	17:H:33:LYS:HA	1.96	0.46
18:I:118:LEU:HB3	18:I:123:ARG:O	2.15	0.46
33:X:70:G:O2'	36:a:55:SER:OG	2.16	0.46
43:h:29:GLY:HA2	43:h:106:ASP:OD2	2.15	0.46
8:7:2130:U:P	8:7:2159:G:H22	2.38	0.46
10:A:83:C:H3'	10:A:84:U:H3'	1.96	0.46
10:A:112:G:H22	10:A:315:A:H2	1.62	0.46
10:A:181:A:H2'	10:A:194:C:N4	2.30	0.46
10:A:983:A:H5''	10:A:984:C:OP2	2.15	0.46
17:H:103:VAL:HG12	17:H:126:ILE:HD13	1.96	0.46
24:O:7:ALA:O	24:O:10:LYS:HG2	2.16	0.46
25:P:8:ARG:HG3	25:P:17:TYR:CE1	2.50	0.46
35:Z:54:LYS:O	35:Z:90:LYS:NZ	2.49	0.46
8:7:754:U:H2'	8:7:755:U:C6	2.50	0.46
14:E:44:GLY:HA2	14:E:76:LEU:HG	1.98	0.46
30:U:39:GLU:HG2	30:U:44:GLU:HB3	1.97	0.46
37:b:98:ASP:OD1	37:b:98:ASP:O	2.34	0.46
44:i:129:GLU:HG2	44:i:129:GLU:O	2.14	0.46
46:k:76:ALA:HB2	46:k:113:LYS:HE2	1.98	0.46
59:x:24:LYS:HB3	59:x:37:GLU:OE1	2.16	0.46
4:3:20:HIS:O	4:3:23:THR:OG1	2.30	0.46
8:7:79:C:O2'	8:7:346:A:N3	2.46	0.46
8:7:468:G:OP2	47:l:37:LYS:NZ	2.44	0.46
8:7:2025:C:H2'	8:7:2026:U:C6	2.51	0.46
8:7:2122:U:OP1	8:7:2168:G:N2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:2698:U:H2'	8:7:2699:C:H6	1.80	0.46
10:A:150:U:H2'	10:A:151:A:H8	1.81	0.46
11:B:130:THR:O	11:B:132:LYS:NZ	2.47	0.46
11:B:149:GLY:O	11:B:152:LYS:HG2	2.16	0.46
48:m:109:LEU:HD23	48:m:118:MET:HB2	1.97	0.46
55:t:44:GLN:NE2	56:u:77:PHE:HD2	2.13	0.46
8:7:2380:C:H2'	8:7:2381:A:C8	2.51	0.46
9:8:42:C:C5	40:e:66:LEU:HD22	2.50	0.46
10:A:219:U:H2'	10:A:220:G:H8	1.81	0.46
28:S:32:ARG:HH21	28:S:57:HIS:CE1	2.32	0.46
33:X:22:A:H5''	33:X:22:A:H8	1.80	0.46
36:a:10:VAL:HG12	36:a:14:LYS:HE3	1.98	0.46
53:r:5:SER:O	53:r:9:ARG:HG3	2.15	0.46
1:0:34:LYS:NZ	8:7:2743:U:OP1	2.48	0.46
6:5:3:VAL:HG22	8:7:2015:A:C2	2.50	0.46
7:6:13:ARG:HH12	50:o:59:ARG:HA	1.81	0.46
8:7:322:A:H5'	8:7:340:A:H1'	1.97	0.46
8:7:1487:U:H2'	8:7:1488:C:C6	2.51	0.46
8:7:1754:A:O2'	54:s:103:ARG:NH2	2.48	0.46
8:7:1827:U:O2'	8:7:1970:A:N3	2.45	0.46
8:7:2127:G:H2'	8:7:2128:G:O4'	2.16	0.46
8:7:2130:U:OP2	36:a:6:LYS:HE2	2.15	0.46
8:7:2185:U:H2'	8:7:2186:G:C8	2.51	0.46
8:7:2291:U:H2'	8:7:2292:U:C6	2.50	0.46
12:C:29:PHE:HZ	23:N:94:PRO:HD2	1.81	0.46
19:J:15:HIS:HB3	19:J:70:HIS:NE2	2.30	0.46
25:P:6:LEU:HD12	25:P:19:VAL:HG22	1.97	0.46
29:T:57:ILE:HG23	29:T:61:GLN:HE22	1.80	0.46
30:U:63:GLU:O	30:U:65:ALA:N	2.44	0.46
34:Y:9:A:H1'	34:Y:45:G:H2'	1.97	0.46
40:e:118:SER:HA	40:e:178:ARG:NE	2.31	0.46
48:m:116:ARG:O	48:m:120:ARG:HG3	2.15	0.46
55:t:83:LEU:HD12	55:t:88:VAL:HG11	1.97	0.46
57:v:13:SER:OG	57:v:16:LYS:HG3	2.16	0.46
58:w:58:VAL:HG22	58:w:85:VAL:HG13	1.97	0.46
7:6:25:LYS:HE3	50:o:64:PHE:HB3	1.97	0.46
8:7:513:A:H1'	55:t:11:ARG:NH1	2.31	0.46
8:7:1131:G:N2	8:7:1132:U:O4	2.39	0.46
8:7:2023:C:H2'	8:7:2024:G:H8	1.81	0.46
8:7:2271:G:H5''	61:z:18:ALA:HB3	1.98	0.46
8:7:2599:G:OP2	37:b:235:GLY:HA2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1047:G:H5''	23:N:4:GLN:NE2	2.31	0.46
10:A:1447:A:OP1	10:A:1448:C:N4	2.45	0.46
26:Q:15:ASP:OD2	26:Q:54:GLY:HA2	2.16	0.46
34:Y:54:5MU:H72	34:Y:55:PSU:C2	2.51	0.46
37:b:78:VAL:HG21	37:b:110:LEU:HD21	1.98	0.46
45:j:97:LYS:HE3	45:j:123:ILE:HG13	1.98	0.46
54:s:14:LYS:NZ	54:s:81:VAL:O	2.34	0.46
56:u:38:VAL:HG22	56:u:59:ILE:HG12	1.98	0.46
7:6:25:LYS:O	50:o:61:LEU:HD12	2.16	0.46
8:7:24:G:H2'	8:7:25:U:H6	1.81	0.46
8:7:1094:U:H1'	8:7:1097:U:H5	1.79	0.46
8:7:1808:A:H3'	8:7:1809:A:C8	2.51	0.46
8:7:2138:G:H3'	8:7:2139:U:H4'	1.98	0.46
10:A:54:C:N4	10:A:352:C:H2'	2.31	0.46
10:A:1456:A:H2'	10:A:1457:G:O4'	2.16	0.46
17:H:26:THR:HG22	17:H:60:GLU:OE1	2.16	0.46
18:I:19:VAL:HG23	18:I:65:ILE:CD1	2.45	0.46
19:J:37:ARG:HB2	19:J:75:ASP:HB2	1.98	0.46
37:b:92:ALA:N	37:b:104:ILE:O	2.33	0.46
38:c:13:ARG:HG2	54:s:56:HIS:CE1	2.51	0.46
41:f:71:LEU:O	41:f:74:SER:OG	2.28	0.46
54:s:6:LYS:HG2	54:s:10:GLN:HE22	1.81	0.46
8:7:1615:C:H2'	8:7:1617:C:C5	2.52	0.45
8:7:1789:A:OP1	37:b:221:ARG:HG3	2.16	0.45
10:A:41:G:H2'	10:A:42:G:H8	1.81	0.45
11:B:90:PHE:CD2	11:B:154:MET:HG3	2.51	0.45
28:S:29:LYS:HE2	28:S:29:LYS:HA	1.98	0.45
31:V:12:A:H2'	31:V:13:C:C6	2.50	0.45
33:X:17:G:H5''	33:X:19:C:H5'	1.97	0.45
54:s:91:ALA:O	54:s:111:LYS:NZ	2.32	0.45
8:7:747:5MU:C5M	8:7:2612:C:H4'	2.46	0.45
8:7:2102:G:H2'	8:7:2103:C:C6	2.51	0.45
8:7:2233:U:H2'	8:7:2234:G:C8	2.51	0.45
10:A:160:A:H1'	10:A:344:A:C5	2.51	0.45
40:e:130:MET:SD	40:e:154:ILE:HD12	2.56	0.45
8:7:851:C:H2'	8:7:852:U:C6	2.51	0.45
8:7:1569:A:H2'	8:7:1570:A:C8	2.52	0.45
8:7:2041:U:H2'	8:7:2042:A:C8	2.52	0.45
8:7:2071:A:H2'	8:7:2072:C:C6	2.51	0.45
8:7:2136:G:H2'	8:7:2137:U:C5	2.51	0.45
13:D:99:ASP:OD1	13:D:100:ASN:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:e:58:ALA:HB2	40:e:65:PRO:HD3	1.97	0.45
46:k:105:GLN:O	46:k:109:ILE:HD12	2.15	0.45
52:q:47:VAL:O	52:q:51:LEU:HD23	2.17	0.45
58:w:1:MET:HG3	58:w:42:GLU:HA	1.97	0.45
59:x:40:ASN:HB2	59:x:65:ILE:HD11	1.98	0.45
8:7:663:G:H5'	50:o:17:LYS:HZ3	1.80	0.45
8:7:1095:A:N6	46:k:26:PRO:HB2	2.32	0.45
8:7:1971:U:OP2	8:7:1971:U:H4'	2.15	0.45
8:7:2638:G:O2'	8:7:2775:G:N2	2.43	0.45
10:A:791:G:N2	10:A:1497:G:H4'	2.32	0.45
10:A:879:C:H2'	10:A:880:C:C6	2.51	0.45
13:D:183:LYS:NZ	13:D:184:ARG:HE	2.14	0.45
39:d:164:LEU:HB2	39:d:167:VAL:HG22	1.99	0.45
54:s:5:ILE:O	54:s:9:GLU:HG2	2.16	0.45
8:7:372:G:O2'	8:7:400:G:O6	2.32	0.45
8:7:714:U:H1'	8:7:717:C:H5	1.80	0.45
8:7:1542:U:H2'	8:7:1543:G:O4'	2.17	0.45
8:7:1992:G:N2	8:7:1996:C:O2'	2.50	0.45
8:7:2657:A:O2'	41:f:160:LYS:NZ	2.49	0.45
10:A:46:G:H2'	10:A:366:A:N7	2.31	0.45
10:A:1308:U:H2'	10:A:1309:G:C8	2.52	0.45
10:A:1396:A:O3'	14:E:29:ARG:NH2	2.50	0.45
11:B:129:LEU:C	11:B:131:LYS:H	2.24	0.45
11:B:186:ILE:HD13	11:B:200:ILE:HB	1.97	0.45
12:C:123:GLN:HG3	12:C:126:ARG:HH22	1.81	0.45
21:L:63:VAL:HG21	21:L:95:TYR:CE2	2.52	0.45
23:N:76:LYS:HG3	23:N:77:PHE:CD2	2.52	0.45
25:P:69:ASP:OD1	25:P:70:ARG:N	2.49	0.45
33:X:9:G:N2	33:X:64:U:O4	2.48	0.45
44:i:100:ALA:HB3	44:i:112:LYS:NZ	2.32	0.45
8:7:1796:U:H2'	8:7:1797:G:H8	1.82	0.45
8:7:2144:G:O5'	8:7:2144:G:H8	2.00	0.45
8:7:2698:U:H2'	8:7:2699:C:C6	2.51	0.45
9:8:9:G:P	53:r:15:ARG:HH21	2.38	0.45
12:C:111:LEU:HD11	12:C:146:ALA:HB2	1.97	0.45
22:M:42:ASP:OD1	22:M:42:ASP:N	2.50	0.45
26:Q:16:LYS:O	26:Q:16:LYS:HD3	2.17	0.45
27:R:11:CYS:SG	27:R:48:ARG:HG2	2.57	0.45
35:Z:11:GLU:HA	35:Z:14:LYS:HZ3	1.81	0.45
39:d:115:GLN:CD	39:d:117:ARG:HD3	2.42	0.45
4:3:27:LEU:HB3	4:3:29:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:584:C:O5'	55:t:6:ARG:NH2	2.47	0.45
8:7:888:C:OP2	8:7:888:C:H4'	2.17	0.45
8:7:2039:U:H2'	8:7:2040:G:C8	2.52	0.45
10:A:68:G:H4'	10:A:171:A:H1'	1.99	0.45
10:A:574:A:H1'	10:A:883:C:H1'	1.99	0.45
10:A:1099:G:H5''	30:U:69:ARG:HH11	1.81	0.45
10:A:1536:C:O2	31:V:13:C:O2'	2.20	0.45
12:C:185:ASN:CG	12:C:186:THR:H	2.25	0.45
25:P:61:VAL:HG22	25:P:67:ILE:HD11	1.99	0.45
44:i:30:LEU:HB3	44:i:36:ALA:HB3	1.99	0.45
46:k:109:ILE:HA	46:k:112:THR:HB	1.97	0.45
46:k:132:THR:O	46:k:136:MET:HG2	2.17	0.45
49:n:61:VAL:HG12	49:n:87:LEU:HD11	1.98	0.45
52:q:2:ARG:HA	52:q:5:LYS:HD2	1.99	0.45
6:5:9:THR:HG21	8:7:2020:A:H5'	1.99	0.45
8:7:1070:A:O2'	8:7:1097:U:O3'	2.33	0.45
8:7:1742:U:H2'	8:7:1743:G:H8	1.82	0.45
10:A:720:C:O3'	27:R:52:GLN:NE2	2.50	0.45
15:F:4:TYR:CD2	15:F:71:ILE:HG13	2.52	0.45
29:T:67:ILE:HD12	29:T:71:LYS:HB3	1.98	0.45
33:X:33:RSP:H2'	33:X:34:U:C6	2.51	0.45
37:b:105:LEU:HD21	37:b:156:ARG:HG3	1.98	0.45
45:j:28:ALA:HB3	45:j:81:LEU:HD23	1.99	0.45
6:5:16:ARG:NH1	8:7:1266:G:OP1	2.48	0.45
8:7:571:U:H3'	56:u:80:ARG:NH1	2.32	0.45
8:7:964:C:O2'	8:7:2273:A:N3	2.41	0.45
10:A:193:C:H1'	29:T:55:GLN:NE2	2.32	0.45
10:A:1060:U:OP1	23:N:85:ARG:NH2	2.46	0.45
10:A:1074:G:OP1	14:E:69:ARG:NH2	2.49	0.45
12:C:23:PHE:CE2	19:J:12:ALA:HA	2.51	0.45
16:G:113:ASP:HB2	16:G:119:ARG:HG3	1.99	0.45
16:G:126:ASP:HB3	16:G:131:LYS:HG3	1.98	0.45
24:O:71:LYS:HE2	24:O:78:TYR:CE2	2.52	0.45
35:Z:24:VAL:HG11	35:Z:72:LEU:HD12	1.97	0.45
37:b:130:LEU:HB2	37:b:135:ILE:HD11	1.99	0.45
43:h:64:TRP:HB2	43:h:104:GLU:HB2	1.97	0.45
45:j:12:VAL:HG21	45:j:62:ARG:HD2	1.99	0.45
50:o:82:LEU:HD22	50:o:90:VAL:HG21	1.99	0.45
2:1:3:ARG:O	2:1:12:PRO:HD3	2.17	0.45
8:7:29:U:H2'	8:7:30:G:C8	2.51	0.45
10:A:1048:G:H5''	23:N:3:LYS:CD	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1112:C:N3	12:C:178:LEU:HD23	2.31	0.45
10:A:1345:U:H5''	18:I:122:ARG:NH1	2.32	0.45
25:P:51:ARG:O	25:P:52:LEU:HD23	2.16	0.45
30:U:67:ARG:HA	35:Z:79:PHE:CE2	2.52	0.45
35:Z:11:GLU:HA	35:Z:14:LYS:NZ	2.31	0.45
39:d:191:ASP:OD1	39:d:191:ASP:N	2.48	0.45
43:h:120:ALA:O	43:h:124:LEU:HD23	2.17	0.45
60:y:75:GLN:HB2	60:y:92:VAL:HG13	1.99	0.45
8:7:2531:A:OP2	41:f:175:LYS:HE3	2.16	0.44
10:A:255:G:H4'	26:Q:19:LYS:HD3	1.98	0.44
12:C:38:LYS:O	12:C:41:GLN:HG2	2.17	0.44
16:G:81:GLY:HA3	31:V:16:U:H5'	1.99	0.44
20:K:24:HIS:HB3	20:K:31:ILE:HB	1.98	0.44
4:3:27:LEU:HD11	4:3:47:MET:HB3	1.99	0.44
8:7:639:U:H2'	8:7:640:C:C6	2.52	0.44
8:7:1184:U:H2'	8:7:1185:G:C8	2.53	0.44
8:7:2159:G:H2'	8:7:2160:C:C6	2.53	0.44
10:A:1201:A:O2'	10:A:1202:U:OP2	2.34	0.44
10:A:1437:A:OP1	29:T:29:ARG:NH1	2.48	0.44
12:C:11:ARG:HH22	12:C:182:ILE:HD11	1.82	0.44
12:C:23:PHE:HZ	19:J:11:LYS:NZ	2.13	0.44
13:D:59:GLN:O	13:D:63:ARG:NE	2.46	0.44
15:F:42:TRP:HB2	15:F:59:TYR:HB2	1.99	0.44
19:J:21:ALA:HB1	19:J:92:LEU:HD21	2.00	0.44
30:U:43:THR:O	30:U:44:GLU:C	2.60	0.44
33:X:86:C:H2'	33:X:87:A:C8	2.51	0.44
49:n:1:MET:N	49:n:65:THR:HG21	2.32	0.44
53:r:54:VAL:HG23	53:r:54:VAL:O	2.17	0.44
8:7:1820:U:C4	37:b:159:GLY:HA3	2.51	0.44
8:7:2178:C:H2'	8:7:2179:C:C6	2.52	0.44
10:A:858:G:O6	10:A:869:G:H3'	2.18	0.44
10:A:946:A:O2'	10:A:1333:A:N3	2.45	0.44
12:C:155:GLY:O	12:C:196:ILE:HG12	2.17	0.44
48:m:78:THR:HG23	48:m:83:GLY:O	2.18	0.44
8:7:373:U:H2'	8:7:374:A:H8	1.83	0.44
8:7:2810:A:H4'	38:c:62:LYS:HD2	1.98	0.44
10:A:1106:G:H5''	12:C:172:ARG:HG3	1.99	0.44
10:A:1464:U:P	54:s:109:ARG:HH22	2.41	0.44
11:B:68:LEU:HD23	11:B:161:LEU:HD11	1.97	0.44
14:E:83:HIS:CG	17:H:96:MET:HE1	2.53	0.44
19:J:28:THR:O	19:J:32:THR:HG22	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Z:76:GLU:HB2	35:Z:80:GLY:HA2	2.00	0.44
53:r:58:ILE:HG13	53:r:58:ILE:O	2.16	0.44
56:u:24:LYS:HD3	56:u:92:TRP:HB3	1.99	0.44
8:7:743:A:OP1	38:c:135:GLY:HA2	2.17	0.44
8:7:1791:A:C5'	37:b:205:LEU:HD11	2.46	0.44
8:7:2047:C:O2'	8:7:2823:A:N1	2.47	0.44
8:7:2112:G:H1'	33:X:20:H2U:N3	2.32	0.44
8:7:2271:G:OP1	61:z:18:ALA:HB1	2.16	0.44
8:7:2514:U:H2'	8:7:2515:C:C6	2.53	0.44
10:A:280:C:O2'	26:Q:40:ARG:NH1	2.51	0.44
11:B:102:THR:HG23	11:B:175:GLU:HB3	1.98	0.44
12:C:73:PRO:O	12:C:77:ILE:HG12	2.17	0.44
12:C:110:GLU:OE1	12:C:110:GLU:N	2.42	0.44
18:I:97:GLU:HG2	18:I:98:LEU:N	2.33	0.44
20:K:63:ALA:HB1	20:K:96:THR:HG23	1.99	0.44
49:n:13:ASN:OD1	49:n:98:ARG:N	2.51	0.44
52:q:24:MET:HB3	52:q:44:LEU:HD13	1.98	0.44
53:r:62:LEU:HD12	53:r:62:LEU:O	2.17	0.44
8:7:554:U:H2'	8:7:555:G:O4'	2.17	0.44
8:7:812:C:H5'	50:o:21:ARG:O	2.18	0.44
8:7:1028:A:OP2	8:7:1126:A:N6	2.43	0.44
8:7:2329:U:H2'	8:7:2330:G:C8	2.53	0.44
8:7:2700:A:H2'	8:7:2701:U:C6	2.53	0.44
8:7:2743:U:O3'	41:f:153:ARG:NH1	2.48	0.44
10:A:362:G:O2'	10:A:364:A:N7	2.48	0.44
10:A:381:C:H2'	10:A:382:A:O4'	2.18	0.44
10:A:384:G:H2'	10:A:385:C:C6	2.53	0.44
10:A:404:G:OP2	13:D:115:ARG:NH2	2.44	0.44
10:A:476:U:H2'	10:A:477:C:C6	2.52	0.44
10:A:882:C:O2'	10:A:883:C:H5'	2.17	0.44
10:A:974:A:O4'	23:N:71:HIS:ND1	2.50	0.44
10:A:1073:U:H4'	11:B:105:LYS:HZ2	1.81	0.44
10:A:1536:C:N3	31:V:14:G:N2	2.58	0.44
11:B:167:ASP:HB2	11:B:191:SER:HA	1.99	0.44
20:K:61:PHE:O	20:K:65:VAL:HG23	2.18	0.44
33:X:20:H2U:H61	33:X:74:G:H21	1.83	0.44
2:1:39:TRP:CD1	44:i:32:PRO:HA	2.52	0.44
8:7:277:G:O2'	8:7:361:G:O6	2.34	0.44
8:7:716:A:H1'	24:O:40:GLN:OE1	2.17	0.44
8:7:2745:C:O2'	41:f:139:GLN:O	2.35	0.44
10:A:537:G:OP1	21:L:110:ARG:NH1	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:784:A:H2'	10:A:785:G:C8	2.53	0.44
10:A:855:U:OP2	10:A:871:U:N3	2.39	0.44
11:B:217:VAL:O	11:B:220:THR:HG22	2.18	0.44
14:E:77:ASN:HB2	14:E:82:GLN:HG2	2.00	0.44
36:a:46:VAL:HG13	36:a:212:VAL:HG22	2.00	0.44
37:b:78:VAL:HG21	37:b:110:LEU:HD11	2.00	0.44
37:b:210:ALA:HA	37:b:213:TRP:CE3	2.53	0.44
41:f:25:THR:C	41:f:26:ILE:HD13	2.42	0.44
5:4:48:GLN:O	5:4:49:ARG:HB2	2.16	0.44
8:7:1100:C:H2'	8:7:1101:U:O4'	2.18	0.44
8:7:2092:U:OP1	8:7:2199:A:O2'	2.31	0.44
8:7:2108:A:OP1	8:7:2150:C:O2'	2.35	0.44
10:A:269:C:H2'	10:A:270:A:C8	2.53	0.44
10:A:1391:U:H2'	10:A:1392:G:C8	2.52	0.44
12:C:179:ARG:HD3	12:C:208:LEU:HD13	2.00	0.44
38:c:129:THR:OG1	38:c:140:HIS:O	2.31	0.44
39:d:126:VAL:HG23	39:d:156:ASN:HB3	2.00	0.44
45:j:46:ARG:NE	46:k:121:ASP:OD1	2.50	0.44
48:m:39:LYS:HE2	48:m:39:LYS:HB3	1.79	0.44
49:n:121:GLU:OE1	49:n:123:LEU:HD23	2.17	0.44
8:7:158:U:O2'	8:7:159:G:OP1	2.34	0.44
8:7:538:A:H5''	48:m:7:LYS:HE2	2.00	0.44
8:7:736:C:H2'	8:7:737:C:C6	2.53	0.44
8:7:927:A:H2'	8:7:928:A:C8	2.53	0.44
8:7:995:C:H42	48:m:2:LYS:HB3	1.83	0.44
8:7:1357:C:H2'	8:7:1358:G:O4'	2.17	0.44
8:7:1900:A:H1'	8:7:1970:A:H2'	2.00	0.44
8:7:1982:U:H2'	8:7:1983:G:H8	1.83	0.44
8:7:2152:G:H8	8:7:2152:G:O5'	2.01	0.44
8:7:2866:U:H4'	8:7:2867:G:H4'	1.99	0.44
10:A:323:U:OP1	29:T:18:ARG:NH2	2.50	0.44
10:A:496:A:H61	10:A:498:A:H62	1.65	0.44
10:A:545:C:H5''	13:D:69:GLU:HG2	1.99	0.44
10:A:922:G:H1'	14:E:24:THR:HG23	1.99	0.44
29:T:18:ARG:NE	29:T:18:ARG:HA	2.33	0.44
38:c:150:GLN:HG2	38:c:150:GLN:O	2.18	0.44
54:s:89:ARG:NH2	54:s:115:ASN:O	2.51	0.44
55:t:102:ASP:OD1	55:t:104:VAL:HG22	2.18	0.44
59:x:14:LEU:HD11	59:x:71:ALA:HB2	1.99	0.44
8:7:1323:C:N4	8:7:1324:G:O6	2.51	0.43
8:7:1432:G:H2'	8:7:1433:A:C8	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:2107:G:H5''	36:a:3:LYS:HE3	2.00	0.43
10:A:427:U:H5''	13:D:10:LYS:HZ1	1.82	0.43
10:A:563:A:H61	10:A:884:U:H3	1.66	0.43
12:C:29:PHE:CZ	23:N:94:PRO:HD2	2.53	0.43
20:K:126:LYS:NZ	30:U:37:PHE:HB2	2.33	0.43
33:X:78:C:H2'	33:X:79:C:C6	2.53	0.43
57:v:35:ILE:O	57:v:39:THR:OG1	2.27	0.43
8:7:96:C:H2'	8:7:97:C:C6	2.53	0.43
8:7:2179:C:H2'	8:7:2180:U:C6	2.53	0.43
8:7:2571:U:O2	38:c:148:GLN:NE2	2.50	0.43
10:A:2:A:H3'	10:A:3:A:C8	2.53	0.43
10:A:222:C:H2'	10:A:223:A:C8	2.53	0.43
10:A:1201:A:H1'	10:A:1202:U:OP2	2.18	0.43
10:A:1537:U:H3	31:V:13:C:H42	1.66	0.43
11:B:97:LEU:N	11:B:100:MET:HE1	2.32	0.43
27:R:42:SER:HA	27:R:45:THR:HG22	2.00	0.43
33:X:2:G:H2'	33:X:3:U:C6	2.53	0.43
48:m:103:ILE:HG13	48:m:104:ALA:N	2.32	0.43
49:n:58:LEU:HD11	49:n:86:LEU:HG	1.99	0.43
49:n:63:VAL:HG12	49:n:107:LEU:HD11	1.99	0.43
8:7:17:G:H4'	55:t:25:TYR:CE1	2.53	0.43
8:7:284:U:H3	8:7:356:G:H1	1.65	0.43
8:7:597:G:O2'	50:o:11:GLY:O	2.28	0.43
8:7:947:A:H2'	8:7:948:C:H6	1.84	0.43
8:7:960:A:H2'	8:7:962:G:H5'	1.99	0.43
8:7:1173:U:O2'	8:7:1176:U:O4	2.33	0.43
8:7:1469:A:H2'	8:7:1470:A:C8	2.54	0.43
8:7:2512:C:H5''	38:c:127:PHE:CE1	2.54	0.43
10:A:414:A:P	10:A:428:G:H22	2.41	0.43
10:A:662:U:OP1	15:F:93:LYS:NZ	2.52	0.43
10:A:1345:U:OP1	18:I:122:ARG:NH1	2.51	0.43
14:E:13:GLU:OE2	14:E:37:THR:OG1	2.19	0.43
17:H:87:LYS:HE2	17:H:87:LYS:HB2	1.69	0.43
19:J:19:ASP:HA	19:J:22:THR:HG22	2.00	0.43
19:J:35:GLN:HE22	19:J:77:VAL:HB	1.82	0.43
19:J:52:LEU:HD11	23:N:81:ARG:HH11	1.82	0.43
24:O:32:LEU:O	24:O:36:ILE:HG12	2.18	0.43
30:U:68:THR:HG22	30:U:69:ARG:H	1.82	0.43
38:c:11:MET:HE2	38:c:11:MET:HB3	1.72	0.43
8:7:532:A:N1	8:7:2020:A:H1'	2.33	0.43
8:7:1230:A:H2'	8:7:1231:U:H6	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:2574:G:H1'	38:c:148:GLN:NE2	2.34	0.43
10:A:345:C:H5''	54:s:39:ARG:NH1	2.33	0.43
10:A:1507:A:H2'	10:A:1508:A:C8	2.54	0.43
16:G:31:MET:HE2	16:G:31:MET:HB3	1.82	0.43
20:K:73:ALA:O	20:K:77:TYR:N	2.37	0.43
24:O:3:LEU:HB2	24:O:35:GLN:OE1	2.18	0.43
34:Y:65:C:H2'	34:Y:66:A:C8	2.54	0.43
37:b:135:ILE:HD12	37:b:192:LEU:HD21	2.01	0.43
8:7:1759:A:O2'	8:7:2714:G:O2'	2.32	0.43
8:7:2106:U:H2'	8:7:2107:G:C8	2.53	0.43
8:7:2167:U:O2	8:7:2169:A:H2'	2.19	0.43
10:A:94:G:H4'	10:A:95:C:H5'	1.99	0.43
10:A:162:A:C5	10:A:163:C:H1'	2.53	0.43
10:A:539:A:H2'	10:A:540:G:C8	2.53	0.43
10:A:1162:C:H2'	10:A:1163:A:C8	2.54	0.43
16:G:146:GLU:OE1	16:G:146:GLU:HA	2.18	0.43
22:M:69:LEU:HD12	22:M:72:GLU:OE2	2.18	0.43
29:T:57:ILE:H	29:T:57:ILE:HD12	1.83	0.43
37:b:172:VAL:O	37:b:183:LYS:HA	2.18	0.43
42:g:39:PHE:HB2	42:g:46:HIS:CE1	2.53	0.43
43:h:42:THR:HG22	43:h:93:VAL:HG12	1.98	0.43
45:j:8:LYS:HD2	45:j:59:LEU:HD21	2.01	0.43
53:r:13:ARG:CZ	53:r:17:LYS:HZ2	2.31	0.43
53:r:33:ARG:O	53:r:65:THR:OG1	2.35	0.43
8:7:191:A:H2'	8:7:192:C:H6	1.84	0.43
8:7:495:G:H21	57:v:61:ASN:ND2	2.15	0.43
8:7:967:U:H2'	8:7:968:C:C6	2.54	0.43
8:7:997:G:OP1	55:t:92:ARG:HD2	2.18	0.43
8:7:1020:A:OP1	8:7:1034:G:N2	2.38	0.43
8:7:1021:A:O2'	8:7:1123:C:OP1	2.32	0.43
10:A:427:U:H5''	13:D:10:LYS:NZ	2.33	0.43
10:A:1513:A:H2'	10:A:1514:G:C8	2.54	0.43
16:G:108:ALA:O	16:G:119:ARG:HD3	2.18	0.43
18:I:34:SER:OG	18:I:36:GLU:OE1	2.36	0.43
33:X:10:G:N2	33:X:27:G:H1'	2.33	0.43
50:o:51:GLU:O	50:o:51:GLU:HG3	2.18	0.43
55:t:45:TYR:HA	55:t:48:ARG:NH1	2.33	0.43
55:t:79:PHE:O	55:t:83:LEU:HD23	2.18	0.43
61:z:21:LEU:HD23	61:z:40:GLN:HA	2.00	0.43
61:z:25:ARG:NH2	61:z:29:GLU:HB3	2.32	0.43
8:7:959:A:N3	8:7:2457:PSU:O2'	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:1309:G:H4'	47:l:7:PRO:HB2	2.00	0.43
8:7:1754:A:H8	8:7:1754:A:O5'	2.01	0.43
10:A:33:A:H5''	10:A:364:A:O2'	2.18	0.43
10:A:219:U:H2'	10:A:220:G:C8	2.53	0.43
10:A:236:A:H2'	10:A:237:G:C8	2.53	0.43
18:I:24:GLY:HA3	18:I:62:ASP:CG	2.44	0.43
24:O:64:ARG:HD2	24:O:67:LEU:HD21	2.01	0.43
34:Y:37:6MZ:H8	34:Y:37:6MZ:O5'	2.19	0.43
49:n:22:ILE:HG22	49:n:40:LYS:C	2.43	0.43
61:z:40:GLN:OE1	61:z:44:LYS:HB2	2.18	0.43
8:7:552:U:H2'	8:7:553:G:C8	2.54	0.43
8:7:675:A:H2'	8:7:676:A:C8	2.54	0.43
8:7:1238:G:H2'	8:7:1239:G:O4'	2.18	0.43
8:7:2116:G:H1	8:7:2164:C:H5'	1.84	0.43
10:A:178:C:H2'	10:A:179:A:H8	1.82	0.43
10:A:324:G:N2	10:A:326:G:H3'	2.34	0.43
11:B:130:THR:O	11:B:131:LYS:HB3	2.18	0.43
12:C:6:HIS:CE1	12:C:184:TYR:CD2	3.06	0.43
13:D:92:ALA:HB1	13:D:185:LYS:HE3	1.99	0.43
17:H:96:MET:HB3	17:H:100:GLY:N	2.32	0.43
25:P:6:LEU:CD1	25:P:71:VAL:HG12	2.46	0.43
32:W:54:5MU:H5''	32:W:55:PSU:OP2	2.19	0.43
35:Z:18:THR:CG2	35:Z:24:VAL:HG12	2.48	0.43
43:h:21:ALA:HB2	43:h:97:GLN:HB2	2.01	0.43
54:s:95:ALA:C	54:s:96:LYS:HD2	2.44	0.43
60:y:77:VAL:HG23	60:y:89:ILE:HG12	2.01	0.43
7:6:52:LYS:NZ	8:7:937:C:OP1	2.36	0.43
8:7:898:C:H2'	8:7:899:A:O4'	2.18	0.43
8:7:2162:G:H4'	8:7:2173:A:C4	2.54	0.43
8:7:2262:U:OP2	61:z:16:SER:OG	2.26	0.43
10:A:723:U:C4	30:U:53:VAL:HG22	2.54	0.43
10:A:1098:C:OP1	11:B:143:LYS:HD3	2.19	0.43
19:J:54:SER:CB	19:J:58:ASN:HB3	2.49	0.43
20:K:23:ILE:N	20:K:85:MET:O	2.49	0.43
21:L:43:LYS:HG2	21:L:44:LYS:H	1.83	0.43
55:t:17:ILE:HG23	55:t:39:VAL:HG21	2.00	0.43
8:7:24:G:H2'	8:7:25:U:C6	2.54	0.43
8:7:1779:U:H5	8:7:1784:A:N7	2.16	0.43
8:7:1954:G:O6	8:7:1986:C:H5''	2.19	0.43
8:7:2574:G:H1'	38:c:148:GLN:HE22	1.83	0.43
10:A:264:C:O3'	26:Q:65:ARG:NH1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:523:A:C2	21:L:88:LYS:HB3	2.54	0.43
10:A:748:G:H2'	10:A:749:A:H8	1.84	0.43
10:A:909:A:OP2	21:L:18:LYS:NZ	2.51	0.43
10:A:1013:G:N2	10:A:1016:A:OP2	2.47	0.43
10:A:1038:C:H2'	10:A:1039:G:C8	2.54	0.43
10:A:1107:C:H5'	12:C:169:ARG:HH22	1.83	0.43
19:J:63:ASP:OD1	23:N:98:LYS:HG3	2.18	0.43
28:S:41:PHE:H	28:S:44:MET:CE	2.32	0.43
34:Y:43:G:H3'	34:Y:44:G:H8	1.84	0.43
39:d:77:ILE:HD12	39:d:77:ILE:H	1.84	0.43
41:f:117:LEU:HD13	41:f:121:ILE:HG22	2.01	0.43
57:v:24:ILE:O	57:v:24:ILE:HG22	2.18	0.43
61:z:25:ARG:HH21	61:z:29:GLU:HB3	1.84	0.43
4:3:7:ILE:HD12	4:3:48:ILE:HD11	2.00	0.42
5:4:5:ILE:HD12	40:e:64:LYS:HD2	2.01	0.42
8:7:1363:C:O2'	8:7:1809:A:N3	2.43	0.42
8:7:1785:A:O2'	8:7:1786:A:H2'	2.18	0.42
8:7:1827:U:OP1	8:7:1971:U:O2'	2.34	0.42
8:7:1827:U:OP2	37:b:221:ARG:NE	2.51	0.42
8:7:2572:A:H2'	38:c:149:ASN:HD21	1.84	0.42
9:8:66:A:N6	9:8:107:G:H2'	2.34	0.42
10:A:463:U:H2'	10:A:464:U:C2	2.53	0.42
13:D:62:ARG:NH2	13:D:68:LEU:HD13	2.34	0.42
23:N:17:ALA:HA	23:N:55:SER:HA	2.00	0.42
32:W:43:C:O2'	32:W:44:G:O5'	2.33	0.42
33:X:10:G:H22	33:X:27:G:H1'	1.84	0.42
34:Y:9:A:H2'	34:Y:11:C:H41	1.83	0.42
38:c:61:THR:OG1	38:c:64:GLU:HG2	2.19	0.42
39:d:127:GLU:H	39:d:127:GLU:CD	2.27	0.42
49:n:7:MET:HA	49:n:20:MET:HA	2.01	0.42
49:n:105:ARG:NH1	54:s:33:VAL:O	2.47	0.42
54:s:48:ILE:HA	54:s:97:LEU:HD12	2.00	0.42
60:y:30:ILE:HD12	60:y:91:PHE:O	2.19	0.42
5:4:60:PHE:CD1	5:4:64:PHE:HD2	2.38	0.42
8:7:482:A:N6	8:7:506:G:O2'	2.52	0.42
8:7:586:A:N1	8:7:809:G:O2'	2.47	0.42
8:7:739:A:H1'	8:7:740:C:H5	1.84	0.42
8:7:2127:G:C2	8:7:2162:G:H8	2.38	0.42
8:7:2769:U:O5'	48:m:95:ARG:NH2	2.52	0.42
8:7:2845:U:H5''	54:s:52:ASN:O	2.18	0.42
10:A:102:G:H2'	10:A:103:U:H6	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:209:U:OP2	10:A:210:C:N4	2.50	0.42
10:A:325:A:H2'	10:A:326:G:O4'	2.19	0.42
10:A:404:G:P	13:D:115:ARG:HH12	2.42	0.42
10:A:405:U:O4	13:D:2:ALA:N	2.52	0.42
10:A:765:G:N1	10:A:812:G:O2'	2.43	0.42
10:A:1373:G:H5''	16:G:36:LYS:HG3	2.01	0.42
15:F:51:ILE:O	15:F:51:ILE:HG13	2.19	0.42
27:R:39:ILE:H	27:R:39:ILE:HD12	1.84	0.42
48:m:117:ALA:HA	48:m:120:ARG:HH11	1.84	0.42
54:s:32:VAL:HB	54:s:39:ARG:HG3	2.00	0.42
4:3:18:PRO:HD3	8:7:968:C:O3'	2.20	0.42
6:5:28:LEU:HD11	57:v:34:ASP:OD1	2.19	0.42
8:7:2869:G:H2'	8:7:2870:C:H6	1.84	0.42
10:A:546:A:P	13:D:69:GLU:HB3	2.58	0.42
10:A:1542:A:H3'	10:A:1542:A:OP2	2.20	0.42
11:B:217:VAL:O	11:B:221:VAL:HG12	2.19	0.42
18:I:116:VAL:HG23	19:J:62:ARG:HH11	1.84	0.42
29:T:71:LYS:HA	29:T:74:ARG:HE	1.84	0.42
31:V:19:G:O5'	31:V:19:G:H8	2.02	0.42
33:X:7:G:N2	33:X:84:C:H1'	2.35	0.42
34:Y:6:A:H2'	34:Y:7:4SU:H6	2.01	0.42
34:Y:14:A:H2'	34:Y:15:G:O4'	2.19	0.42
41:f:95:ARG:HG3	41:f:128:GLN:HG3	2.01	0.42
53:r:16:ARG:HA	53:r:16:ARG:HH11	1.84	0.42
2:1:3:ARG:HD3	2:1:30:LEU:HD12	2.01	0.42
6:5:55:ILE:HG22	6:5:57:LYS:H	1.84	0.42
8:7:94:A:H2'	8:7:95:A:C8	2.54	0.42
8:7:587:C:O2	50:o:33:ARG:NH1	2.52	0.42
8:7:1801:A:N6	8:7:2201:G:O2'	2.53	0.42
8:7:2709:G:H2'	8:7:2710:C:C6	2.55	0.42
10:A:739:C:O2'	24:O:42:HIS:ND1	2.50	0.42
10:A:1100:C:OP2	11:B:95:ARG:HD2	2.19	0.42
10:A:1151:A:O2'	10:A:1152:A:O5'	2.35	0.42
12:C:23:PHE:CZ	19:J:11:LYS:NZ	2.88	0.42
35:Z:66:ASP:OD1	35:Z:67:GLU:N	2.53	0.42
50:o:19:LEU:HB2	50:o:31:GLY:HA2	2.02	0.42
8:7:571:U:P	56:u:80:ARG:HH22	2.43	0.42
8:7:858:G:H3'	8:7:859:G:C8	2.53	0.42
8:7:995:C:O2	48:m:3:THR:OG1	2.24	0.42
8:7:1081:U:H5'	46:k:127:ARG:NH1	2.34	0.42
8:7:1283:G:N1	8:7:1286:A:OP2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:1779:U:O2	8:7:1783:A:N6	2.52	0.42
8:7:2757:A:N1	41:f:67:THR:OG1	2.46	0.42
10:A:994:A:H1'	23:N:9:ARG:NH2	2.34	0.42
10:A:1025:U:O3'	10:A:1026:G:H8	2.02	0.42
10:A:1525:G:OP2	30:U:40:LYS:NZ	2.53	0.42
12:C:123:GLN:HG3	12:C:126:ARG:NH2	2.35	0.42
21:L:80:ILE:HG22	21:L:81:LEU:N	2.35	0.42
32:W:10:G:H2'	32:W:11:C:C6	2.54	0.42
39:d:124:PHE:O	39:d:157:LEU:HD11	2.20	0.42
41:f:152:ARG:HD3	41:f:152:ARG:HA	1.83	0.42
43:h:30:SER:N	43:h:106:ASP:OD1	2.53	0.42
49:n:8:LEU:N	49:n:19:VAL:O	2.44	0.42
4:3:14:ILE:HD11	8:7:989:G:C4	2.53	0.42
8:7:81:G:O2'	8:7:295:G:O2'	2.37	0.42
8:7:1527:G:N1	8:7:1544:A:OP2	2.49	0.42
8:7:1638:C:O2	8:7:2698:U:O2'	2.35	0.42
8:7:2899:A:H5'	48:m:136:GLN:NE2	2.35	0.42
10:A:842:U:H3'	10:A:843:U:H4'	2.02	0.42
19:J:15:HIS:HB3	19:J:70:HIS:CD2	2.55	0.42
37:b:142:HIS:ND1	37:b:193:GLY:O	2.46	0.42
41:f:42:GLU:HB3	41:f:55:ARG:NE	2.34	0.42
41:f:103:ILE:HG22	41:f:105:LEU:HD12	2.02	0.42
56:u:79:ARG:O	56:u:81:LYS:HG2	2.19	0.42
8:7:1398:C:H2'	8:7:1399:C:C6	2.54	0.42
8:7:1703:G:H2'	8:7:1704:C:C6	2.55	0.42
8:7:2150:C:H2'	8:7:2151:U:H6	1.85	0.42
8:7:2799:A:N7	8:7:2801:G:C8	2.88	0.42
10:A:274:A:H4'	26:Q:16:LYS:NZ	2.35	0.42
10:A:791:G:O6	10:A:792:A:N6	2.50	0.42
10:A:1004:A:H8	10:A:1025:U:O2'	2.02	0.42
13:D:54:GLN:HB3	13:D:203:LEU:HD13	2.01	0.42
20:K:123:PRO:HG2	30:U:38:TYR:HB2	2.01	0.42
25:P:21:VAL:O	25:P:33:ILE:N	2.45	0.42
39:d:105:LEU:HD23	39:d:105:LEU:HA	1.85	0.42
8:7:587:C:C2	50:o:19:LEU:HD21	2.54	0.42
8:7:617:G:OP1	39:d:102:ARG:NH1	2.53	0.42
8:7:698:C:O2'	8:7:734:A:N6	2.43	0.42
8:7:1153:C:H2'	8:7:1154:G:O4'	2.19	0.42
8:7:2251:OMG:H1'	8:7:2251:OMG:HM23	1.60	0.42
10:A:1349:A:H5''	18:I:123:ARG:CG	2.45	0.42
11:B:104:TRP:HA	11:B:107:VAL:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:65:VAL:O	20:K:68:GLU:HG2	2.19	0.42
26:Q:71:LYS:HE2	26:Q:71:LYS:HB3	1.84	0.42
27:R:45:THR:HG23	27:R:47:THR:HG23	2.01	0.42
27:R:57:ARG:O	27:R:61:ARG:HG3	2.20	0.42
34:Y:75:C:H2'	34:Y:76:A:C8	2.55	0.42
46:k:75:PRO:O	46:k:79:LEU:HG	2.20	0.42
1:0:17:VAL:HG12	1:0:19:ARG:H	1.83	0.42
3:2:19:LEU:HD23	3:2:19:LEU:HA	1.89	0.42
8:7:322:A:OP2	39:d:163:ASN:HB2	2.20	0.42
8:7:807:U:H2'	8:7:808:G:H8	1.84	0.42
8:7:963:U:H2'	8:7:964:C:C6	2.55	0.42
8:7:1047:G:N2	8:7:1110:G:O2'	2.53	0.42
8:7:2014:A:H2'	8:7:2015:A:C8	2.55	0.42
8:7:2333:A:H4'	8:7:2334:U:O5'	2.20	0.42
8:7:2834:G:H2'	8:7:2879:A:H61	1.85	0.42
10:A:59:A:H3'	10:A:331:G:H22	1.85	0.42
10:A:331:G:H5'	10:A:331:G:H8	1.85	0.42
10:A:334:C:O2'	10:A:1434:A:O2'	2.31	0.42
10:A:1227:A:C8	22:M:116:ILE:HG13	2.55	0.42
10:A:1318:A:H5''	28:S:3:ARG:HH12	1.84	0.42
10:A:1497:G:H1'	10:A:1518:MA6:C2	2.50	0.42
12:C:185:ASN:CG	12:C:186:THR:N	2.77	0.42
15:F:10:VAL:HB	15:F:58:HIS:HB3	2.01	0.42
15:F:29:ILE:HD13	15:F:64:VAL:HG11	2.02	0.42
23:N:11:VAL:HA	23:N:14:VAL:HG12	2.02	0.42
31:V:31:U:H2'	31:V:32:U:C2	2.55	0.42
33:X:5:A:H2'	33:X:6:G:C8	2.55	0.42
38:c:85:ALA:HB3	38:c:88:GLU:CD	2.44	0.42
39:d:120:VAL:HA	39:d:188:MET:O	2.20	0.42
40:e:29:PRO:HB2	40:e:169:LEU:HD22	2.01	0.42
42:g:32:GLU:OE1	42:g:32:GLU:N	2.49	0.42
48:m:114:LEU:HB3	48:m:118:MET:HE2	2.02	0.42
8:7:324:A:OP2	8:7:1205:A:N6	2.53	0.42
8:7:371:A:H3'	8:7:371:A:OP1	2.20	0.42
8:7:395:U:O2'	8:7:396:G:N7	2.48	0.42
8:7:1486:U:H2'	8:7:1487:U:C6	2.55	0.42
8:7:1505:A:H2'	8:7:1506:U:C6	2.55	0.42
8:7:2246:G:H2'	8:7:2247:A:C8	2.55	0.42
9:8:66:A:H61	9:8:107:G:H2'	1.85	0.42
10:A:154:U:H2'	10:A:155:A:C8	2.55	0.42
10:A:1402:4OC:O5'	10:A:1402:4OC:H6	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1445:U:O5'	10:A:1445:U:H6	2.02	0.42
20:K:84:VAL:HG11	20:K:97:ILE:HD11	2.00	0.42
30:U:28:VAL:O	30:U:32:VAL:HG23	2.19	0.42
33:X:41:G:H2'	33:X:42:G:C8	2.55	0.42
33:X:75:A:H1'	33:X:77:U:C5'	2.50	0.42
41:f:30:ASN:ND2	41:f:79:VAL:O	2.37	0.42
48:m:99:ARG:HH11	48:m:99:ARG:HA	1.85	0.42
56:u:27:ILE:O	56:u:66:HIS:NE2	2.52	0.42
60:y:6:ALA:HB2	60:y:63:ILE:HD11	2.01	0.42
8:7:1475:G:HO2'	8:7:1476:U:P	2.38	0.41
8:7:2118:U:H5''	8:7:2148:G:O2'	2.20	0.41
8:7:2134:A:OP1	8:7:2134:A:H3'	2.19	0.41
8:7:2233:U:H2'	8:7:2234:G:H8	1.85	0.41
8:7:2512:C:H2'	8:7:2513:A:O4'	2.19	0.41
10:A:376:G:H2'	10:A:377:G:H8	1.85	0.41
10:A:885:G:O2'	10:A:914:A:N1	2.45	0.41
10:A:927:G:O2'	10:A:1503:A:N6	2.47	0.41
10:A:1148:U:H2'	10:A:1149:C:O4'	2.20	0.41
10:A:1216:A:OP1	23:N:3:LYS:NZ	2.33	0.41
10:A:1273:C:H2'	10:A:1274:A:O4'	2.20	0.41
10:A:1537:U:H1'	10:A:1538:C:C6	2.54	0.41
14:E:134:ILE:HG13	14:E:135:ASN:N	2.35	0.41
14:E:164:ILE:HG13	14:E:165:LEU:N	2.35	0.41
15:F:78:PHE:HA	15:F:84:VAL:HG11	2.01	0.41
19:J:49:PHE:HE2	23:N:77:PHE:HD2	1.68	0.41
19:J:56:HIS:ND1	19:J:57:VAL:HG13	2.35	0.41
22:M:113:ARG:HD3	22:M:113:ARG:C	2.43	0.41
30:U:13:ASP:O	30:U:17:ARG:HG2	2.20	0.41
39:d:106:LYS:HZ2	39:d:200:LEU:HD22	1.85	0.41
43:h:42:THR:HA	43:h:93:VAL:HA	2.01	0.41
54:s:16:ASP:OD1	54:s:16:ASP:N	2.53	0.41
8:7:829:A:N7	8:7:2248:C:H5'	2.35	0.41
8:7:1556:C:H2'	8:7:1557:C:C6	2.56	0.41
8:7:1847:A:O2'	8:7:1848:A:P	2.78	0.41
8:7:2173:A:H2'	8:7:2174:C:C6	2.55	0.41
8:7:2522:U:O2'	8:7:2647:U:OP1	2.25	0.41
8:7:2636:C:O2'	38:c:45:TYR:OH	2.27	0.41
8:7:2798:U:H5''	8:7:2799:A:C2	2.55	0.41
26:Q:77:ARG:CZ	26:Q:77:ARG:HB3	2.50	0.41
38:c:121:THR:HB	38:c:127:PHE:HD2	1.85	0.41
49:n:121:GLU:OE2	49:n:123:LEU:HB3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:o:9:ALA:O	50:o:12:SER:OG	2.38	0.41
50:o:35:HIS:C	50:o:36:LYS:HG2	2.46	0.41
50:o:77:ILE:HG22	50:o:109:LYS:O	2.20	0.41
8:7:245:G:O2'	8:7:384:A:N1	2.50	0.41
8:7:1475:G:O2'	8:7:1476:U:P	2.78	0.41
10:A:173:U:H5''	10:A:197:A:O4'	2.20	0.41
10:A:456:A:H61	10:A:476:U:H3	1.67	0.41
10:A:831:A:H2'	10:A:832:G:H8	1.84	0.41
10:A:1147:C:O3'	18:I:7:TYR:OH	2.34	0.41
17:H:95:VAL:CG2	17:H:102:ALA:HB2	2.50	0.41
31:V:25:U:H2'	31:V:26:G:C8	2.55	0.41
34:Y:39:G:H2'	34:Y:40:G:C8	2.55	0.41
40:e:111:ILE:HD13	40:e:137:ILE:HG21	2.02	0.41
5:4:55:GLY:O	5:4:59:ARG:N	2.35	0.41
8:7:2059:A:H2'	8:7:2503:2MA:N1	2.35	0.41
8:7:2489:U:O2	8:7:2491:U:N3	2.53	0.41
8:7:2523:G:O2'	8:7:2764:A:O2'	2.26	0.41
8:7:2728:U:O2'	8:7:2729:G:H8	2.03	0.41
10:A:169:C:H2'	10:A:170:U:C6	2.55	0.41
10:A:237:G:OP1	26:Q:42:THR:OG1	2.28	0.41
10:A:881:G:P	21:L:9:ARG:HH22	2.43	0.41
10:A:1330:U:H4'	22:M:23:TYR:CE1	2.55	0.41
10:A:1351:U:H2'	10:A:1352:C:C6	2.55	0.41
12:C:58:GLU:OE2	19:J:94:ALA:HB3	2.20	0.41
27:R:34:THR:HG22	27:R:38:LYS:O	2.21	0.41
27:R:64:TYR:HD2	27:R:65:LEU:HD22	1.84	0.41
37:b:120:VAL:HG12	37:b:131:PRO:HG2	2.02	0.41
43:h:105:MET:SD	43:h:108:VAL:HG21	2.61	0.41
6:5:28:LEU:HD12	6:5:37:LYS:HE2	2.02	0.41
8:7:176:A:H3'	8:7:177:G:N2	2.36	0.41
8:7:631:A:N3	8:7:2415:G:O2'	2.50	0.41
8:7:833:A:H2'	8:7:834:G:H8	1.85	0.41
8:7:1032:A:H2	8:7:1122:G:H22	1.68	0.41
8:7:1824:G:O2'	37:b:246:THR:HG22	2.21	0.41
8:7:2333:A:OP1	61:z:77:ARG:NH1	2.51	0.41
8:7:2481:G:O2'	8:7:2482:A:H8	2.02	0.41
10:A:294:U:OP1	10:A:610:U:O2'	2.27	0.41
12:C:14:ILE:O	12:C:211:MET:HG2	2.21	0.41
29:T:44:LYS:HG2	29:T:86:LEU:HD22	2.02	0.41
52:q:96:ARG:O	52:q:113:ILE:HD12	2.20	0.41
8:7:221:A:N1	8:7:265:A:O2'	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:1129:A:H1'	8:7:2516:A:H1'	2.02	0.41
8:7:1246:A:H2'	8:7:1247:A:O4'	2.21	0.41
8:7:1475:G:HO2'	8:7:1476:U:C5'	2.31	0.41
8:7:1794:A:H2'	8:7:1795:C:C6	2.56	0.41
8:7:2748:A:H5'	41:f:4:VAL:HG21	2.03	0.41
10:A:748:G:H2'	10:A:749:A:C8	2.55	0.41
10:A:1442:G:H4'	54:s:114:LEU:HD11	2.02	0.41
13:D:67:VAL:HG21	13:D:94:LEU:HD22	2.02	0.41
17:H:127:CYS:SG	17:H:128:TYR:N	2.93	0.41
37:b:111:LYS:HE2	37:b:111:LYS:HB2	1.86	0.41
40:e:165:GLU:H	40:e:165:GLU:CD	2.28	0.41
45:j:116:GLU:OE2	45:j:125:ARG:NH2	2.53	0.41
53:r:4:LYS:O	53:r:5:SER:C	2.64	0.41
54:s:14:LYS:HB2	54:s:77:HIS:HD2	1.86	0.41
2:1:31:PRO:HB2	2:1:33:LEU:HG	2.02	0.41
5:4:34:LEU:CD2	40:e:106:ILE:HD12	2.49	0.41
8:7:82:U:H2'	8:7:83:A:C8	2.56	0.41
8:7:101:A:H2'	8:7:101:A:N3	2.35	0.41
8:7:1880:U:H2'	8:7:1881:C:C6	2.56	0.41
8:7:2262:U:OP1	8:7:2387:U:O2'	2.37	0.41
8:7:2872:A:H2'	8:7:2873:A:H5''	2.02	0.41
10:A:824:G:H2'	10:A:825:A:C8	2.56	0.41
10:A:1411:C:H2'	10:A:1412:C:C6	2.56	0.41
11:B:23:TRP:CZ3	11:B:25:PRO:HA	2.56	0.41
15:F:4:TYR:CE2	15:F:71:ILE:HG13	2.56	0.41
31:V:8:A:N3	31:V:8:A:H2'	2.35	0.41
33:X:38:12A:C5'	33:X:38:12A:H8	2.51	0.41
35:Z:36:VAL:N	35:Z:48:ILE:O	2.45	0.41
37:b:165:VAL:HG21	37:b:181:MET:HE1	2.02	0.41
39:d:102:ARG:HB3	39:d:106:LYS:NZ	2.35	0.41
40:e:34:ILE:HB	40:e:91:LEU:HB2	2.02	0.41
48:m:37:ARG:HH21	48:m:39:LYS:HG3	1.85	0.41
50:o:115:GLU:OE1	50:o:117:THR:HG23	2.21	0.41
54:s:44:GLU:O	54:s:63:LYS:HE2	2.20	0.41
60:y:48:MET:HE3	60:y:48:MET:HB3	1.82	0.41
2:1:56:MET:HE3	2:1:56:MET:HB3	1.93	0.41
8:7:2026:U:H2'	8:7:2027:G:O4'	2.21	0.41
8:7:2108:A:H8	8:7:2108:A:O5'	2.04	0.41
8:7:2138:G:H5''	8:7:2139:U:O2'	2.20	0.41
10:A:109:A:C8	10:A:326:G:H2'	2.56	0.41
10:A:516:PSU:C2	10:A:517:G:C6	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:736:C:H2'	10:A:737:C:C6	2.56	0.41
11:B:199:VAL:O	11:B:200:ILE:HD13	2.20	0.41
13:D:163:GLU:HA	13:D:167:LYS:HE3	2.02	0.41
25:P:68:SER:HB3	25:P:71:VAL:HG22	2.01	0.41
26:Q:7:THR:HG22	26:Q:62:ARG:HB3	2.02	0.41
26:Q:57:ASP:OD1	26:Q:81:LYS:HD2	2.21	0.41
49:n:105:ARG:NH2	54:s:33:VAL:O	2.46	0.41
3:2:17:GLU:OE1	3:2:17:GLU:HA	2.21	0.41
8:7:371:A:H5'	8:7:423:A:C2	2.56	0.41
8:7:560:C:H2'	8:7:561:G:C8	2.56	0.41
8:7:704:G:H1'	8:7:726:G:N2	2.36	0.41
8:7:780:G:O2'	8:7:783:A:N6	2.51	0.41
8:7:817:C:H2'	8:7:818:G:H8	1.86	0.41
8:7:878:A:H3'	8:7:879:G:H8	1.86	0.41
8:7:987:C:H2'	8:7:988:A:O4'	2.20	0.41
8:7:2562:U:H1'	49:n:23:LYS:HZ3	1.86	0.41
8:7:2667:C:H1'	41:f:109:PHE:CD1	2.56	0.41
10:A:17:U:H2'	10:A:18:C:C6	2.56	0.41
10:A:41:G:H2'	10:A:42:G:C8	2.56	0.41
10:A:57:G:H2'	10:A:58:C:C6	2.56	0.41
10:A:193:C:H2'	10:A:194:C:C6	2.56	0.41
10:A:346:G:OP1	54:s:39:ARG:NH1	2.54	0.41
10:A:427:U:O2'	10:A:541:G:OP1	2.39	0.41
10:A:439:U:H4'	13:D:121:LYS:HD2	2.03	0.41
10:A:1095:U:P	10:A:1108:G:H1	2.43	0.41
10:A:1144:G:N2	10:A:1146:A:H62	2.17	0.41
10:A:1368:A:OP2	18:I:114:LYS:NZ	2.38	0.41
10:A:1519:MA6:H8	10:A:1519:MA6:O5'	2.20	0.41
11:B:20:THR:O	11:B:23:TRP:HD1	2.04	0.41
11:B:118:GLU:OE2	11:B:141:LEU:HD11	2.21	0.41
12:C:150:LYS:HB2	12:C:173:VAL:HG21	2.03	0.41
17:H:111:MET:HB2	17:H:115:ALA:HB3	2.03	0.41
26:Q:60:GLU:O	26:Q:61:ILE:HD13	2.20	0.41
34:Y:16:C:O2'	34:Y:18:G:OP2	2.38	0.41
34:Y:37:6MZ:H2'	34:Y:38:A:O4'	2.21	0.41
42:g:11:LEU:HD23	42:g:51:GLU:HA	2.02	0.41
43:h:77:PRO:HB2	43:h:80:VAL:HG21	2.03	0.41
44:i:94:ILE:HB	44:i:122:LEU:HD23	2.03	0.41
44:i:114:GLU:OE2	44:i:132:PHE:HB3	2.21	0.41
46:k:72:LYS:NZ	46:k:73:THR:HG22	2.36	0.41
47:l:10:LEU:HD11	47:l:14:ARG:NH2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:t:3:ARG:NH2	55:t:5:LYS:HE3	2.36	0.41
59:x:4:LYS:O	59:x:94:ARG:NH1	2.48	0.41
1:0:8:LYS:HD3	1:0:9:LYS:H	1.86	0.41
8:7:513:A:N3	55:t:11:ARG:NH2	2.56	0.41
8:7:570:G:N2	8:7:2030:6MZ:O4'	2.54	0.41
8:7:1265:A:H4'	8:7:1266:G:H4'	2.02	0.41
8:7:1569:A:O2'	37:b:36:LYS:HG2	2.21	0.41
8:7:1751:U:H2'	8:7:1752:C:C6	2.56	0.41
8:7:2129:C:H6	8:7:2129:C:O5'	2.04	0.41
8:7:2591:C:H2'	8:7:2592:G:C8	2.56	0.41
8:7:2870:C:H2'	8:7:2871:U:O4'	2.20	0.41
10:A:1108:G:H5'	12:C:176:HIS:CE1	2.56	0.41
10:A:1463:U:H2'	10:A:1464:U:C6	2.56	0.41
11:B:23:TRP:HZ3	11:B:25:PRO:HA	1.85	0.41
12:C:13:GLY:HA3	23:N:97:LYS:HE3	2.01	0.41
15:F:67:PRO:O	15:F:71:ILE:HG12	2.21	0.41
17:H:96:MET:HG3	17:H:99:LEU:HB2	2.03	0.41
20:K:86:VAL:O	20:K:113:VAL:N	2.35	0.41
33:X:3:U:H2'	33:X:4:G:H8	1.86	0.41
33:X:38:12A:OO	33:X:38:12A:HB	2.21	0.41
34:Y:23:A:H2'	34:Y:24:G:C8	2.56	0.41
37:b:241:GLY:O	37:b:242:LYS:HG3	2.21	0.41
41:f:4:VAL:HG13	41:f:69:ARG:HD2	2.02	0.41
46:k:105:GLN:HE21	46:k:109:ILE:HD11	1.86	0.41
49:n:78:ARG:HG3	54:s:71:GLU:HB2	2.02	0.41
53:r:99:TYR:OH	53:r:111:ARG:NH2	2.54	0.41
54:s:4:ILE:O	54:s:8:LEU:HD23	2.21	0.41
1:0:2:LYS:HB2	1:0:35:GLN:HG3	2.03	0.40
3:2:10:SER:HB2	3:2:13:GLU:OE1	2.21	0.40
8:7:351:C:H2'	8:7:352:A:C8	2.56	0.40
8:7:796:C:H2'	8:7:797:G:C8	2.56	0.40
8:7:1084:A:C5'	45:j:53:ARG:HH21	2.35	0.40
8:7:1586:A:H2'	8:7:1587:G:O4'	2.21	0.40
8:7:2532:G:N2	8:7:2663:G:O2'	2.55	0.40
10:A:347:G:H2'	10:A:348:G:O4'	2.22	0.40
10:A:714:G:H2'	10:A:715:A:C8	2.56	0.40
10:A:1318:A:H5''	28:S:3:ARG:NH1	2.37	0.40
20:K:21:ALA:N	20:K:83:GLU:O	2.48	0.40
24:O:4:SER:O	24:O:8:THR:HG23	2.20	0.40
33:X:20:H2U:H52	33:X:74:G:N2	2.36	0.40
41:f:47:ASP:CG	41:f:48:ASN:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:14:LEU:HD22	3:2:53:VAL:HG23	2.03	0.40
8:7:598:U:H2'	8:7:599:A:C8	2.56	0.40
8:7:680:C:H2'	8:7:681:G:C8	2.56	0.40
8:7:687:C:H5''	47:l:2:LYS:HE2	2.03	0.40
8:7:780:G:H1	37:b:229:ASP:CG	2.28	0.40
8:7:1127:A:N6	8:7:2488:G:H21	2.19	0.40
8:7:1799:G:C8	37:b:180:GLU:OE2	2.74	0.40
8:7:2126:A:C2	8:7:2162:G:H1'	2.56	0.40
8:7:2247:A:H2'	8:7:2248:C:C6	2.55	0.40
8:7:2836:U:H2'	8:7:2837:A:C8	2.56	0.40
10:A:1080:A:OP1	14:E:52:LYS:HE2	2.20	0.40
10:A:1160:G:H22	10:A:1176:A:H2	1.70	0.40
10:A:1436:U:H2'	10:A:1437:A:C8	2.56	0.40
16:G:125:SER:O	16:G:129:GLU:HG2	2.20	0.40
26:Q:26:GLU:HG2	26:Q:26:GLU:O	2.21	0.40
36:a:173:THR:HG21	36:a:192:LEU:HD21	2.03	0.40
37:b:225:MET:SD	37:b:230:HIS:HB2	2.62	0.40
47:l:43:THR:OG1	47:l:44:VAL:N	2.54	0.40
49:n:9:ASN:OD1	49:n:18:ARG:NH1	2.54	0.40
55:t:94:ILE:HD12	55:t:94:ILE:N	2.35	0.40
8:7:672:C:H5	50:o:42:SER:HB3	1.86	0.40
8:7:679:C:H2'	8:7:680:C:C6	2.55	0.40
8:7:782:A:N1	37:b:225:MET:HE2	2.36	0.40
8:7:981:A:OP2	8:7:982:C:N4	2.48	0.40
8:7:1169:A:N6	8:7:1180:U:H3	2.19	0.40
8:7:1243:C:H2'	8:7:1244:A:C8	2.55	0.40
8:7:1599:U:OP1	58:w:40:LYS:HG3	2.21	0.40
8:7:2296:U:OP2	53:r:9:ARG:NH1	2.46	0.40
8:7:2339:C:H2'	8:7:2340:A:C8	2.57	0.40
8:7:2691:C:H2'	8:7:2692:G:C8	2.52	0.40
10:A:6:G:H1	14:E:99:ALA:HA	1.87	0.40
11:B:21:ARG:CZ	11:B:21:ARG:HB3	2.52	0.40
13:D:202:GLU:HB2	14:E:112:ARG:HH22	1.86	0.40
14:E:166:GLY:HA3	17:H:114:ARG:HH22	1.86	0.40
23:N:53:ARG:HH21	28:S:37:ARG:NH2	2.18	0.40
33:X:5:A:H2'	33:X:6:G:H8	1.86	0.40
41:f:96:ALA:CB	41:f:131:ILE:HD11	2.51	0.40
42:g:50:LYS:HE2	42:g:50:LYS:HB2	1.87	0.40
48:m:134:ALA:O	48:m:136:GLN:NE2	2.54	0.40
2:1:51:VAL:HG12	2:1:52:SER:O	2.22	0.40
10:A:134:G:H2'	10:A:135:C:C6	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1099:G:H5''	30:U:69:ARG:NH1	2.37	0.40
10:A:1401:G:H2'	10:A:1402:4OC:O4'	2.21	0.40
11:B:207:ILE:O	11:B:210:VAL:HG12	2.22	0.40
30:U:63:GLU:C	30:U:65:ALA:N	2.79	0.40
31:V:21:U:H6	31:V:21:U:O5'	2.04	0.40
34:Y:50:G:N2	34:Y:64:U:O2	2.54	0.40
34:Y:73:A:N3	34:Y:73:A:H2'	2.36	0.40
41:f:55:ARG:HD3	41:f:55:ARG:HA	1.90	0.40
44:i:111:ALA:HB3	44:i:114:GLU:HB2	2.04	0.40
53:r:78:VAL:HA	53:r:81:ARG:HD2	2.04	0.40
1:0:32:LYS:HE3	1:0:32:LYS:HB3	1.78	0.40
5:4:45:THR:C	5:4:47:LYS:H	2.29	0.40
8:7:175:G:H2'	8:7:176:A:O4'	2.21	0.40
8:7:876:C:H2'	8:7:877:A:O4'	2.21	0.40
8:7:1076:C:H2'	8:7:1077:A:C8	2.56	0.40
8:7:1999:C:H2'	8:7:2000:C:H6	1.86	0.40
8:7:2010:G:H2'	8:7:2011:U:C6	2.56	0.40
10:A:376:G:H2'	10:A:377:G:C8	2.57	0.40
10:A:389:A:N3	10:A:389:A:H2'	2.37	0.40
10:A:977:A:O2'	10:A:979:C:OP2	2.33	0.40
11:B:131:LYS:HB3	11:B:131:LYS:HE2	1.87	0.40
12:C:28:GLU:OE1	12:C:28:GLU:N	2.54	0.40
12:C:112:ASP:O	12:C:116:VAL:HG22	2.21	0.40
17:H:18:GLN:HE21	17:H:72:VAL:H	1.68	0.40
18:I:40:GLY:HA2	18:I:45:ARG:HH21	1.86	0.40
19:J:8:ILE:HB	19:J:74:VAL:HG23	2.04	0.40
21:L:89:ASP:C	21:L:90:LEU:HD22	2.47	0.40
38:c:115:GLY:HA2	38:c:166:GLY:HA3	2.03	0.40
38:c:124:ARG:HG3	38:c:165:MET:CG	2.52	0.40
48:m:69:ARG:O	48:m:89:PHE:HB3	2.22	0.40
50:o:17:LYS:O	50:o:18:ARG:C	2.65	0.40
53:r:60:GLU:N	53:r:60:GLU:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
2	1	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
3	2	61/63 (97%)	60 (98%)	0	1 (2%)	7	31
4	3	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	2	17
5	4	65/70 (93%)	49 (75%)	16 (25%)	0	100	100
6	5	54/57 (95%)	54 (100%)	0	0	100	100
7	6	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
11	B	222/241 (92%)	209 (94%)	12 (5%)	1 (0%)	24	55
12	C	210/233 (90%)	208 (99%)	2 (1%)	0	100	100
13	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
14	E	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
15	F	104/135 (77%)	103 (99%)	1 (1%)	0	100	100
16	G	153/179 (86%)	149 (97%)	4 (3%)	0	100	100
17	H	127/130 (98%)	127 (100%)	0	0	100	100
18	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
19	J	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
20	K	116/129 (90%)	102 (88%)	11 (10%)	3 (3%)	4	23
21	L	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
22	M	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
23	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
24	O	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	10	37
25	P	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
26	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
27	R	72/75 (96%)	63 (88%)	7 (10%)	2 (3%)	4	21
28	S	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
29	T	84/87 (97%)	84 (100%)	0	0	100	100
30	U	68/71 (96%)	61 (90%)	7 (10%)	0	100	100
35	Z	168/557 (30%)	161 (96%)	7 (4%)	0	100	100
36	a	130/234 (56%)	126 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	b	269/273 (98%)	262 (97%)	6 (2%)	1 (0%)	30	60
38	c	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
39	d	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
40	e	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
41	f	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
42	g	50/55 (91%)	50 (100%)	0	0	100	100
43	h	135/136 (99%)	134 (99%)	1 (1%)	0	100	100
44	i	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	18	49
45	j	133/165 (81%)	122 (92%)	11 (8%)	0	100	100
46	k	132/142 (93%)	124 (94%)	8 (6%)	0	100	100
47	l	44/46 (96%)	44 (100%)	0	0	100	100
48	m	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
49	n	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
50	o	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
51	p	4/18 (22%)	3 (75%)	1 (25%)	0	100	100
52	q	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
53	r	114/117 (97%)	105 (92%)	7 (6%)	2 (2%)	6	29
54	s	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
55	t	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
56	u	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	12	40
57	v	108/110 (98%)	96 (89%)	11 (10%)	1 (1%)	14	43
58	w	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
59	x	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
60	y	92/94 (98%)	92 (100%)	0	0	100	100
61	z	82/85 (96%)	77 (94%)	5 (6%)	0	100	100
All	All	6208/7029 (88%)	5944 (96%)	248 (4%)	16 (0%)	37	65

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	v	64	ALA
4	3	21	LYS
20	K	70	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	K	80	LYS
53	r	5	SER
3	2	9	LYS
11	B	131	LYS
27	R	16	GLU
53	r	3	LYS
4	3	20	HIS
20	K	74	VAL
24	O	75	VAL
37	b	247	PRO
56	u	49	ILE
27	R	37	GLY
44	i	121	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	34/34 (100%)	34 (100%)	0	100	100
2	1	67/68 (98%)	67 (100%)	0	100	100
3	2	55/55 (100%)	55 (100%)	0	100	100
4	3	48/49 (98%)	48 (100%)	0	100	100
5	4	60/62 (97%)	60 (100%)	0	100	100
6	5	47/48 (98%)	47 (100%)	0	100	100
7	6	51/52 (98%)	51 (100%)	0	100	100
11	B	186/199 (94%)	186 (100%)	0	100	100
12	C	172/190 (90%)	172 (100%)	0	100	100
13	D	172/173 (99%)	172 (100%)	0	100	100
14	E	120/126 (95%)	120 (100%)	0	100	100
15	F	92/116 (79%)	92 (100%)	0	100	100
16	G	128/147 (87%)	127 (99%)	1 (1%)	73	79
17	H	104/105 (99%)	104 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	I	105/107 (98%)	105 (100%)	0	100	100
19	J	88/90 (98%)	88 (100%)	0	100	100
20	K	91/99 (92%)	91 (100%)	0	100	100
21	L	103/104 (99%)	103 (100%)	0	100	100
22	M	93/96 (97%)	90 (97%)	3 (3%)	34	60
23	N	83/84 (99%)	83 (100%)	0	100	100
24	O	76/77 (99%)	76 (100%)	0	100	100
25	P	65/65 (100%)	65 (100%)	0	100	100
26	Q	74/78 (95%)	74 (100%)	0	100	100
27	R	64/65 (98%)	64 (100%)	0	100	100
28	S	72/79 (91%)	72 (100%)	0	100	100
29	T	65/66 (98%)	65 (100%)	0	100	100
30	U	59/61 (97%)	59 (100%)	0	100	100
35	Z	143/461 (31%)	143 (100%)	0	100	100
36	a	110/181 (61%)	110 (100%)	0	100	100
37	b	216/218 (99%)	216 (100%)	0	100	100
38	c	164/164 (100%)	164 (100%)	0	100	100
39	d	165/165 (100%)	165 (100%)	0	100	100
40	e	149/150 (99%)	149 (100%)	0	100	100
41	f	137/138 (99%)	137 (100%)	0	100	100
42	g	47/49 (96%)	47 (100%)	0	100	100
43	h	110/109 (101%)	110 (100%)	0	100	100
44	i	114/114 (100%)	114 (100%)	0	100	100
45	j	103/123 (84%)	103 (100%)	0	100	100
46	k	104/110 (94%)	104 (100%)	0	100	100
47	l	38/38 (100%)	38 (100%)	0	100	100
48	m	116/116 (100%)	116 (100%)	0	100	100
49	n	104/104 (100%)	104 (100%)	0	100	100
50	o	103/103 (100%)	103 (100%)	0	100	100
51	p	4/4 (100%)	4 (100%)	0	100	100
52	q	100/103 (97%)	100 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	r	86/87 (99%)	86 (100%)	0	100	100
54	s	99/100 (99%)	99 (100%)	0	100	100
55	t	89/90 (99%)	89 (100%)	0	100	100
56	u	84/84 (100%)	84 (100%)	0	100	100
57	v	93/93 (100%)	93 (100%)	0	100	100
58	w	80/84 (95%)	80 (100%)	0	100	100
59	x	83/85 (98%)	83 (100%)	0	100	100
60	y	78/78 (100%)	78 (100%)	0	100	100
61	z	62/63 (98%)	62 (100%)	0	100	100
All	All	5155/5709 (90%)	5151 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	G	86	GLN
22	M	104	THR
22	M	105	ASN
22	M	113	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	34	HIS
2	1	36	HIS
3	2	15	ASN
3	2	38	GLN
4	3	9	GLN
5	4	33	ASN
11	B	168	HIS
15	F	14	GLN
15	F	17	GLN
16	G	9	GLN
17	H	16	ASN
20	K	22	HIS
20	K	119	ASN
21	L	29	GLN
23	N	43	ASN
27	R	52	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	T	55	GLN
36	a	24	ASN
37	b	226	ASN
38	c	173	GLN
39	d	9	GLN
39	d	92	HIS
39	d	94	GLN
39	d	115	GLN
40	e	81	GLN
41	f	101	ASN
41	f	115	HIS
42	g	19	HIS
44	i	133	GLN
46	k	43	ASN
46	k	105	GLN
48	m	80	HIS
50	o	104	GLN
53	r	100	HIS
54	s	10	GLN
54	s	77	HIS
57	v	9	HIS
57	v	57	ASN
57	v	61	ASN
61	z	50	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1541/1542 (99%)	249 (16%)	20 (1%)
31	V	29/30 (96%)	14 (48%)	3 (10%)
32	W	75/76 (98%)	24 (32%)	2 (2%)
33	X	76/78 (97%)	26 (34%)	4 (5%)
34	Y	75/76 (98%)	26 (34%)	7 (9%)
8	7	2902/2903 (99%)	496 (17%)	55 (1%)
9	8	119/120 (99%)	14 (11%)	1 (0%)
All	All	4817/4825 (99%)	849 (17%)	92 (1%)

All (849) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	10	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	15	G
8	7	28	A
8	7	34	U
8	7	44	A
8	7	46	G
8	7	55	G
8	7	71	A
8	7	74	A
8	7	75	G
8	7	96	C
8	7	101	A
8	7	102	U
8	7	103	A
8	7	118	A
8	7	119	A
8	7	120	U
8	7	121	G
8	7	125	A
8	7	135	U
8	7	139	U
8	7	141	G
8	7	142	A
8	7	159	G
8	7	163	C
8	7	174	U
8	7	176	A
8	7	177	G
8	7	178	G
8	7	181	A
8	7	196	A
8	7	199	A
8	7	215	G
8	7	216	A
8	7	221	A
8	7	222	A
8	7	248	G
8	7	252	G
8	7	275	C
8	7	277	G
8	7	278	A
8	7	279	A
8	7	283	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	284	U
8	7	285	G
8	7	286	U
8	7	294	A
8	7	295	G
8	7	311	A
8	7	330	A
8	7	341	C
8	7	343	C
8	7	345	A
8	7	353	C
8	7	359	G
8	7	361	G
8	7	362	A
8	7	386	G
8	7	395	U
8	7	396	G
8	7	401	A
8	7	405	U
8	7	412	A
8	7	455	C
8	7	456	C
8	7	457	A
8	7	470	A
8	7	473	G
8	7	474	G
8	7	475	C
8	7	481	G
8	7	491	G
8	7	504	A
8	7	505	A
8	7	506	G
8	7	509	C
8	7	510	C
8	7	513	A
8	7	514	A
8	7	527	C
8	7	529	A
8	7	532	A
8	7	547	A
8	7	549	G
8	7	563	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	573	U
8	7	575	A
8	7	603	A
8	7	613	A
8	7	614	A
8	7	615	U
8	7	637	A
8	7	645	C
8	7	646	U
8	7	647	G
8	7	654	A
8	7	655	A
8	7	686	U
8	7	717	C
8	7	726	G
8	7	729	G
8	7	730	A
8	7	747	5MU
8	7	748	G
8	7	749	A
8	7	764	A
8	7	765	C
8	7	775	G
8	7	776	G
8	7	782	A
8	7	784	G
8	7	785	G
8	7	805	G
8	7	812	C
8	7	819	A
8	7	827	U
8	7	828	U
8	7	830	G
8	7	831	G
8	7	845	A
8	7	846	U
8	7	847	U
8	7	858	G
8	7	859	G
8	7	869	G
8	7	878	A
8	7	883	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	885	C
8	7	887	U
8	7	888	C
8	7	891	G
8	7	895	U
8	7	896	A
8	7	897	C
8	7	902	C
8	7	907	G
8	7	910	A
8	7	917	A
8	7	919	U
8	7	931	U
8	7	932	U
8	7	941	A
8	7	946	C
8	7	961	C
8	7	962	G
8	7	974	G
8	7	983	A
8	7	989	G
8	7	990	A
8	7	995	C
8	7	996	A
8	7	999	U
8	7	1005	C
8	7	1012	U
8	7	1013	C
8	7	1021	A
8	7	1022	G
8	7	1025	G
8	7	1026	G
8	7	1027	A
8	7	1033	U
8	7	1046	A
8	7	1047	G
8	7	1055	G
8	7	1060	U
8	7	1070	A
8	7	1081	U
8	7	1083	U
8	7	1084	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	1085	A
8	7	1087	G
8	7	1088	A
8	7	1090	A
8	7	1097	U
8	7	1112	G
8	7	1130	U
8	7	1132	U
8	7	1133	A
8	7	1134	A
8	7	1135	C
8	7	1136	G
8	7	1142	A
8	7	1149	G
8	7	1161	C
8	7	1169	A
8	7	1172	C
8	7	1173	U
8	7	1174	U
8	7	1176	U
8	7	1178	C
8	7	1179	G
8	7	1180	U
8	7	1184	U
8	7	1236	G
8	7	1247	A
8	7	1248	G
8	7	1249	U
8	7	1250	G
8	7	1253	A
8	7	1256	G
8	7	1262	A
8	7	1266	G
8	7	1267	U
8	7	1271	G
8	7	1272	A
8	7	1273	U
8	7	1300	G
8	7	1301	A
8	7	1321	A
8	7	1329	U
8	7	1341	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	1342	A
8	7	1344	U
8	7	1345	C
8	7	1352	U
8	7	1365	A
8	7	1368	G
8	7	1379	U
8	7	1380	G
8	7	1383	A
8	7	1396	U
8	7	1398	C
8	7	1416	G
8	7	1417	C
8	7	1419	A
8	7	1420	A
8	7	1428	C
8	7	1434	A
8	7	1452	G
8	7	1453	A
8	7	1454	C
8	7	1455	G
8	7	1461	C
8	7	1476	U
8	7	1482	G
8	7	1488	C
8	7	1490	A
8	7	1491	G
8	7	1493	C
8	7	1494	A
8	7	1497	U
8	7	1503	A
8	7	1508	A
8	7	1509	A
8	7	1515	A
8	7	1524	G
8	7	1532	A
8	7	1539	U
8	7	1566	A
8	7	1569	A
8	7	1578	U
8	7	1581	G
8	7	1583	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	1584	U
8	7	1602	U
8	7	1608	A
8	7	1610	A
8	7	1618	6MZ
8	7	1647	U
8	7	1648	U
8	7	1649	G
8	7	1674	G
8	7	1714	U
8	7	1715	G
8	7	1716	U
8	7	1717	A
8	7	1727	C
8	7	1729	U
8	7	1730	C
8	7	1731	G
8	7	1738	G
8	7	1754	A
8	7	1755	A
8	7	1756	G
8	7	1764	C
8	7	1773	A
8	7	1784	A
8	7	1786	A
8	7	1791	A
8	7	1799	G
8	7	1800	C
8	7	1801	A
8	7	1807	G
8	7	1808	A
8	7	1811	G
8	7	1816	C
8	7	1848	A
8	7	1870	C
8	7	1872	A
8	7	1873	G
8	7	1901	A
8	7	1906	G
8	7	1907	G
8	7	1929	G
8	7	1930	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	1940	U
8	7	1954	G
8	7	1955	U
8	7	1960	A
8	7	1966	A
8	7	1967	C
8	7	1970	A
8	7	1971	U
8	7	1972	G
8	7	1975	G
8	7	1982	U
8	7	1991	U
8	7	1992	G
8	7	1993	U
8	7	1997	C
8	7	2016	U
8	7	2021	C
8	7	2022	U
8	7	2023	C
8	7	2030	6MZ
8	7	2031	A
8	7	2032	G
8	7	2033	A
8	7	2043	C
8	7	2055	C
8	7	2056	G
8	7	2060	A
8	7	2061	G
8	7	2062	A
8	7	2069	G7M
8	7	2072	C
8	7	2093	G
8	7	2101	A
8	7	2102	G
8	7	2110	G
8	7	2111	U
8	7	2112	G
8	7	2114	A
8	7	2117	A
8	7	2118	U
8	7	2120	G
8	7	2121	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	2123	G
8	7	2124	G
8	7	2126	A
8	7	2130	U
8	7	2131	U
8	7	2132	U
8	7	2133	G
8	7	2134	A
8	7	2136	G
8	7	2137	U
8	7	2139	U
8	7	2140	G
8	7	2141	G
8	7	2146	C
8	7	2148	G
8	7	2149	U
8	7	2153	C
8	7	2154	A
8	7	2156	G
8	7	2161	C
8	7	2162	G
8	7	2163	A
8	7	2164	C
8	7	2165	C
8	7	2166	U
8	7	2170	A
8	7	2171	A
8	7	2172	U
8	7	2173	A
8	7	2176	A
8	7	2177	C
8	7	2178	C
8	7	2182	U
8	7	2190	G
8	7	2198	A
8	7	2204	G
8	7	2211	A
8	7	2212	A
8	7	2214	C
8	7	2225	A
8	7	2238	G
8	7	2239	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	2243	U
8	7	2251	OMG
8	7	2268	A
8	7	2278	A
8	7	2279	G
8	7	2283	C
8	7	2287	A
8	7	2305	U
8	7	2308	G
8	7	2309	A
8	7	2311	A
8	7	2312	U
8	7	2319	G
8	7	2321	U
8	7	2322	A
8	7	2325	G
8	7	2333	A
8	7	2335	A
8	7	2336	A
8	7	2345	G
8	7	2347	C
8	7	2350	C
8	7	2361	G
8	7	2372	U
8	7	2375	G
8	7	2379	G
8	7	2383	G
8	7	2385	C
8	7	2391	G
8	7	2402	U
8	7	2403	C
8	7	2406	A
8	7	2410	G
8	7	2423	U
8	7	2425	A
8	7	2429	G
8	7	2430	A
8	7	2431	U
8	7	2441	U
8	7	2447	G
8	7	2448	A
8	7	2464	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	2475	C
8	7	2476	A
8	7	2478	A
8	7	2482	A
8	7	2484	G
8	7	2492	U
8	7	2494	G
8	7	2498	OMC
8	7	2502	G
8	7	2503	2MA
8	7	2504	PSU
8	7	2505	G
8	7	2506	U
8	7	2518	A
8	7	2529	G
8	7	2535	G
8	7	2537	U
8	7	2547	A
8	7	2554	U
8	7	2555	U
8	7	2566	A
8	7	2567	G
8	7	2572	A
8	7	2573	C
8	7	2581	G
8	7	2582	G
8	7	2602	A
8	7	2603	G
8	7	2609	U
8	7	2613	U
8	7	2614	A
8	7	2615	U
8	7	2629	U
8	7	2630	G
8	7	2663	G
8	7	2689	U
8	7	2690	U
8	7	2711	A
8	7	2713	U
8	7	2714	G
8	7	2716	C
8	7	2718	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	2726	A
8	7	2732	G
8	7	2733	A
8	7	2739	U
8	7	2743	U
8	7	2744	G
8	7	2748	A
8	7	2751	G
8	7	2757	A
8	7	2765	A
8	7	2778	A
8	7	2779	U
8	7	2798	U
8	7	2800	A
8	7	2818	U
8	7	2820	A
8	7	2821	A
8	7	2832	U
8	7	2835	A
8	7	2849	U
8	7	2850	A
8	7	2858	C
8	7	2861	U
8	7	2867	G
8	7	2870	C
8	7	2873	A
8	7	2879	A
8	7	2880	C
8	7	2883	A
8	7	2884	U
8	7	2885	G
8	7	2886	A
8	7	2891	U
9	8	4	C
9	8	9	G
9	8	15	A
9	8	16	G
9	8	35	C
9	8	50	A
9	8	51	G
9	8	66	A
9	8	67	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	8	89	U
9	8	90	C
9	8	91	C
9	8	99	A
9	8	109	A
10	A	3	A
10	A	4	U
10	A	5	U
10	A	7	A
10	A	9	G
10	A	22	G
10	A	32	A
10	A	33	A
10	A	39	G
10	A	47	C
10	A	48	C
10	A	49	U
10	A	50	A
10	A	51	A
10	A	52	C
10	A	60	A
10	A	65	A
10	A	71	A
10	A	72	A
10	A	75	G
10	A	78	A
10	A	79	G
10	A	82	G
10	A	83	C
10	A	84	U
10	A	85	U
10	A	86	G
10	A	87	C
10	A	88	U
10	A	91	U
10	A	92	U
10	A	95	C
10	A	131	A
10	A	134	G
10	A	137	U
10	A	141	G
10	A	143	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	144	G
10	A	163	C
10	A	171	A
10	A	174	A
10	A	182	A
10	A	183	C
10	A	184	G
10	A	192	A
10	A	193	C
10	A	197	A
10	A	204	G
10	A	208	U
10	A	209	U
10	A	210	C
10	A	215	C
10	A	226	G
10	A	245	U
10	A	247	G
10	A	250	A
10	A	251	G
10	A	252	U
10	A	266	G
10	A	267	C
10	A	281	G
10	A	289	G
10	A	300	A
10	A	305	G
10	A	315	A
10	A	316	C
10	A	322	C
10	A	323	U
10	A	325	A
10	A	327	A
10	A	328	C
10	A	329	A
10	A	330	C
10	A	331	G
10	A	345	C
10	A	347	G
10	A	348	G
10	A	351	G
10	A	352	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	354	G
10	A	367	U
10	A	372	C
10	A	398	U
10	A	406	G
10	A	411	A
10	A	412	A
10	A	413	G
10	A	421	U
10	A	424	G
10	A	429	U
10	A	458	U
10	A	459	A
10	A	460	A
10	A	462	G
10	A	463	U
10	A	465	A
10	A	467	U
10	A	468	A
10	A	469	C
10	A	479	U
10	A	484	G
10	A	485	U
10	A	486	U
10	A	499	A
10	A	509	A
10	A	511	C
10	A	518	C
10	A	523	A
10	A	527	G7M
10	A	531	U
10	A	532	A
10	A	533	A
10	A	535	A
10	A	547	A
10	A	559	A
10	A	562	U
10	A	572	A
10	A	573	A
10	A	575	G
10	A	576	C
10	A	577	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	633	G
10	A	653	U
10	A	665	A
10	A	703	G
10	A	718	A
10	A	723	U
10	A	724	G
10	A	734	G
10	A	748	G
10	A	755	G
10	A	777	A
10	A	793	U
10	A	794	A
10	A	815	A
10	A	817	C
10	A	821	G
10	A	828	U
10	A	829	G
10	A	841	C
10	A	842	U
10	A	843	U
10	A	844	G
10	A	845	A
10	A	846	G
10	A	902	G
10	A	914	A
10	A	926	G
10	A	933	G
10	A	934	C
10	A	935	A
10	A	960	U
10	A	961	U
10	A	969	A
10	A	971	G
10	A	975	A
10	A	976	G
10	A	977	A
10	A	983	A
10	A	993	G
10	A	994	A
10	A	1004	A
10	A	1008	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1016	A
10	A	1020	G
10	A	1024	G
10	A	1026	G
10	A	1028	C
10	A	1029	U
10	A	1031	C
10	A	1032	G
10	A	1033	G
10	A	1034	G
10	A	1035	A
10	A	1044	A
10	A	1045	C
10	A	1065	U
10	A	1085	U
10	A	1094	G
10	A	1095	U
10	A	1101	A
10	A	1124	G
10	A	1125	U
10	A	1133	G
10	A	1135	U
10	A	1136	C
10	A	1137	C
10	A	1138	G
10	A	1139	G
10	A	1140	C
10	A	1141	C
10	A	1152	A
10	A	1154	G
10	A	1158	C
10	A	1159	U
10	A	1168	U
10	A	1169	A
10	A	1182	G
10	A	1183	U
10	A	1184	G
10	A	1191	A
10	A	1196	A
10	A	1197	A
10	A	1200	C
10	A	1201	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1202	U
10	A	1212	U
10	A	1213	A
10	A	1227	A
10	A	1228	C
10	A	1238	A
10	A	1239	A
10	A	1258	G
10	A	1260	G
10	A	1280	A
10	A	1282	C
10	A	1286	U
10	A	1287	A
10	A	1300	G
10	A	1302	C
10	A	1305	G
10	A	1317	C
10	A	1320	C
10	A	1336	C
10	A	1346	A
10	A	1347	G
10	A	1363	A
10	A	1368	A
10	A	1370	G
10	A	1429	A
10	A	1432	G
10	A	1433	A
10	A	1441	A
10	A	1446	A
10	A	1448	C
10	A	1454	G
10	A	1487	G
10	A	1492	A
10	A	1499	A
10	A	1503	A
10	A	1506	U
10	A	1507	A
10	A	1517	G
10	A	1529	G
10	A	1530	G
10	A	1537	U
10	A	1538	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1539	C
10	A	1542	A
31	V	6	A
31	V	8	A
31	V	9	A
31	V	10	G
31	V	11	G
31	V	14	G
31	V	15	G
31	V	17	G
31	V	18	A
31	V	21	U
31	V	28	C
31	V	29	A
31	V	30	A
31	V	33	A
32	W	2	C
32	W	4	C
32	W	8	4SU
32	W	11	C
32	W	15	G
32	W	16	H2U
32	W	17	H2U
32	W	18	G
32	W	19	G
32	W	20	H2U
32	W	22	G
32	W	35	A
32	W	37	MIA
32	W	44	G
32	W	46	G7M
32	W	47	U
32	W	48	C
32	W	49	C
32	W	52	G
32	W	54	5MU
32	W	58	A
32	W	72	C
32	W	74	C
32	W	76	A
33	X	2	G
33	X	3	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	X	7	G
33	X	8	4SU
33	X	9	G
33	X	13	G
33	X	16	A
33	X	17	G
33	X	18	G
33	X	19	C
33	X	20	H2U
33	X	21	G
33	X	22	A
33	X	34	U
33	X	38	12A
33	X	46	A
33	X	47	U
33	X	64	U
33	X	65	C
33	X	66	C
33	X	75	A
33	X	77	U
33	X	82	G
33	X	89	C
33	X	90	G
33	X	93	A
34	Y	7	4SU
34	Y	8	U
34	Y	10	G
34	Y	11	C
34	Y	16	C
34	Y	17	U
34	Y	18	G
34	Y	19	G
34	Y	20	G
34	Y	46	7MG
34	Y	47	U
34	Y	48	C
34	Y	49	G
34	Y	53	G
34	Y	56	C
34	Y	57	G
34	Y	58	A
34	Y	59	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	Y	60	C
34	Y	61	C
34	Y	62	C
34	Y	64	U
34	Y	65	C
34	Y	73	A
34	Y	74	C
34	Y	75	C

All (92) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	43	G
8	7	120	U
8	7	134	G
8	7	158	U
8	7	177	G
8	7	277	G
8	7	285	G
8	7	352	A
8	7	404	A
8	7	474	G
8	7	613	A
8	7	748	G
8	7	784	G
8	7	827	U
8	7	829	A
8	7	830	G
8	7	989	G
8	7	1020	A
8	7	1046	A
8	7	1060	U
8	7	1128	G
8	7	1133	A
8	7	1266	G
8	7	1344	U
8	7	1416	G
8	7	1419	A
8	7	1475	G
8	7	1490	A
8	7	1580	A
8	7	1602	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	1647	U
8	7	1713	A
8	7	1714	U
8	7	1755	A
8	7	1847	A
8	7	1939	5MU
8	7	2031	A
8	7	2110	G
8	7	2136	G
8	7	2138	G
8	7	2139	U
8	7	2148	G
8	7	2162	G
8	7	2163	A
8	7	2176	A
8	7	2177	C
8	7	2210	U
8	7	2211	A
8	7	2430	A
8	7	2474	U
8	7	2491	U
8	7	2506	U
8	7	2581	G
8	7	2710	C
8	7	2756	U
9	8	3	C
10	A	48	C
10	A	84	U
10	A	85	U
10	A	181	A
10	A	251	G
10	A	315	A
10	A	351	G
10	A	428	G
10	A	457	G
10	A	522	C
10	A	845	A
10	A	1027	C
10	A	1124	G
10	A	1137	C
10	A	1190	G
10	A	1201	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1281	C
10	A	1345	U
10	A	1397	C
10	A	1432	G
31	V	8	A
31	V	28	C
31	V	32	U
32	W	10	G
32	W	43	C
33	X	2	G
33	X	19	C
33	X	21	G
33	X	46	A
34	Y	7	4SU
34	Y	10	G
34	Y	18	G
34	Y	47	U
34	Y	57	G
34	Y	59	U
34	Y	64	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

55 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	$\# Z > 2$
33	12A	X	38	10,33	33,36,37	4.19	18 (54%)	47,52,55	3.08	16 (34%)
10	MA6	A	1519	10	23,26,27	0.27	0	34,38,41	0.63	1 (2%)
8	3TD	7	1915	8	19,22,23	0.83	1 (5%)	21,32,35	0.59	0
10	G7M	A	527	10	23,26,27	0.71	1 (4%)	35,39,42	0.56	0
10	2MG	A	1516	10	23,26,27	0.35	0	32,38,41	0.38	0
32	MIA	W	37	32	28,31,32	2.44	5 (17%)	40,44,47	2.78	12 (30%)
10	PSU	A	516	10,63	18,21,22	0.89	1 (5%)	22,30,33	1.14	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	4SU	Y	7	34	18,21,22	0.37	0	26,30,33	1.35	3 (11%)
8	H2U	7	2449	8	18,21,22	4.41	14 (77%)	21,30,33	2.21	5 (23%)
10	5MC	A	1407	10	18,22,23	0.33	0	26,32,35	0.58	0
32	PSU	W	55	32	18,21,22	0.90	1 (5%)	22,30,33	0.70	0
8	6MZ	7	1618	8	22,25,26	0.32	0	30,36,39	0.61	0
32	H2U	W	17	32	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
32	5MU	W	54	32	19,22,23	0.25	0	28,32,35	0.37	0
8	5MU	7	747	8	19,22,23	0.23	0	28,32,35	0.33	0
8	2MG	7	2445	8	23,26,27	0.34	0	32,38,41	0.39	0
8	1MG	7	745	8	22,26,27	0.52	0	33,39,42	0.57	0
8	5MC	7	1962	8	18,22,23	0.33	0	26,32,35	0.52	0
8	G7M	7	2069	8	23,26,27	0.69	1 (4%)	35,39,42	0.63	0
8	2MA	7	2503	8	22,25,26	0.83	1 (4%)	33,37,40	1.13	4 (12%)
8	PSU	7	2605	8	18,21,22	0.86	1 (5%)	22,30,33	0.54	0
34	7MG	Y	46	34	22,26,27	3.88	10 (45%)	29,39,42	2.08	9 (31%)
8	PSU	7	746	8,63	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
32	PSU	W	32	32	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
8	2MG	7	1835	8	23,26,27	0.35	0	32,38,41	0.41	0
33	RSP	X	33	33	17,21,22	4.18	7 (41%)	22,30,33	0.72	0
8	5MU	7	1939	8,63	19,22,23	0.27	0	28,32,35	0.40	0
33	PSU	X	72	33	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
32	4SU	W	8	32	18,21,22	3.79	7 (38%)	26,30,33	2.23	5 (19%)
32	G7M	W	46	32	23,26,27	2.85	8 (34%)	35,39,42	1.94	8 (22%)
34	PSU	Y	55	34	18,21,22	0.88	1 (5%)	22,30,33	0.58	0
33	4SU	X	8	33	18,21,22	3.81	7 (38%)	26,30,33	2.26	4 (15%)
10	4OC	A	1402	10	20,23,24	0.38	0	26,32,35	0.41	0
33	5MU	X	71	33	19,22,23	0.25	0	28,32,35	0.27	0
10	UR3	A	1498	10	19,22,23	0.30	0	26,32,35	0.67	0
10	MA6	A	1518	10	23,26,27	0.26	0	34,38,41	0.67	1 (2%)
8	PSU	7	2504	8	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
32	PSU	W	39	32	18,21,22	4.65	8 (44%)	22,30,33	1.89	5 (22%)
8	OMU	7	2552	8	19,22,23	0.21	0	26,31,34	0.50	0
8	PSU	7	2604	8	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
8	PSU	7	955	8	18,21,22	0.86	1 (5%)	22,30,33	0.59	0
10	5MC	A	967	10	18,22,23	4.04	7 (38%)	26,32,35	1.01	2 (7%)
10	2MG	A	966	10	23,26,27	3.10	8 (34%)	32,38,41	2.53	12 (37%)
33	H2U	X	20	33	18,21,22	3.07	5 (27%)	21,30,33	2.05	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PSU	7	2457	8	18,21,22	0.85	1 (5%)	22,30,33	0.78	1 (4%)
8	PSU	7	2580	8	18,21,22	0.85	1 (5%)	22,30,33	0.97	1 (4%)
34	CM0	Y	34	34	23,26,27	1.11	1 (4%)	27,37,40	0.56	0
8	6MZ	7	2030	8	22,25,26	0.37	0	30,36,39	0.74	1 (3%)
32	H2U	W	16	32	18,21,22	3.08	5 (27%)	21,30,33	2.03	5 (23%)
34	6MZ	Y	37	34	22,25,26	0.28	0	30,36,39	0.43	0
34	5MU	Y	54	34	19,22,23	0.24	0	28,32,35	0.21	0
32	H2U	W	20	32	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
8	OMG	7	2251	8,32	23,26,27	0.30	0	33,38,41	0.39	0
10	2MG	A	1207	10	23,26,27	0.34	0	32,38,41	0.62	1 (3%)
8	OMC	7	2498	8,63	19,22,23	0.30	0	26,31,34	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	12A	X	38	10,33	-	9/25/43/44	0/3/3/3
10	MA6	A	1519	10	-	4/11/29/30	0/3/3/3
8	3TD	7	1915	8	-	0/7/25/26	0/2/2/2
10	G7M	A	527	10	-	2/7/25/26	0/3/3/3
10	2MG	A	1516	10	-	1/9/27/28	0/3/3/3
32	MIA	W	37	32	-	4/15/33/34	0/3/3/3
10	PSU	A	516	10,63	-	0/7/25/26	0/2/2/2
34	4SU	Y	7	34	-	0/7/25/26	0/2/2/2
8	H2U	7	2449	8	-	0/7/38/39	0/2/2/2
10	5MC	A	1407	10	-	0/7/25/26	0/2/2/2
32	PSU	W	55	32	-	0/7/25/26	0/2/2/2
8	6MZ	7	1618	8	-	2/9/27/28	0/3/3/3
32	H2U	W	17	32	-	6/7/38/39	0/2/2/2
32	5MU	W	54	32	-	4/7/25/26	0/2/2/2
8	5MU	7	747	8	-	0/7/25/26	0/2/2/2
8	2MG	7	2445	8	-	2/9/27/28	0/3/3/3
8	1MG	7	745	8	-	0/7/25/26	0/3/3/3
8	5MC	7	1962	8	-	4/7/25/26	0/2/2/2
8	G7M	7	2069	8	-	1/7/25/26	0/3/3/3
8	2MA	7	2503	8	-	2/7/25/26	0/3/3/3
8	PSU	7	2605	8	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	7MG	Y	46	34	-	1/7/37/38	0/3/3/3
8	PSU	7	746	8,63	-	6/7/25/26	0/2/2/2
32	PSU	W	32	32	-	0/7/25/26	0/2/2/2
8	2MG	7	1835	8	-	1/9/27/28	0/3/3/3
33	RSP	X	33	33	-	1/7/25/26	0/2/2/2
8	5MU	7	1939	8,63	-	0/7/25/26	0/2/2/2
33	PSU	X	72	33	-	0/7/25/26	0/2/2/2
32	4SU	W	8	32	-	2/7/25/26	0/2/2/2
32	G7M	W	46	32	-	5/7/25/26	0/3/3/3
34	PSU	Y	55	34	-	4/7/25/26	0/2/2/2
33	4SU	X	8	33	-	2/7/25/26	0/2/2/2
10	4OC	A	1402	10	-	0/9/29/30	0/2/2/2
33	5MU	X	71	33	-	0/7/25/26	0/2/2/2
10	UR3	A	1498	10	-	2/7/25/26	0/2/2/2
10	MA6	A	1518	10	-	0/11/29/30	0/3/3/3
8	PSU	7	2504	8	-	0/7/25/26	0/2/2/2
32	PSU	W	39	32	-	0/7/25/26	0/2/2/2
8	OMU	7	2552	8	-	0/9/27/28	0/2/2/2
8	PSU	7	2604	8	-	0/7/25/26	0/2/2/2
8	PSU	7	955	8	-	0/7/25/26	0/2/2/2
10	5MC	A	967	10	-	0/7/25/26	0/2/2/2
10	2MG	A	966	10	-	0/9/27/28	0/3/3/3
33	H2U	X	20	33	-	5/7/38/39	0/2/2/2
8	PSU	7	2457	8	-	0/7/25/26	0/2/2/2
8	PSU	7	2580	8	-	0/7/25/26	0/2/2/2
34	CM0	Y	34	34	-	2/12/30/31	0/2/2/2
8	6MZ	7	2030	8	-	1/9/27/28	0/3/3/3
32	H2U	W	16	32	-	1/7/38/39	0/2/2/2
34	6MZ	Y	37	34	-	0/9/27/28	0/3/3/3
34	5MU	Y	54	34	-	0/7/25/26	0/2/2/2
32	H2U	W	20	32	-	3/7/38/39	0/2/2/2
8	OMG	7	2251	8,32	-	3/9/27/28	0/3/3/3
10	2MG	A	1207	10	-	0/9/27/28	0/3/3/3
8	OMC	7	2498	8,63	-	2/9/27/28	0/2/2/2

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	38	12A	C2-S2	14.59	1.88	1.75
32	W	32	PSU	C6-C5	12.17	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	39	PSU	C6-C5	12.14	1.49	1.35
33	X	33	RSP	C2-N3	11.88	1.49	1.36
33	X	38	12A	C2'-C3'	-10.51	1.24	1.53
8	7	2449	H2U	C2'-C3'	-10.35	1.25	1.53
10	A	967	5MC	C6-C5	9.89	1.50	1.34
34	Y	46	7MG	C8-N9	9.86	1.51	1.46
33	X	20	H2U	C2-N1	9.61	1.49	1.35
32	W	39	PSU	C2-N1	9.55	1.49	1.36
32	W	32	PSU	C2-N1	9.54	1.49	1.36
32	W	20	H2U	C2-N1	9.47	1.49	1.35
32	W	16	H2U	C2-N1	9.45	1.49	1.35
32	W	17	H2U	C2-N1	9.41	1.49	1.35
8	7	2449	H2U	C2-N1	9.25	1.48	1.35
33	X	8	4SU	C4-N3	8.95	1.47	1.37
32	W	8	4SU	C4-N3	8.84	1.47	1.37
32	W	32	PSU	C2-N3	8.26	1.51	1.37
32	W	39	PSU	C2-N3	8.23	1.51	1.37
10	A	966	2MG	C2-N3	8.19	1.47	1.31
32	W	37	MIA	C6-N6	8.10	1.47	1.34
34	Y	46	7MG	C5-N7	7.85	1.44	1.35
32	W	37	MIA	C2-S10	7.82	1.82	1.75
33	X	38	12A	O3'-C3'	7.75	1.61	1.43
10	A	967	5MC	C4-N3	7.48	1.46	1.34
10	A	966	2MG	C4-N3	6.95	1.50	1.34
10	A	967	5MC	C2-N3	6.95	1.50	1.36
32	W	8	4SU	C2-N3	6.95	1.50	1.38
33	X	33	RSP	C6-C5	6.91	1.51	1.35
33	X	8	4SU	C2-N3	6.89	1.50	1.38
32	W	46	G7M	C4-N3	6.77	1.50	1.34
33	X	33	RSP	C4-N4	6.67	1.49	1.33
32	W	46	G7M	C2-N2	6.57	1.49	1.34
32	W	17	H2U	C2-N3	6.53	1.49	1.38
32	W	16	H2U	C2-N3	6.51	1.49	1.38
32	W	20	H2U	C2-N3	6.51	1.49	1.38
10	A	966	2MG	C2-N2	6.44	1.47	1.33
33	X	20	H2U	C2-N3	6.40	1.49	1.38
8	7	2449	H2U	C2-N3	6.29	1.49	1.38
33	X	8	4SU	C4-S4	-6.10	1.56	1.68
32	W	8	4SU	C4-S4	-6.01	1.57	1.68
34	Y	46	7MG	C2-N3	5.92	1.47	1.33
34	Y	46	7MG	C4-N9	5.90	1.44	1.37
33	X	8	4SU	C2-N1	5.89	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	46	G7M	C2-N3	5.87	1.47	1.33
32	W	32	PSU	C6-N1	5.86	1.46	1.36
32	W	8	4SU	C6-C5	5.80	1.48	1.35
32	W	39	PSU	C6-N1	5.78	1.45	1.36
33	X	8	4SU	C6-C5	5.77	1.48	1.35
32	W	8	4SU	C2-N1	5.77	1.47	1.38
33	X	38	12A	CC-N	5.75	1.48	1.35
10	A	967	5MC	C4-N4	5.71	1.49	1.34
34	Y	46	7MG	C4-N3	5.57	1.47	1.34
10	A	967	5MC	C6-N1	5.55	1.47	1.38
10	A	966	2MG	C2-N1	5.35	1.45	1.36
33	X	33	RSP	C4-N3	5.31	1.45	1.34
32	W	17	H2U	C4-N3	4.99	1.46	1.37
32	W	20	H2U	C4-N3	4.98	1.46	1.37
32	W	16	H2U	C4-N3	4.94	1.46	1.37
33	X	38	12A	O4'-C1'	-4.78	1.30	1.42
34	Y	46	7MG	C2-N2	4.77	1.45	1.34
33	X	20	H2U	C4-N3	4.72	1.45	1.37
8	7	2449	H2U	C4-N3	4.71	1.45	1.37
34	Y	34	CM0	C6-C5	4.66	1.39	1.34
33	X	38	12A	C3'-C4'	4.60	1.64	1.53
8	7	2449	H2U	O4'-C1'	-4.58	1.31	1.42
10	A	967	5MC	C2-N1	4.57	1.49	1.40
32	W	32	PSU	C4-N3	4.39	1.47	1.38
32	W	39	PSU	C4-N3	4.37	1.46	1.38
32	W	46	G7M	C5-N7	-4.31	1.34	1.39
33	X	38	12A	C2'-C1'	4.16	1.66	1.53
32	W	46	G7M	C5-C6	3.93	1.54	1.43
34	Y	46	7MG	C2-N1	3.80	1.47	1.37
33	X	33	RSP	C5-C4	3.60	1.51	1.42
34	Y	46	7MG	C5-C6	3.54	1.52	1.43
32	W	8	4SU	C5-C4	3.51	1.47	1.42
32	W	55	PSU	C6-C5	3.51	1.39	1.35
33	X	8	4SU	C5-C4	3.45	1.47	1.42
32	W	8	4SU	C6-N1	3.44	1.46	1.38
34	Y	55	PSU	C6-C5	3.43	1.39	1.35
33	X	8	4SU	C6-N1	3.42	1.46	1.38
8	7	1915	3TD	C6-C5	3.39	1.39	1.35
34	Y	46	7MG	C6-N1	3.37	1.45	1.38
33	X	72	PSU	C6-C5	3.37	1.39	1.35
8	7	746	PSU	C6-C5	3.35	1.39	1.35
8	7	2449	H2U	C5'-C4'	-3.35	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	2504	PSU	C6-C5	3.33	1.39	1.35
8	7	955	PSU	C6-C5	3.30	1.39	1.35
8	7	2605	PSU	C6-C5	3.28	1.39	1.35
8	7	2580	PSU	C6-C5	3.28	1.39	1.35
8	7	2457	PSU	C6-C5	3.27	1.39	1.35
8	7	2604	PSU	C6-C5	3.26	1.39	1.35
33	X	38	12A	O4'-C4'	3.26	1.52	1.45
33	X	33	RSP	C6-N1	3.26	1.45	1.38
33	X	38	12A	C4-N3	3.25	1.38	1.34
8	7	2449	H2U	C2'-C1'	3.24	1.63	1.53
33	X	33	RSP	C2-S2	-3.21	1.59	1.67
8	7	2449	H2U	O3'-C3'	3.19	1.50	1.43
32	W	39	PSU	O4-C4	-3.19	1.17	1.23
10	A	516	PSU	C6-C5	3.17	1.39	1.35
32	W	32	PSU	O4-C4	-3.12	1.17	1.23
33	X	38	12A	C6-N6	3.04	1.45	1.39
32	W	46	G7M	C6-N1	2.99	1.44	1.38
32	W	46	G7M	C2-N1	2.97	1.45	1.37
10	A	966	2MG	C5-C6	2.94	1.55	1.44
10	A	966	2MG	C5-N7	-2.79	1.33	1.39
32	W	37	MIA	C5-N7	-2.78	1.33	1.39
33	X	38	12A	CA-N	2.76	1.51	1.45
10	A	966	2MG	C6-N1	2.74	1.43	1.38
33	X	38	12A	CC-N6	2.70	1.43	1.37
32	W	32	PSU	C1'-C5	2.69	1.56	1.50
33	X	38	12A	C5-C4	-2.64	1.34	1.39
32	W	39	PSU	C1'-C5	2.64	1.56	1.50
8	7	2449	H2U	O2'-C2'	2.57	1.49	1.43
33	X	38	12A	C8-N9	-2.56	1.32	1.37
33	X	38	12A	O-C	2.55	1.29	1.22
32	W	39	PSU	O2-C2	-2.55	1.18	1.23
32	W	32	PSU	O2-C2	-2.54	1.18	1.23
10	A	527	G7M	C8-N7	2.53	1.37	1.33
33	X	38	12A	C5-N7	-2.51	1.34	1.39
34	Y	46	7MG	O6-C6	-2.46	1.18	1.23
33	X	20	H2U	O2-C2	-2.46	1.18	1.23
8	7	2449	H2U	O4-C4	-2.45	1.18	1.23
8	7	2069	G7M	C8-N7	2.45	1.37	1.33
32	W	46	G7M	O6-C6	-2.44	1.18	1.23
8	7	2449	H2U	O2-C2	-2.43	1.18	1.23
8	7	2503	2MA	C6-N6	-2.40	1.28	1.34
8	7	2449	H2U	C3'-C4'	2.40	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	38	12A	O2'-C2'	2.35	1.48	1.43
10	A	966	2MG	O6-C6	-2.32	1.19	1.23
8	7	2449	H2U	O4'-C4'	2.27	1.50	1.45
32	W	17	H2U	O2-C2	-2.27	1.18	1.23
33	X	38	12A	C5'-C4'	-2.27	1.44	1.51
32	W	37	MIA	C5-C4	-2.27	1.34	1.39
32	W	16	H2U	O2-C2	-2.25	1.18	1.23
10	A	967	5MC	O2-C2	-2.23	1.19	1.23
8	7	2449	H2U	C1'-N1	-2.23	1.42	1.46
33	X	20	H2U	O4-C4	-2.21	1.18	1.23
32	W	20	H2U	O2-C2	-2.20	1.19	1.23
32	W	16	H2U	O4-C4	-2.15	1.18	1.23
32	W	17	H2U	O4-C4	-2.13	1.18	1.23
32	W	20	H2U	O4-C4	-2.13	1.18	1.23
32	W	37	MIA	C8-N9	-2.05	1.33	1.37

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	37	MIA	C11-S10-C2	9.96	109.70	102.27
33	X	38	12A	C2M-S2-C2	9.30	109.21	102.27
33	X	38	12A	C5-C6-N6	8.45	141.05	118.71
33	X	8	4SU	C4-N3-C2	-7.94	119.63	127.34
32	W	8	4SU	C4-N3-C2	-7.83	119.74	127.34
8	7	2449	H2U	C4-N3-C2	-7.64	119.46	125.79
33	X	38	12A	C5-C4-N3	-7.25	119.03	127.19
32	W	37	MIA	C5-C4-N3	-7.23	119.06	127.19
32	W	16	H2U	C4-N3-C2	-7.15	119.86	125.79
32	W	17	H2U	C4-N3-C2	-6.95	120.03	125.79
32	W	20	H2U	C4-N3-C2	-6.95	120.03	125.79
10	A	966	2MG	C2-N3-C4	6.91	120.61	112.04
33	X	20	H2U	C4-N3-C2	-6.71	120.22	125.79
33	X	38	12A	N6-C6-N1	-5.88	98.72	118.44
33	X	8	4SU	C5-C4-N3	5.86	120.13	114.69
33	X	38	12A	C4-C5-C6	5.86	121.35	116.81
10	A	966	2MG	C5-C4-N3	-5.65	119.30	128.46
32	W	8	4SU	C5-C4-N3	5.48	119.78	114.69
32	W	37	MIA	C4-C5-C6	5.39	120.98	116.81
33	X	38	12A	N3-C4-N9	5.25	134.28	126.99
34	Y	46	7MG	C5-C6-N1	5.00	119.81	110.99
32	W	46	G7M	C2-N3-C4	4.97	121.15	112.30
10	A	966	2MG	C1'-N9-C4	-4.91	111.92	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	966	2MG	C1'-N9-C8	4.80	140.35	126.70
32	W	46	G7M	C5-C4-N3	-4.72	119.09	128.15
32	W	37	MIA	N3-C4-N9	4.72	133.53	126.99
32	W	39	PSU	C4-N3-C2	-4.64	119.65	126.34
10	A	966	2MG	C2-N1-C6	-4.61	119.17	124.48
33	X	38	12A	N6-CC-N	4.57	120.14	113.76
34	Y	46	7MG	C2-N3-C4	4.54	120.38	112.30
32	W	32	PSU	C4-N3-C2	-4.47	119.90	126.34
34	Y	7	4SU	C4-N3-C2	-4.41	123.06	127.34
34	Y	46	7MG	C5-C4-N3	-4.24	120.06	128.13
32	W	39	PSU	N1-C2-N3	4.22	119.91	115.13
32	W	46	G7M	C5-C6-N1	4.15	120.45	111.79
32	W	32	PSU	N1-C2-N3	4.08	119.75	115.13
33	X	38	12A	N9-C8-N7	-4.07	108.34	113.91
32	W	46	G7M	N9-C4-N3	3.93	133.84	125.94
32	W	37	MIA	N9-C8-N7	-3.87	108.62	113.91
32	W	8	4SU	N3-C2-N1	3.82	119.97	114.89
33	X	8	4SU	N3-C2-N1	3.67	119.77	114.89
33	X	20	H2U	N3-C2-N1	3.64	120.50	116.65
32	W	37	MIA	C12-C13-C14	-3.62	120.09	127.14
33	X	8	4SU	C5-C4-S4	-3.61	119.82	124.47
33	X	38	12A	OO-CC-N6	-3.55	117.62	123.62
10	A	966	2MG	N9-C4-N3	3.48	132.93	125.94
32	W	37	MIA	N3-C2-N1	-3.48	120.57	126.95
32	W	8	4SU	C5-C4-S4	-3.45	120.03	124.47
32	W	46	G7M	O6-C6-C5	-3.42	120.35	128.06
32	W	39	PSU	C6-C5-C4	3.38	120.56	118.20
10	A	967	5MC	C5-C6-N1	-3.33	119.92	123.34
8	7	2580	PSU	C3'-C2'-C1'	3.29	105.46	101.64
32	W	16	H2U	N3-C2-N1	3.25	120.09	116.65
8	7	2449	H2U	C5-C4-N3	3.25	120.30	116.65
34	Y	46	7MG	C4-C5-N7	3.23	110.01	105.53
32	W	46	G7M	C2-N1-C6	-3.19	119.28	125.10
33	X	38	12A	CA-N-CC	3.18	127.23	121.94
8	7	2449	H2U	N3-C2-N1	3.17	120.01	116.65
32	W	17	H2U	N3-C2-N1	3.16	120.00	116.65
32	W	20	H2U	N3-C2-N1	3.13	119.97	116.65
32	W	32	PSU	C6-C5-C4	3.08	120.36	118.20
10	A	516	PSU	C4-N3-C2	-3.05	121.94	126.34
32	W	37	MIA	C5-N7-C8	3.04	107.83	103.51
33	X	38	12A	O3'-C3'-C4'	3.03	119.80	111.05
10	A	1518	MA6	C2-N1-C6	2.96	118.74	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	37	MIA	S10-C2-N3	2.94	126.19	116.01
33	X	20	H2U	C5-C6-N1	2.93	121.26	111.61
34	Y	46	7MG	N9-C4-N3	2.91	129.82	125.47
32	W	32	PSU	C6-N1-C2	-2.91	119.71	122.68
34	Y	46	7MG	C5-C4-N9	2.91	110.12	106.35
10	A	1519	MA6	C2-N1-C6	2.90	118.60	111.75
32	W	37	MIA	C2-N3-C4	2.89	119.95	112.35
34	Y	46	7MG	C2-N1-C6	-2.88	119.85	125.10
34	Y	7	4SU	C5-C4-N3	2.87	117.35	114.69
32	W	39	PSU	C6-N1-C2	-2.84	119.78	122.68
32	W	16	H2U	C5-C4-N3	2.83	119.83	116.65
34	Y	46	7MG	O6-C6-C5	-2.82	120.62	127.54
34	Y	7	4SU	C3'-C2'-C1'	2.80	106.74	101.43
32	W	20	H2U	C5-C4-N3	2.78	119.78	116.65
10	A	966	2MG	C5-C6-N1	2.77	120.23	113.19
32	W	17	H2U	C5-C4-N3	2.74	119.72	116.65
32	W	46	G7M	CN7-N7-C5	2.73	130.16	126.77
8	7	2503	2MA	C5-C4-N3	-2.72	124.13	127.19
33	X	38	12A	C5-N7-C8	2.71	107.36	103.51
33	X	38	12A	N3-C2-N1	-2.70	122.00	126.95
33	X	38	12A	C6-C5-N7	-2.70	129.47	132.39
8	7	2503	2MA	C2-N1-C6	2.70	122.29	118.08
8	7	2503	2MA	CM2-C2-N1	2.69	121.35	117.15
32	W	20	H2U	C5-C6-N1	2.67	120.42	111.61
10	A	966	2MG	N9-C8-N7	-2.67	108.36	113.39
32	W	17	H2U	C5-C6-N1	2.66	120.39	111.61
32	W	16	H2U	C5-C6-N1	2.62	120.25	111.61
8	7	2449	H2U	C5-C6-N1	2.61	120.23	111.61
33	X	38	12A	C2-N3-C4	2.59	119.17	112.35
33	X	20	H2U	C5-C4-N3	2.59	119.56	116.65
10	A	966	2MG	O6-C6-C5	-2.57	119.79	126.60
32	W	39	PSU	O2-C2-N1	-2.53	120.01	122.79
32	W	32	PSU	O2-C2-N1	-2.51	120.03	122.79
33	X	38	12A	C4-N9-C8	2.49	108.42	105.73
32	W	16	H2U	O2-C2-N1	-2.46	120.02	123.11
10	A	966	2MG	N1-C2-N3	-2.45	120.16	123.95
34	Y	46	7MG	N9-C8-N7	2.41	106.83	103.38
32	W	37	MIA	C16-C14-C15	2.40	119.91	114.60
8	7	2449	H2U	O2-C2-N1	-2.38	120.12	123.11
8	7	2503	2MA	N3-C2-N1	-2.36	121.38	125.72
8	7	2457	PSU	C3'-C2'-C1'	2.35	104.38	101.64
8	7	2030	6MZ	C9-N6-C6	-2.34	120.86	122.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	17	H2U	O2-C2-N1	-2.29	120.23	123.11
32	W	20	H2U	O2-C2-N1	-2.24	120.29	123.11
32	W	37	MIA	N6-C6-N1	-2.22	115.67	118.50
10	A	1207	2MG	CM2-N2-C2	-2.21	118.99	123.86
10	A	516	PSU	C5-C6-N1	-2.19	118.82	122.11
10	A	967	5MC	CM5-C5-C6	-2.12	120.01	122.85
10	A	966	2MG	CM2-N2-C2	-2.11	119.19	123.86
10	A	516	PSU	N1-C2-N3	2.08	117.49	115.13
32	W	46	G7M	CN7-N7-C8	-2.07	121.64	124.84
10	A	966	2MG	C8-N7-C5	2.06	107.97	104.24
32	W	8	4SU	O2-C2-N1	-2.02	120.10	122.79

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	527	G7M	O4'-C4'-C5'-O5'
10	A	527	G7M	C3'-C4'-C5'-O5'
10	A	1516	2MG	N3-C2-N2-CM2
10	A	1519	MA6	C5-C6-N6-C10
8	7	746	PSU	C2'-C1'-C5-C4
8	7	746	PSU	C2'-C1'-C5-C6
8	7	2251	OMG	C1'-C2'-O2'-CM2
32	W	17	H2U	O4'-C1'-N1-C6
32	W	17	H2U	C2'-C1'-N1-C2
32	W	17	H2U	C2'-C1'-N1-C6
32	W	37	MIA	O4'-C4'-C5'-O5'
32	W	37	MIA	C3'-C4'-C5'-O5'
32	W	37	MIA	N1-C2-S10-C11
32	W	37	MIA	N3-C2-S10-C11
33	X	8	4SU	C3'-C4'-C5'-O5'
33	X	8	4SU	O4'-C4'-C5'-O5'
33	X	20	H2U	C4'-C5'-O5'-P
33	X	20	H2U	O4'-C4'-C5'-O5'
33	X	20	H2U	C3'-C4'-C5'-O5'
33	X	20	H2U	O4'-C1'-N1-C6
33	X	38	12A	C3'-C4'-C5'-O5'
33	X	38	12A	N1-C2-S2-C2M
33	X	38	12A	N3-C2-S2-C2M
33	X	38	12A	CB-CA-N-CC
33	X	38	12A	N-CA-CB-OG1
33	X	38	12A	N-CA-CB-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	X	38	12A	C-CA-CB-OG1
33	X	38	12A	C-CA-CB-CG2
34	Y	34	CM0	O5-C7-C8-O8
34	Y	55	PSU	C2'-C1'-C5-C4
34	Y	34	CM0	O5-C7-C8-O9
8	7	2498	OMC	C3'-C4'-C5'-O5'
8	7	2498	OMC	O4'-C4'-C5'-O5'
32	W	8	4SU	O4'-C4'-C5'-O5'
33	X	38	12A	O4'-C4'-C5'-O5'
33	X	20	H2U	O4'-C1'-N1-C2
10	A	1498	UR3	O4'-C4'-C5'-O5'
8	7	2251	OMG	O4'-C4'-C5'-O5'
8	7	2445	2MG	C3'-C4'-C5'-O5'
32	W	8	4SU	C3'-C4'-C5'-O5'
10	A	1498	UR3	C3'-C4'-C5'-O5'
8	7	1618	6MZ	O4'-C4'-C5'-O5'
8	7	2251	OMG	C3'-C4'-C5'-O5'
32	W	46	G7M	C2'-C1'-N9-C4
10	A	1519	MA6	C5-C6-N6-C9
8	7	2030	6MZ	O4'-C4'-C5'-O5'
8	7	2445	2MG	O4'-C4'-C5'-O5'
10	A	1519	MA6	N1-C6-N6-C10
32	W	17	H2U	C4'-C5'-O5'-P
32	W	46	G7M	C4'-C5'-O5'-P
34	Y	46	7MG	C4'-C5'-O5'-P
8	7	1618	6MZ	C3'-C4'-C5'-O5'
32	W	46	G7M	O4'-C4'-C5'-O5'
32	W	46	G7M	C2'-C1'-N9-C8
32	W	54	5MU	C4'-C5'-O5'-P
32	W	17	H2U	O4'-C1'-N1-C2
32	W	54	5MU	C3'-C4'-C5'-O5'
32	W	16	H2U	C4'-C5'-O5'-P
8	7	746	PSU	O4'-C1'-C5-C4
34	Y	55	PSU	O4'-C1'-C5-C4
8	7	1962	5MC	O4'-C1'-N1-C6
32	W	54	5MU	C2'-C1'-N1-C2
8	7	1962	5MC	C2'-C1'-N1-C6
32	W	54	5MU	C2'-C1'-N1-C6
8	7	2069	G7M	O4'-C4'-C5'-O5'
8	7	2503	2MA	O4'-C1'-N9-C4
34	Y	55	PSU	O4'-C4'-C5'-O5'
8	7	2503	2MA	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	7	1835	2MG	O4'-C4'-C5'-O5'
32	W	17	H2U	O4'-C4'-C5'-O5'
8	7	746	PSU	O4'-C1'-C5-C6
32	W	20	H2U	O4'-C1'-N1-C6
32	W	20	H2U	C2'-C1'-N1-C2
34	Y	55	PSU	O4'-C1'-C5-C6
8	7	1962	5MC	O4'-C1'-N1-C2
32	W	20	H2U	C4'-C5'-O5'-P
8	7	746	PSU	O4'-C4'-C5'-O5'
8	7	746	PSU	C3'-C4'-C5'-O5'
32	W	46	G7M	C3'-C4'-C5'-O5'
10	A	1519	MA6	O4'-C4'-C5'-O5'
33	X	33	RSP	C3'-C4'-C5'-O5'
8	7	1962	5MC	C2'-C1'-N1-C2

There are no ring outliers.

27 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	38	12A	3	0
10	A	1519	MA6	2	0
8	7	1915	3TD	1	0
32	W	37	MIA	2	0
10	A	516	PSU	1	0
34	Y	7	4SU	1	0
32	W	55	PSU	2	0
32	W	54	5MU	1	0
8	7	747	5MU	2	0
8	7	2503	2MA	1	0
33	X	33	RSP	1	0
33	X	72	PSU	1	0
34	Y	55	PSU	2	0
10	A	1402	4OC	2	0
33	X	71	5MU	1	0
10	A	1498	UR3	1	0
10	A	1518	MA6	2	0
8	7	2552	OMU	1	0
10	A	966	2MG	1	0
33	X	20	H2U	4	0
8	7	2457	PSU	1	0
34	Y	34	CM0	2	0
8	7	2030	6MZ	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	Y	37	6MZ	2	0
34	Y	54	5MU	1	0
8	7	2251	OMG	1	0
8	7	2498	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 264 ligands modelled in this entry, 262 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	ATP	7	3194	-	29,33,33	3.20	11 (37%)	44,52,52	2.20	13 (29%)
64	ATP	7	3193	-	29,33,33	3.21	12 (41%)	44,52,52	2.26	16 (36%)

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
64	ATP	7	3194	-	-	4/22/38/38	0/3/3/3
64	ATP	7	3193	-	-	6/22/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	7	3194	ATP	C2'-C3'	-10.66	1.24	1.53
64	7	3193	ATP	C2'-C3'	-10.60	1.24	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	7	3193	ATP	O4'-C4'	-6.45	1.30	1.45
64	7	3194	ATP	O4'-C4'	-6.22	1.31	1.45
64	7	3194	ATP	C3'-C4'	5.45	1.66	1.53
64	7	3193	ATP	C3'-C4'	5.39	1.66	1.53
64	7	3193	ATP	C1'-N9	-4.91	1.32	1.46
64	7	3194	ATP	C1'-N9	-4.77	1.32	1.46
64	7	3193	ATP	C6-N6	4.66	1.45	1.34
64	7	3194	ATP	C6-N6	4.65	1.45	1.34
64	7	3194	ATP	O4'-C1'	4.00	1.51	1.42
64	7	3193	ATP	O4'-C1'	4.00	1.51	1.42
64	7	3194	ATP	O2'-C2'	3.32	1.50	1.43
64	7	3193	ATP	O2'-C2'	3.30	1.50	1.43
64	7	3194	ATP	C5-C4	-2.72	1.33	1.39
64	7	3193	ATP	C5-C4	-2.71	1.33	1.39
64	7	3194	ATP	C5-N7	-2.50	1.34	1.39
64	7	3193	ATP	C5-N7	-2.49	1.34	1.39
64	7	3193	ATP	C2'-C1'	2.42	1.61	1.53
64	7	3194	ATP	C2'-C1'	2.28	1.60	1.53
64	7	3193	ATP	O3'-C3'	2.19	1.48	1.43
64	7	3194	ATP	O3'-C3'	2.19	1.48	1.43
64	7	3193	ATP	C8-N9	-2.01	1.33	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	7	3194	ATP	N3-C2-N1	-5.45	120.08	128.60
64	7	3193	ATP	N3-C2-N1	-5.41	120.14	128.60
64	7	3193	ATP	C5-C4-N3	-5.29	119.84	126.75
64	7	3194	ATP	C5-C4-N3	-5.27	119.87	126.75
64	7	3193	ATP	C1'-N9-C8	-4.62	116.69	127.14
64	7	3194	ATP	C1'-N9-C8	-4.42	117.15	127.14
64	7	3193	ATP	N9-C8-N7	-4.26	108.08	113.91
64	7	3194	ATP	N9-C8-N7	-4.17	108.20	113.91
64	7	3193	ATP	N6-C6-N1	-4.10	109.38	118.35
64	7	3194	ATP	N6-C6-N1	-4.09	109.39	118.35
64	7	3193	ATP	C4-N9-C1'	3.66	135.31	126.59
64	7	3194	ATP	C2-N3-C4	3.53	120.10	111.75
64	7	3193	ATP	C2-N3-C4	3.53	120.09	111.75
64	7	3194	ATP	C4-N9-C1'	3.53	134.99	126.59
64	7	3193	ATP	C5-C6-N6	3.23	130.46	123.43
64	7	3194	ATP	C5-C6-N6	3.20	130.39	123.43
64	7	3193	ATP	C5-N7-C8	3.13	107.96	103.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	7	3193	ATP	N3-C4-N9	3.13	132.23	127.08
64	7	3194	ATP	N3-C4-N9	3.07	132.14	127.08
64	7	3194	ATP	C5-N7-C8	3.06	107.86	103.51
64	7	3194	ATP	PB-O3B-PG	-2.66	123.71	132.83
64	7	3193	ATP	PB-O3B-PG	-2.65	123.74	132.83
64	7	3193	ATP	PA-O3A-PB	-2.64	123.77	132.83
64	7	3193	ATP	C3'-C2'-C1'	2.13	105.47	101.43
64	7	3194	ATP	PA-O3A-PB	-2.12	125.54	132.83
64	7	3193	ATP	C4-C5-N7	-2.12	108.03	110.62
64	7	3193	ATP	C4-N9-C8	2.10	108.00	105.73
64	7	3194	ATP	C4-C5-N7	-2.07	108.10	110.62
64	7	3193	ATP	C6-C5-C4	2.01	119.88	117.18

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	7	3193	ATP	C5'-O5'-PA-O1A
64	7	3194	ATP	C5'-O5'-PA-O3A
64	7	3193	ATP	C3'-C4'-C5'-O5'
64	7	3193	ATP	C5'-O5'-PA-O3A
64	7	3193	ATP	C5'-O5'-PA-O2A
64	7	3194	ATP	C5'-O5'-PA-O1A
64	7	3194	ATP	C5'-O5'-PA-O2A
64	7	3193	ATP	O4'-C4'-C5'-O5'
64	7	3193	ATP	PG-O3B-PB-O2B
64	7	3194	ATP	PG-O3B-PB-O2B

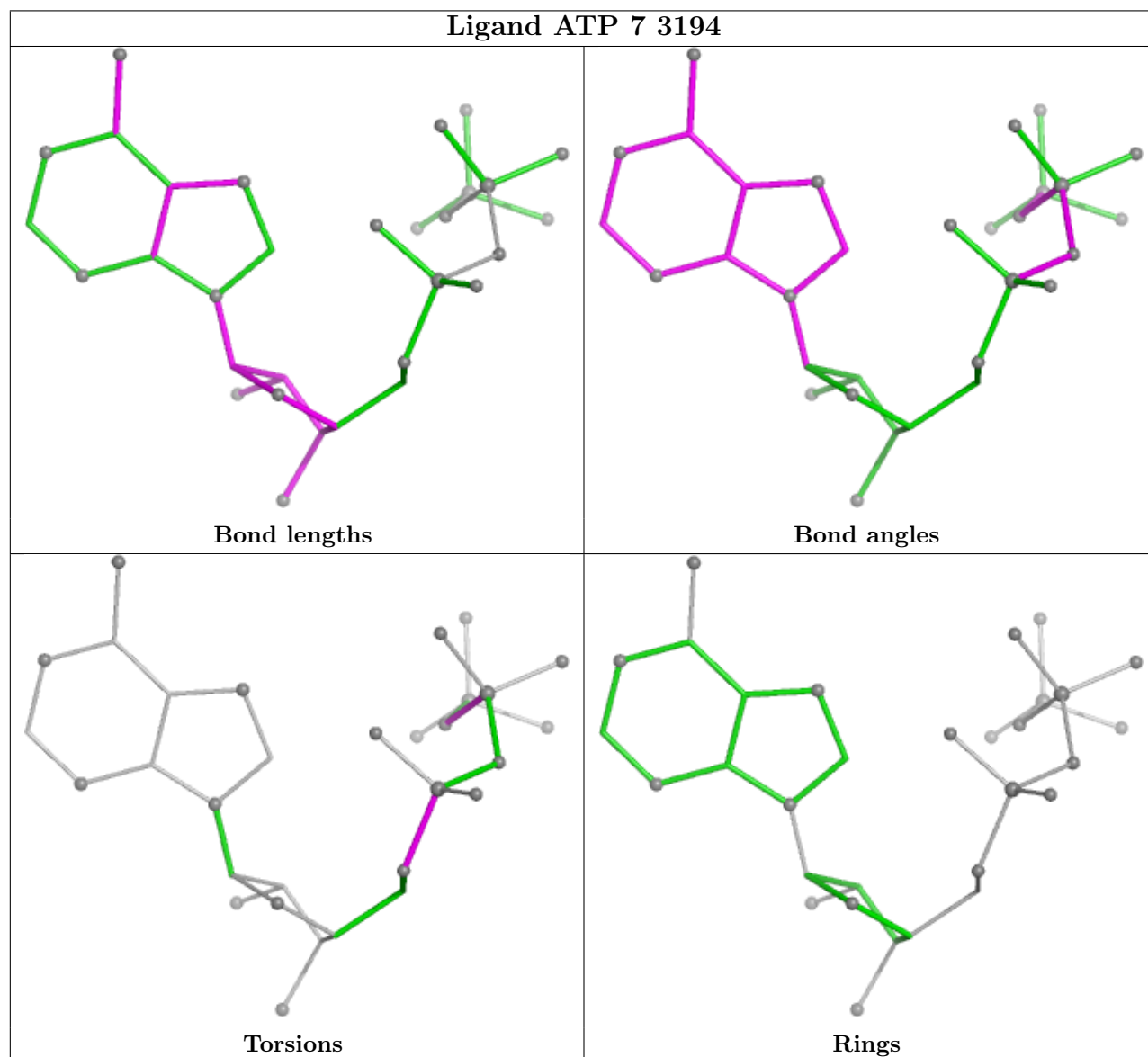
There are no ring outliers.

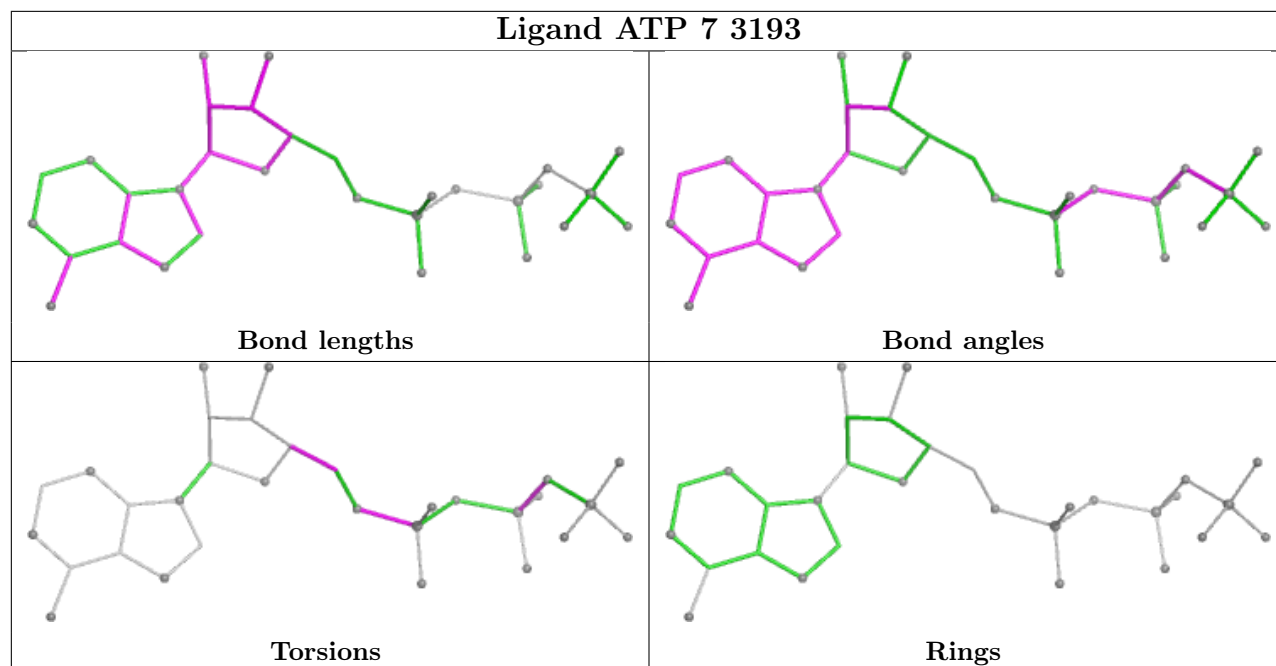
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	7	3193	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	47:U	O3'	63:A	P	17.15

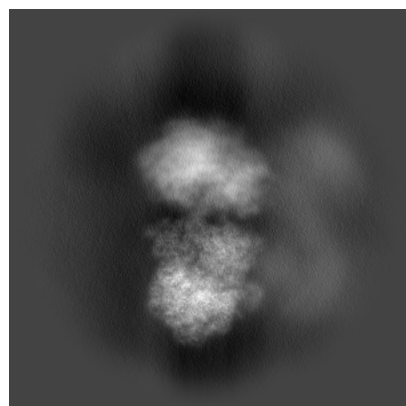
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17631. These allow visual inspection of the internal detail of the map and identification of artifacts.

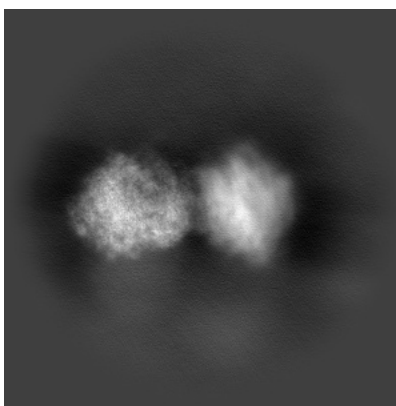
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

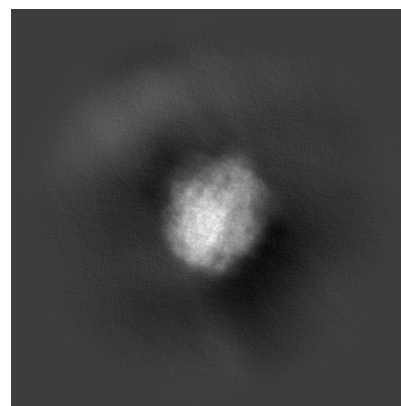
6.1.1 Primary map



X

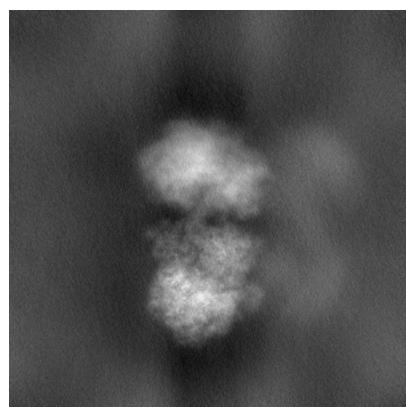


Y

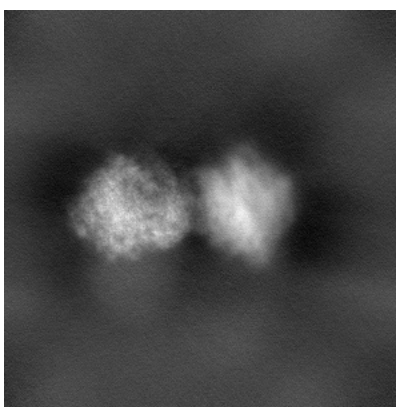


Z

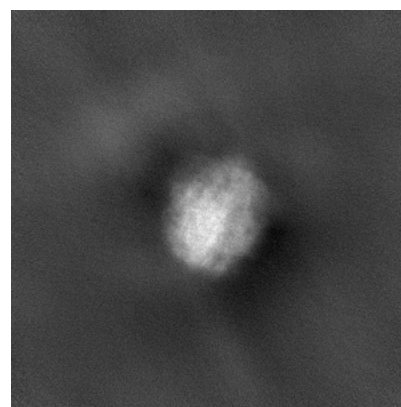
6.1.2 Raw map



X



Y

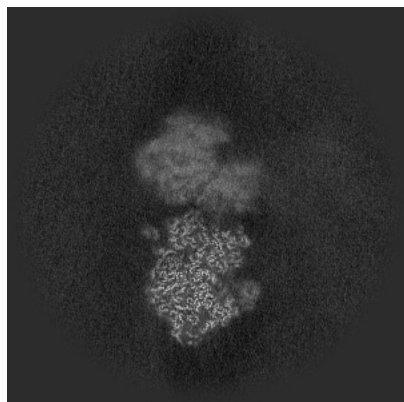


Z

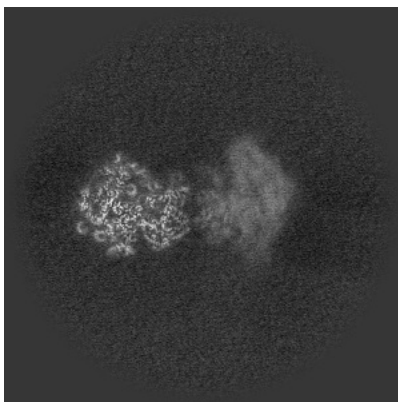
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

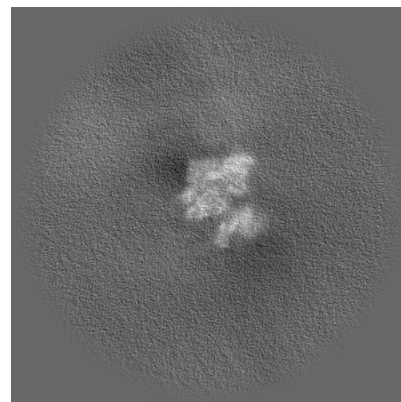
6.2.1 Primary map



X Index: 351

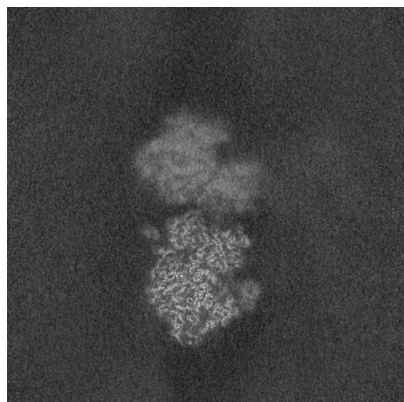


Y Index: 351

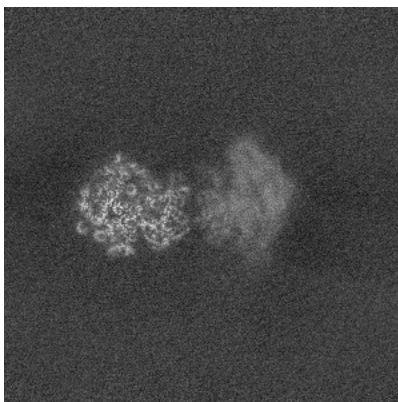


Z Index: 351

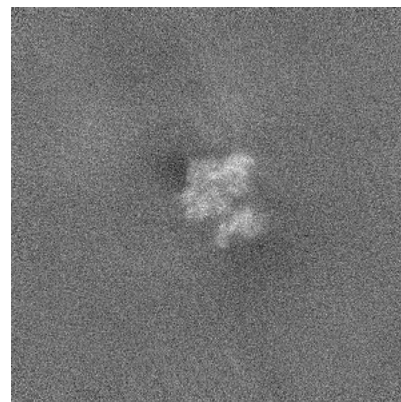
6.2.2 Raw map



X Index: 351



Y Index: 351

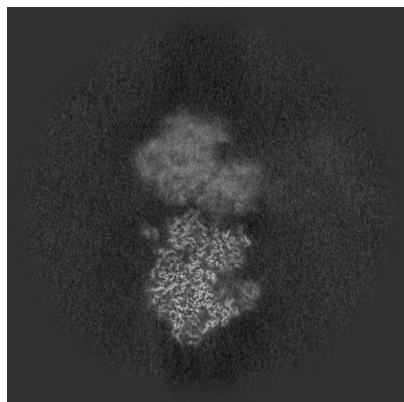


Z Index: 351

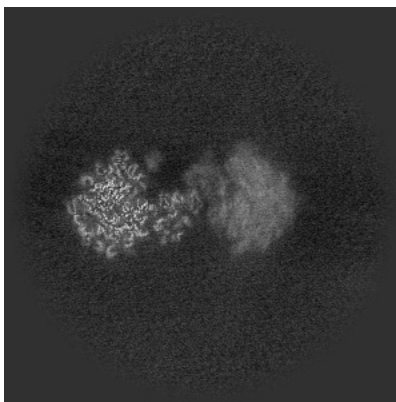
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

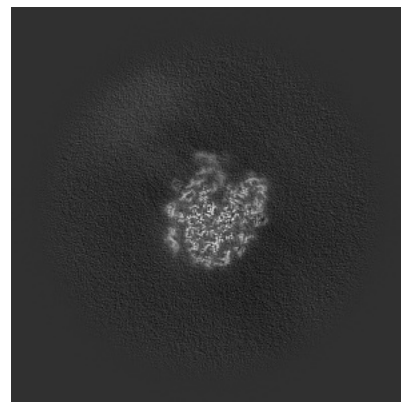
6.3.1 Primary map



X Index: 352

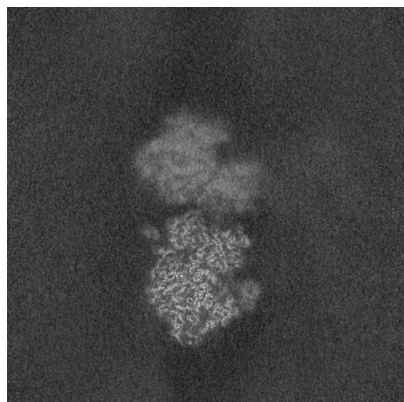


Y Index: 324

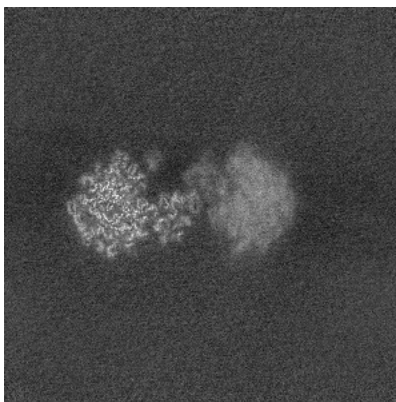


Z Index: 202

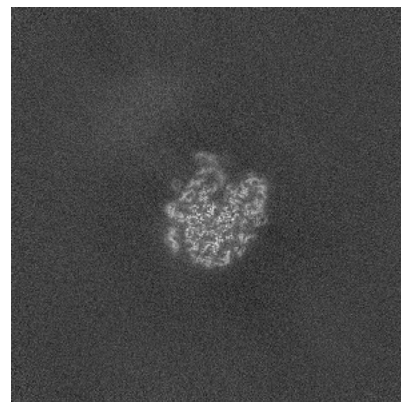
6.3.2 Raw map



X Index: 351



Y Index: 323

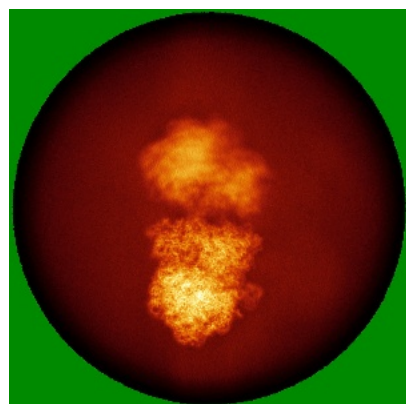


Z Index: 202

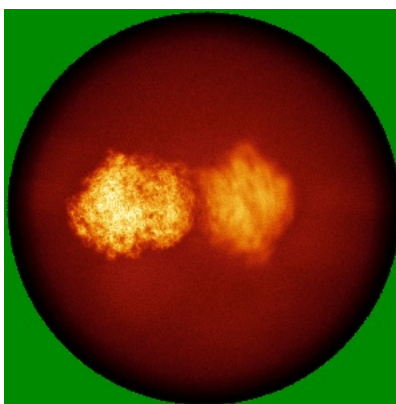
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

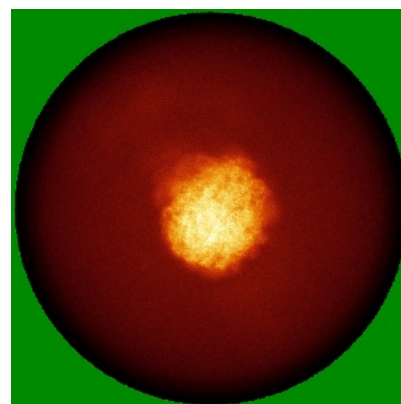
6.4.1 Primary map



X

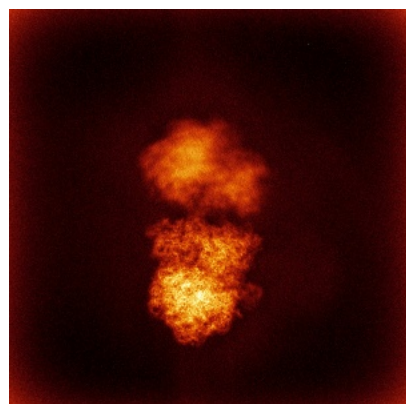


Y

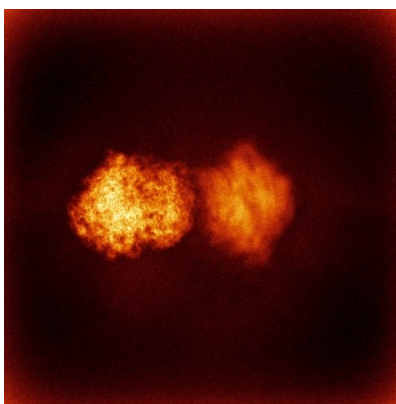


Z

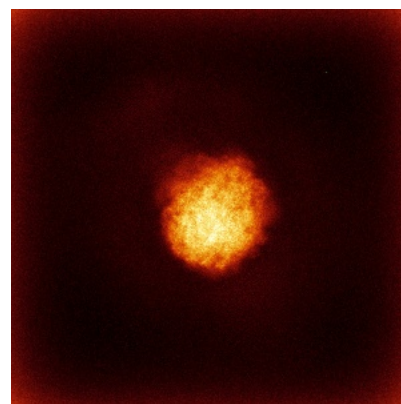
6.4.2 Raw map



X



Y

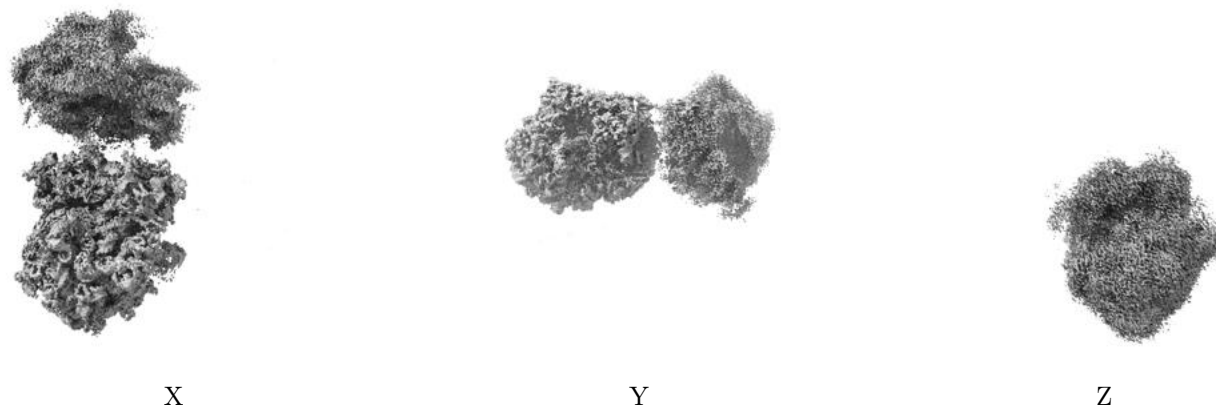


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

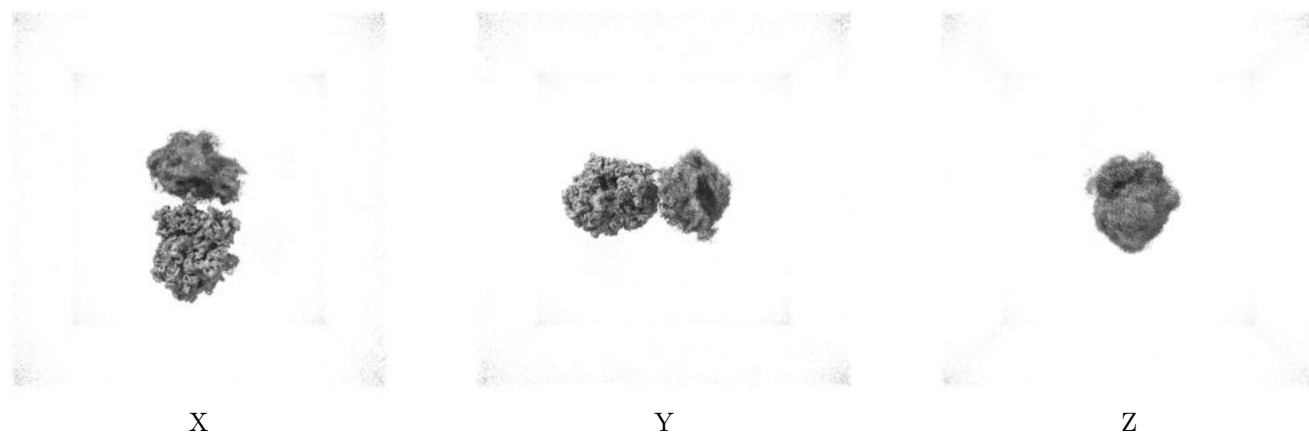
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

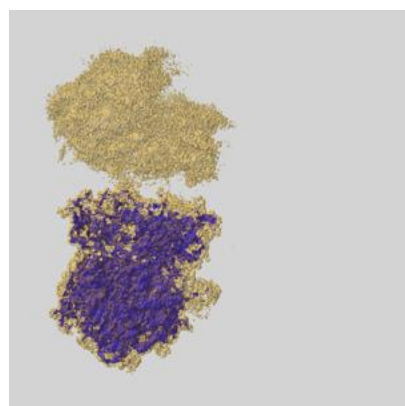
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

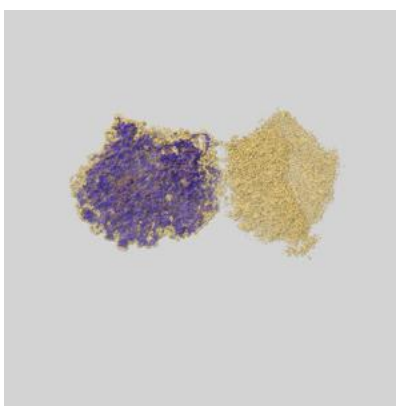
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

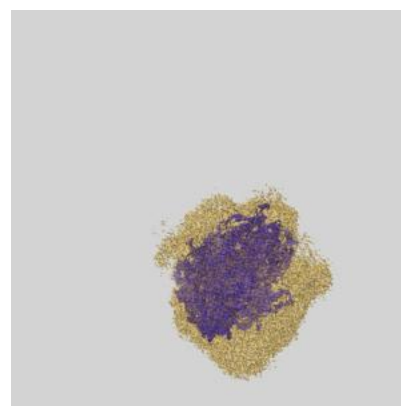
6.6.1 emd_17631_msk_1.map [i](#)



X



Y

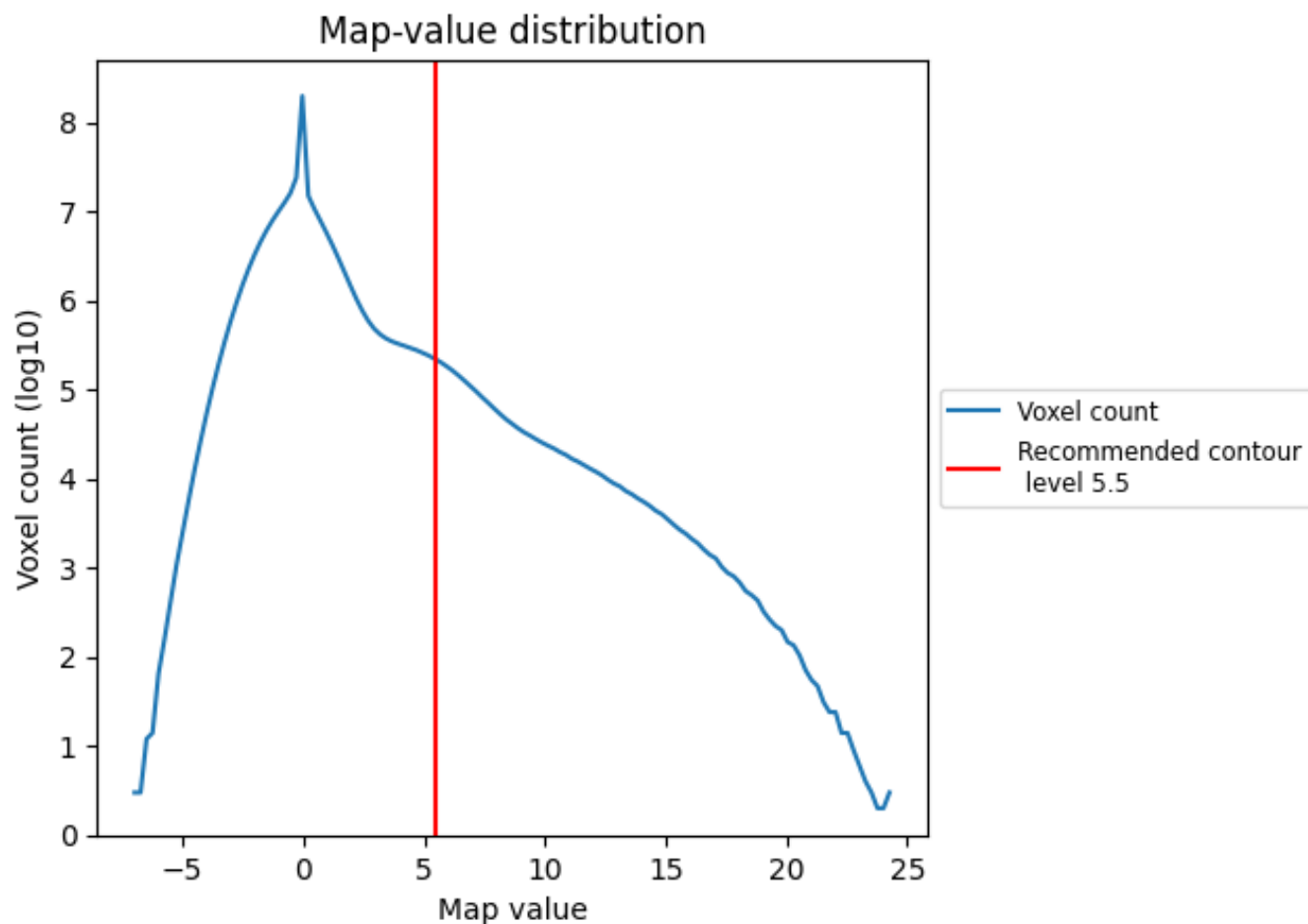


Z

7 Map analysis [i](#)

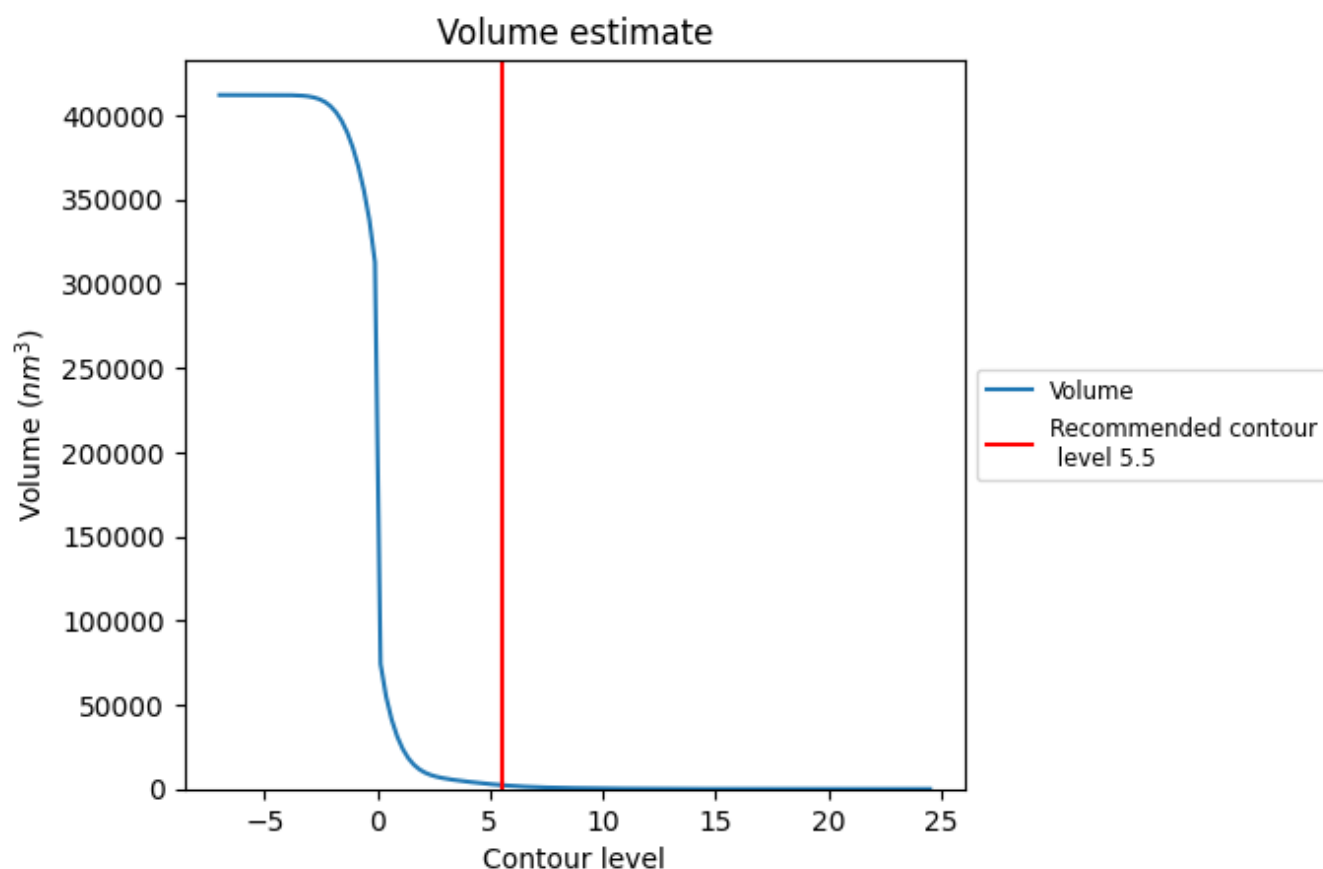
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

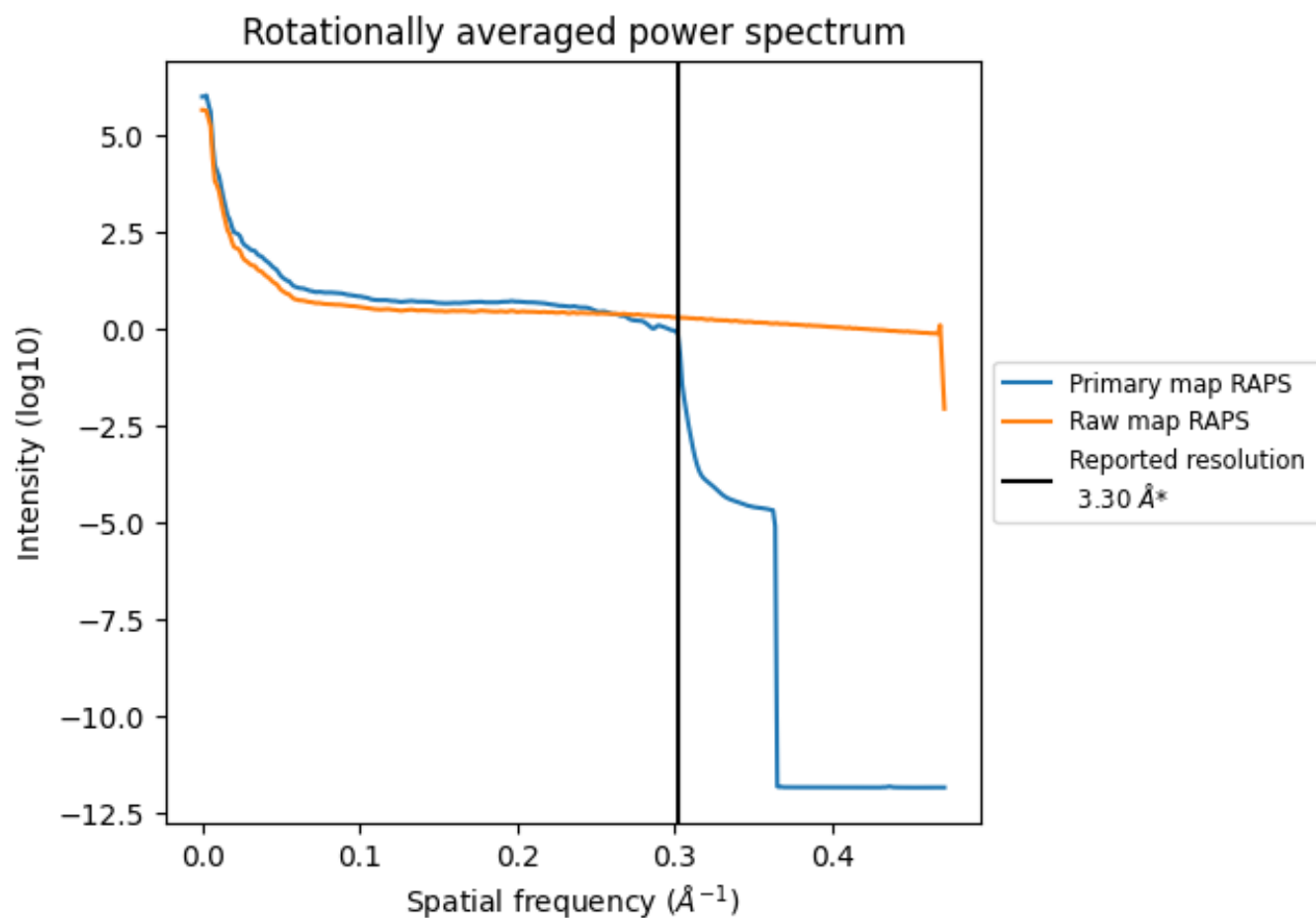
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2321 nm³; this corresponds to an approximate mass of 2097 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

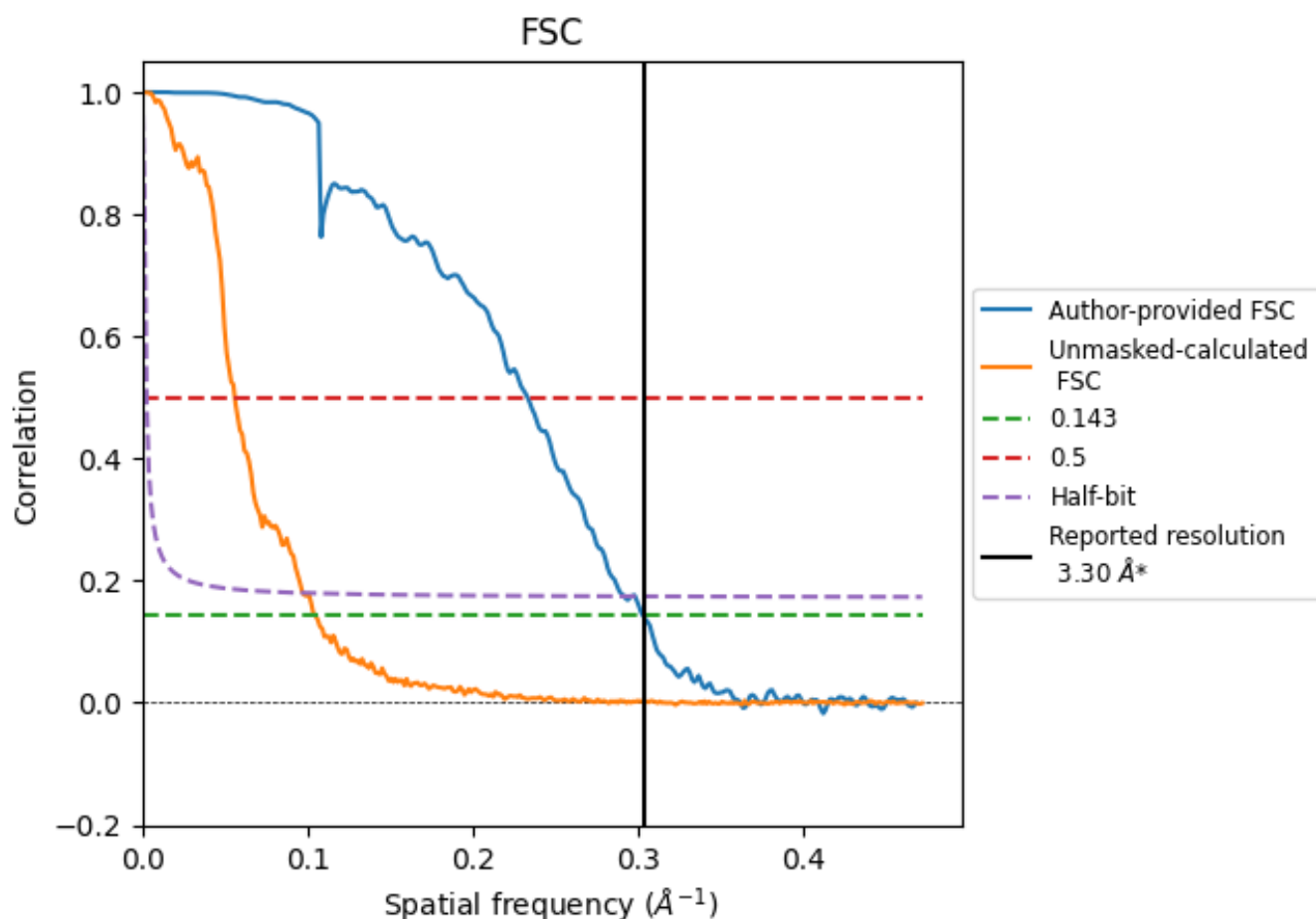


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

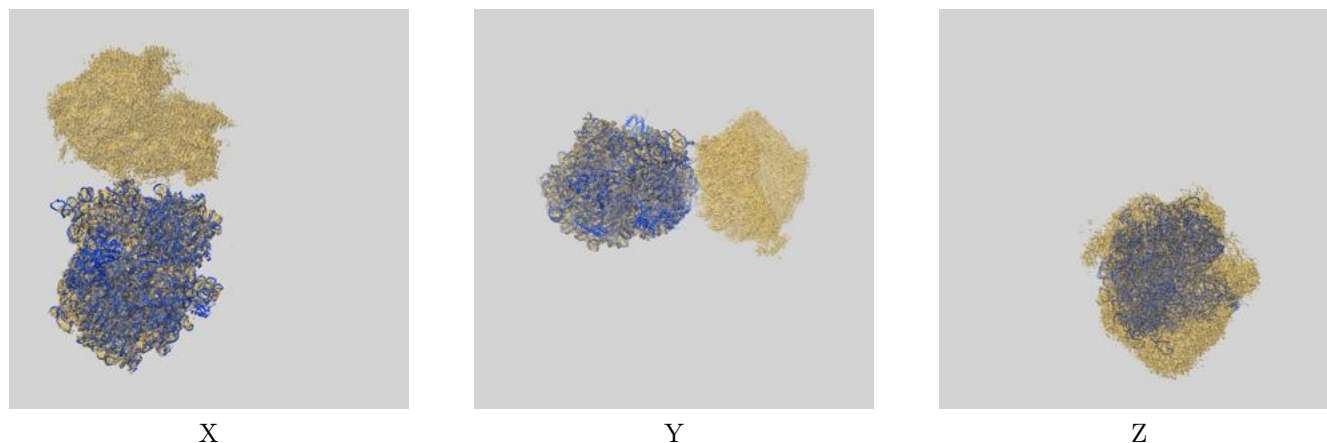
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	4.29	3.43
Unmasked-calculated*	9.55	17.86	10.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.55 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

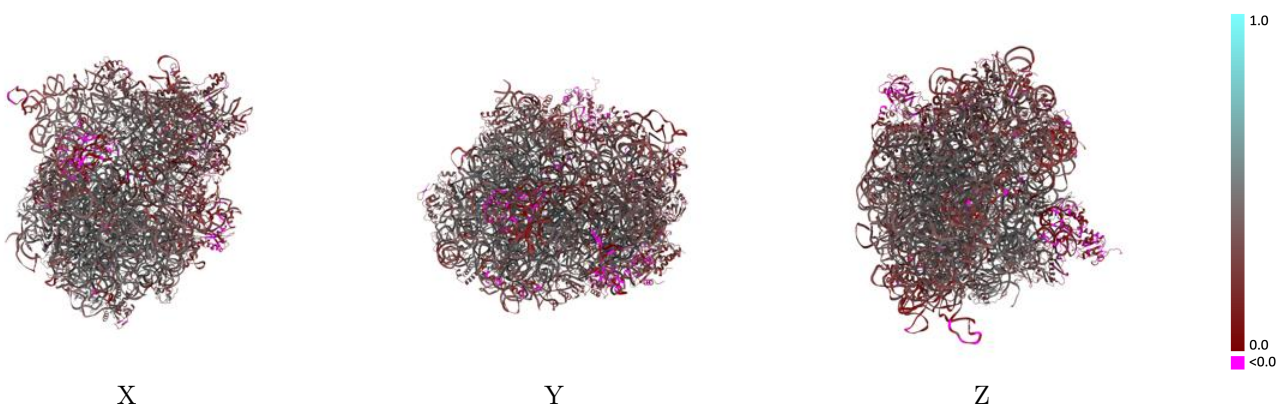
This section contains information regarding the fit between EMDB map EMD-17631 and PDB model 8PEG. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



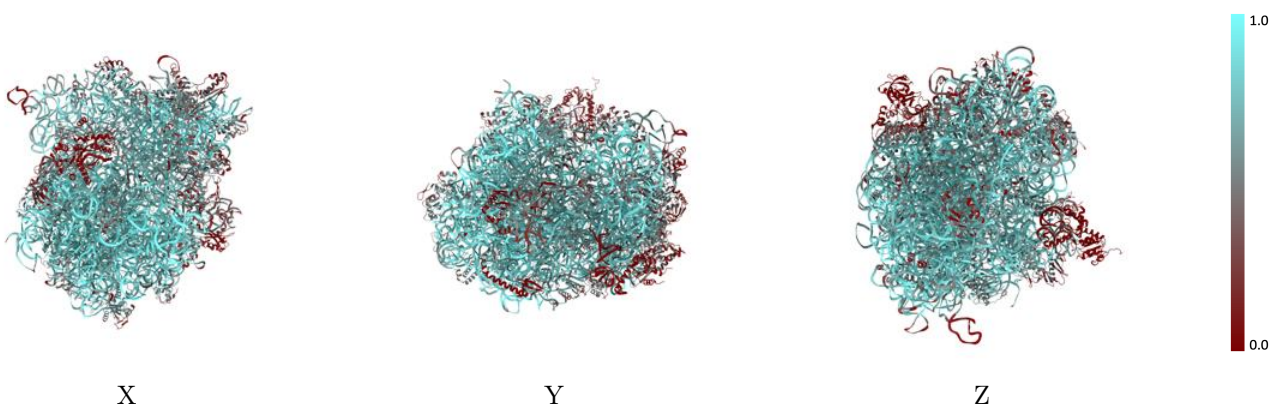
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



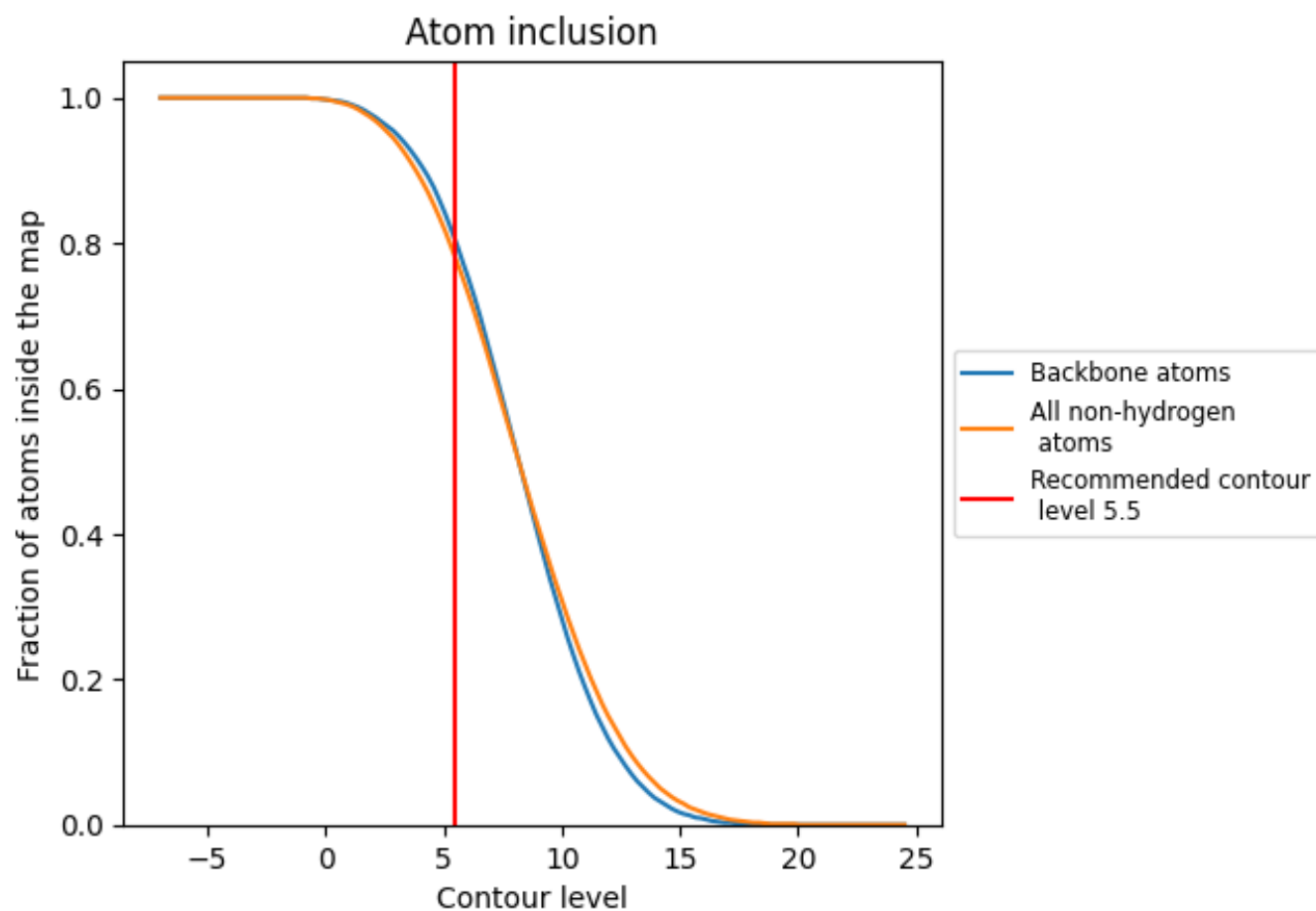
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.3630
0	 0.7610	 0.4130
1	 0.8090	 0.4020
2	 0.6320	 0.3090
3	 0.7210	 0.3630
4	 0.3780	 0.2010
5	 0.7900	 0.3470
6	 0.8290	 0.4340
7	 0.9180	 0.4110
8	 0.8780	 0.3560
A	 0.8640	 0.3640
B	 0.3460	 0.2990
C	 0.5230	 0.3260
D	 0.3700	 0.2740
E	 0.5380	 0.3610
F	 0.4930	 0.3070
G	 0.5300	 0.2790
H	 0.5780	 0.3240
I	 0.5290	 0.2840
J	 0.4160	 0.2480
K	 0.5900	 0.3500
L	 0.6450	 0.3460
M	 0.5820	 0.2860
N	 0.5870	 0.2680
O	 0.6460	 0.3180
P	 0.4820	 0.2940
Q	 0.6110	 0.3030
R	 0.5390	 0.3110
S	 0.5630	 0.3100
T	 0.6430	 0.2560
U	 0.4550	 0.2610
V	 0.4770	 0.1880
W	 0.8510	 0.3100
X	 0.4590	 0.1490
Y	 0.7860	 0.3090



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	 0.0000	 0.0600
a	 0.0440	 0.0890
b	 0.8440	 0.4280
c	 0.6940	 0.4050
d	 0.6410	 0.3650
e	 0.5680	 0.2820
f	 0.4000	 0.2980
g	 0.6710	 0.3550
h	 0.6920	 0.3990
i	 0.1790	 0.2430
j	 0.0010	 0.0690
k	 0.0000	 0.0560
l	 0.9240	 0.4250
m	 0.7660	 0.3850
n	 0.6460	 0.4050
o	 0.6890	 0.3830
p	 0.8810	 0.3740
q	 0.8200	 0.3690
r	 0.6260	 0.3100
s	 0.6730	 0.3780
t	 0.7740	 0.4070
u	 0.5970	 0.3880
v	 0.7640	 0.4130
w	 0.7300	 0.3440
x	 0.6170	 0.3450
y	 0.5380	 0.3360
z	 0.8090	 0.3960