



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 05:43 PM JST

PDB ID : 8ZFF / pdb_00008zff
EMDB ID : EMD-60059
Title : Structure of the Bacterial Ribosome without hypoxia-induced rRNA modifications
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Ito, T.; Suzuki, T.
Deposited on : 2024-05-07
Resolution : 2.59 Å(reported)
Based on initial model : 7K00

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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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

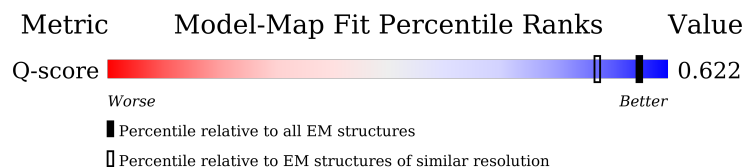
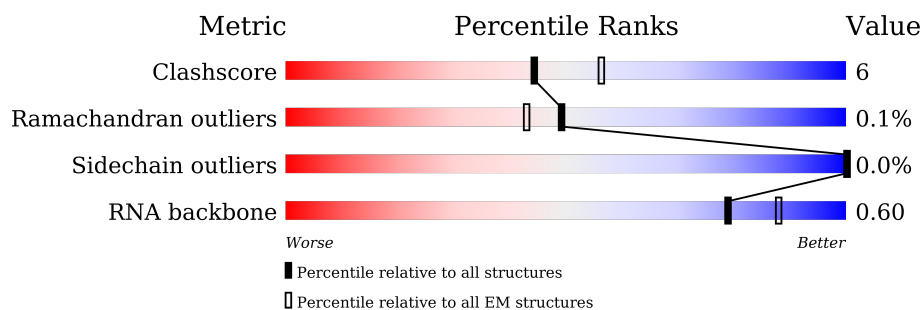
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

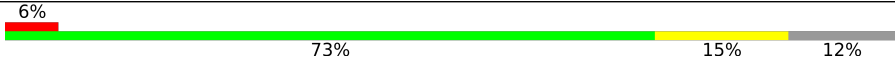
The reported resolution of this entry is 2.59 Å.

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	7741 (2.09 - 3.09)

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	A	1542	
2	B	241	
3	C	233	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	X	66	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	Z	77	8% 56% 35% 8%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 140322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0
			32466	14487	5964	10503	1512		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2761	Total	C	N	O	P	0	0
			59301	26460	10925	19155	2761		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 36 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 42 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 44 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 49 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 50 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	6	Total	C	N	O	P	0	0
			130	58	25	41	6		

- Molecule 54 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Z	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

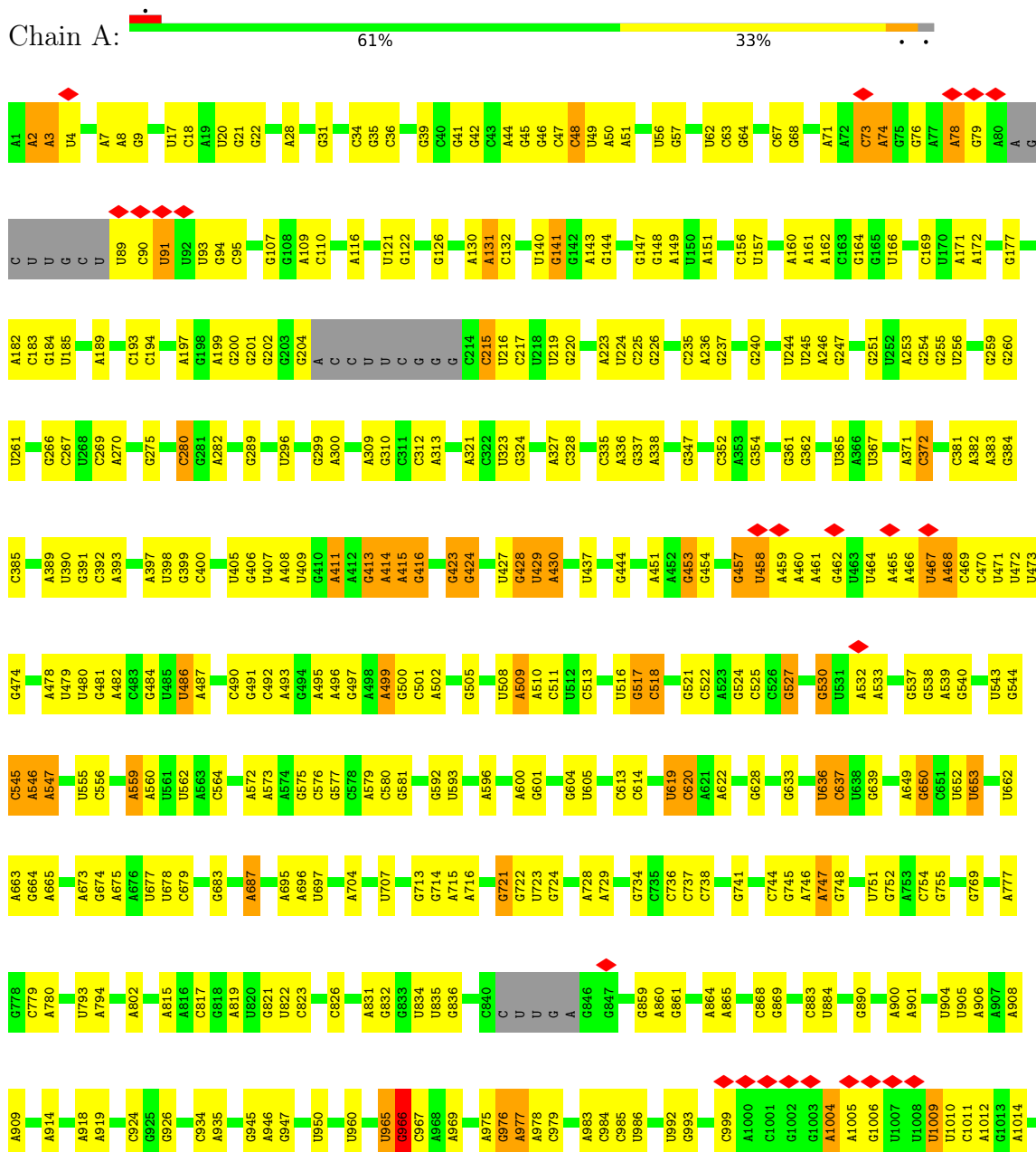
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

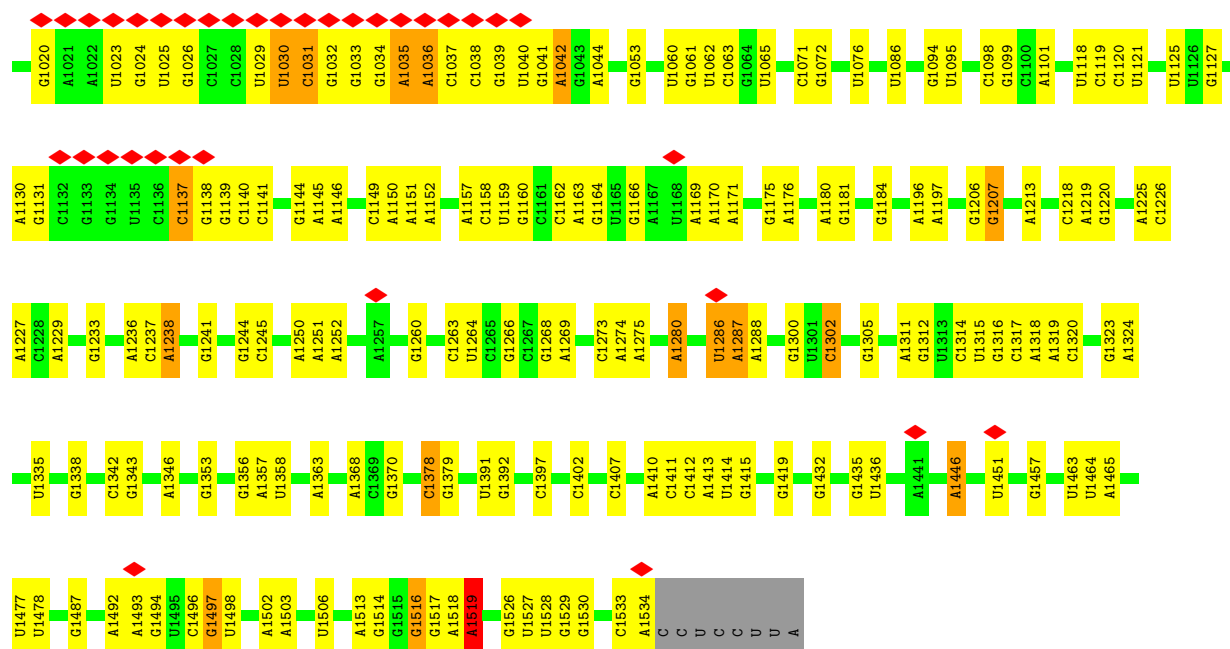
Mol	Chain	Residues	Atoms		AltConf
55	A	119	Total	Mg	0
			119	119	
55	a	328	Total	Mg	0
			328	328	
55	b	6	Total	Mg	0
			6	6	
55	c	1	Total	Mg	0
			1	1	
55	d	1	Total	Mg	0
			1	1	
55	z	1	Total	Mg	0
			1	1	
55	Z	1	Total	Mg	0
			1	1	

3 Residue-property plots

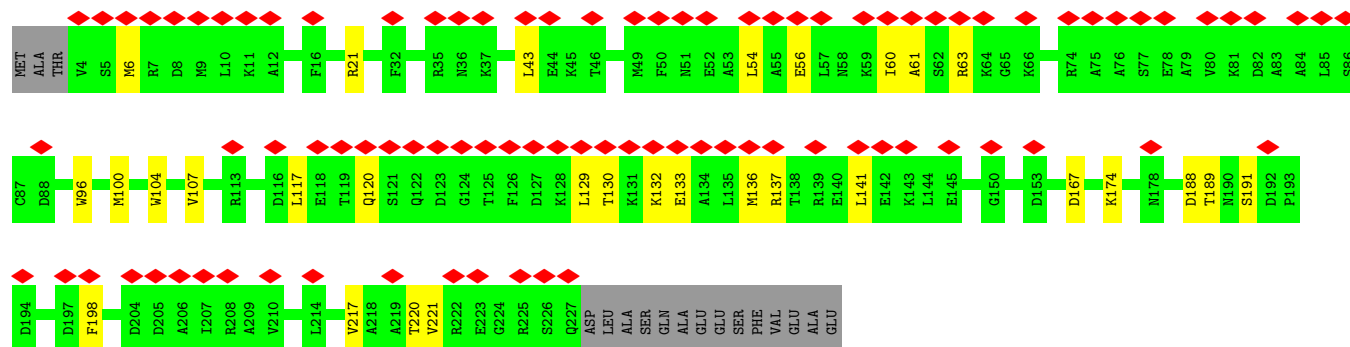
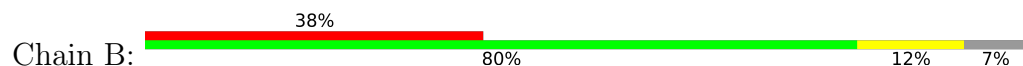
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

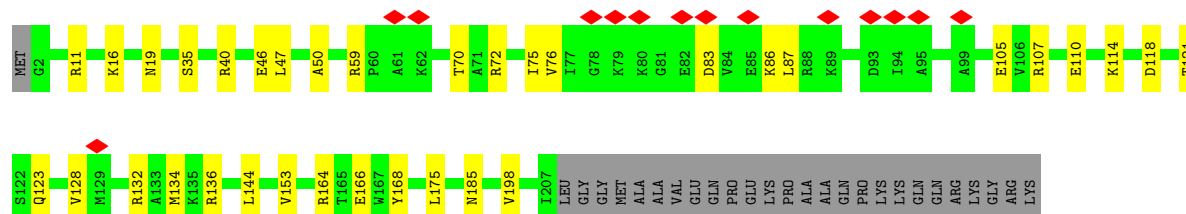
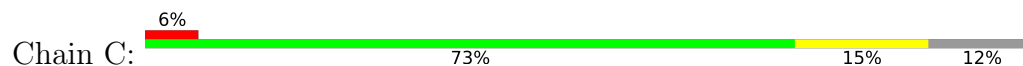




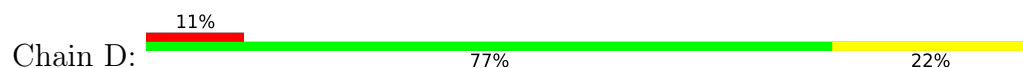
• Molecule 2: Small ribosomal subunit protein uS2

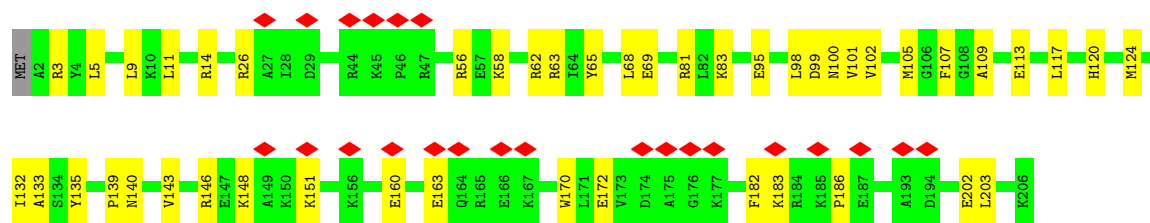


• Molecule 3: Small ribosomal subunit protein uS3

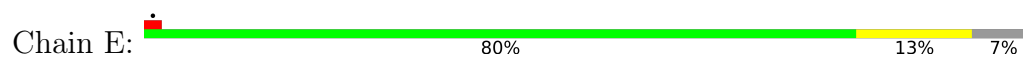


• Molecule 4: Small ribosomal subunit protein uS4

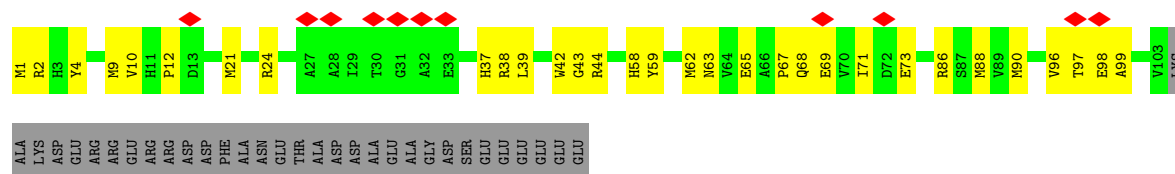




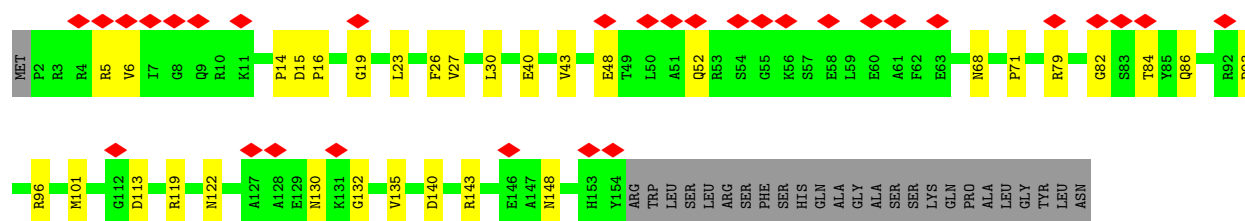
- Molecule 5: Small ribosomal subunit protein uS5



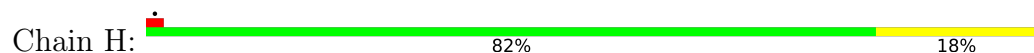
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



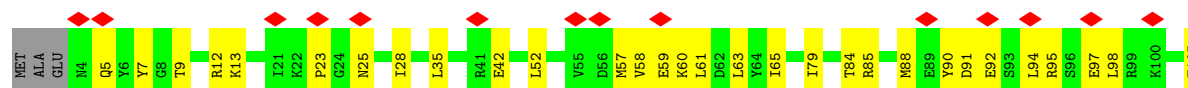
- Molecule 7: Small ribosomal subunit protein uS7



- Molecule 8: Small ribosomal subunit protein uS8

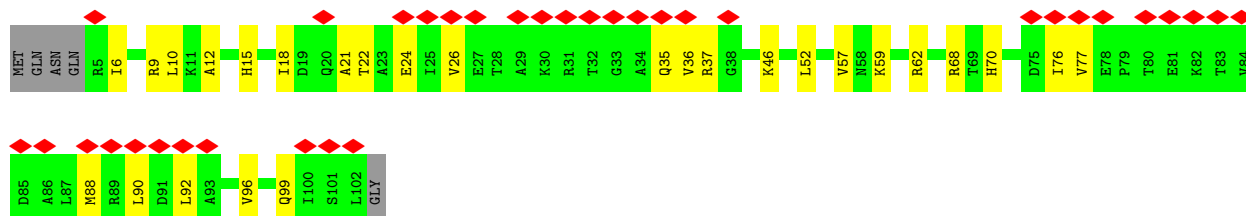


- Molecule 9: Small ribosomal subunit protein uS9





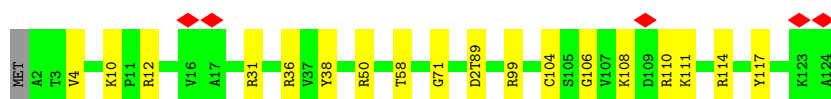
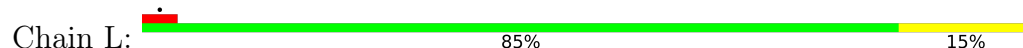
- Molecule 10: Small ribosomal subunit protein uS10



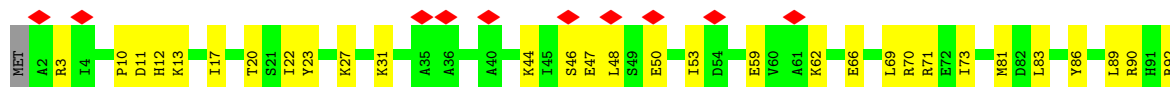
- Molecule 11: Small ribosomal subunit protein uS11



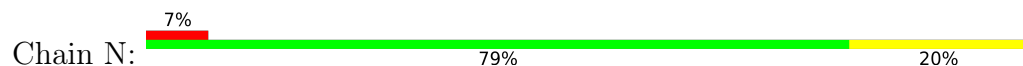
- Molecule 12: Small ribosomal subunit protein uS12

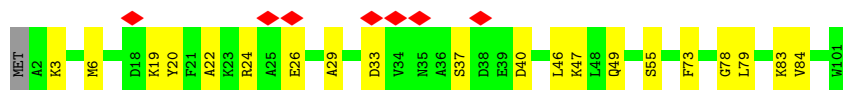


- Molecule 13: Small ribosomal subunit protein uS13

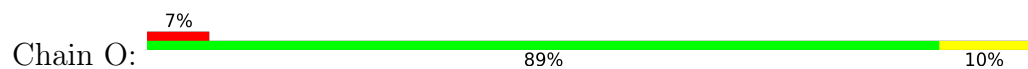


- Molecule 14: Small ribosomal subunit protein uS14

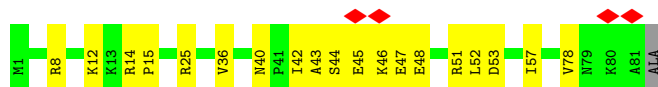
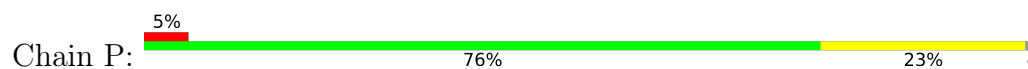




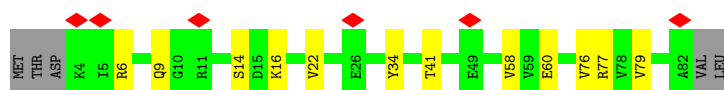
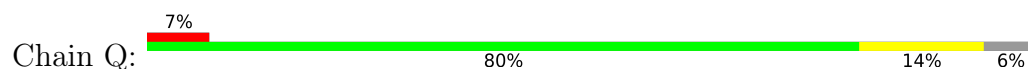
- Molecule 15: Small ribosomal subunit protein uS15



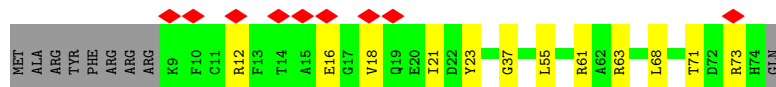
- Molecule 16: Small ribosomal subunit protein bS16



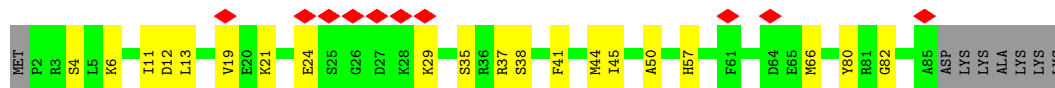
- Molecule 17: Small ribosomal subunit protein uS17



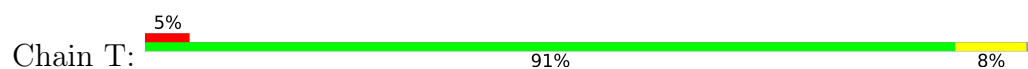
- Molecule 18: Small ribosomal subunit protein bS18



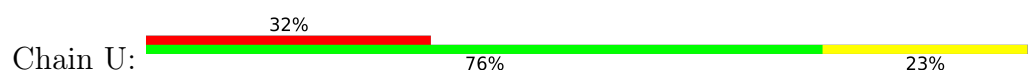
- Molecule 19: Small ribosomal subunit protein uS19



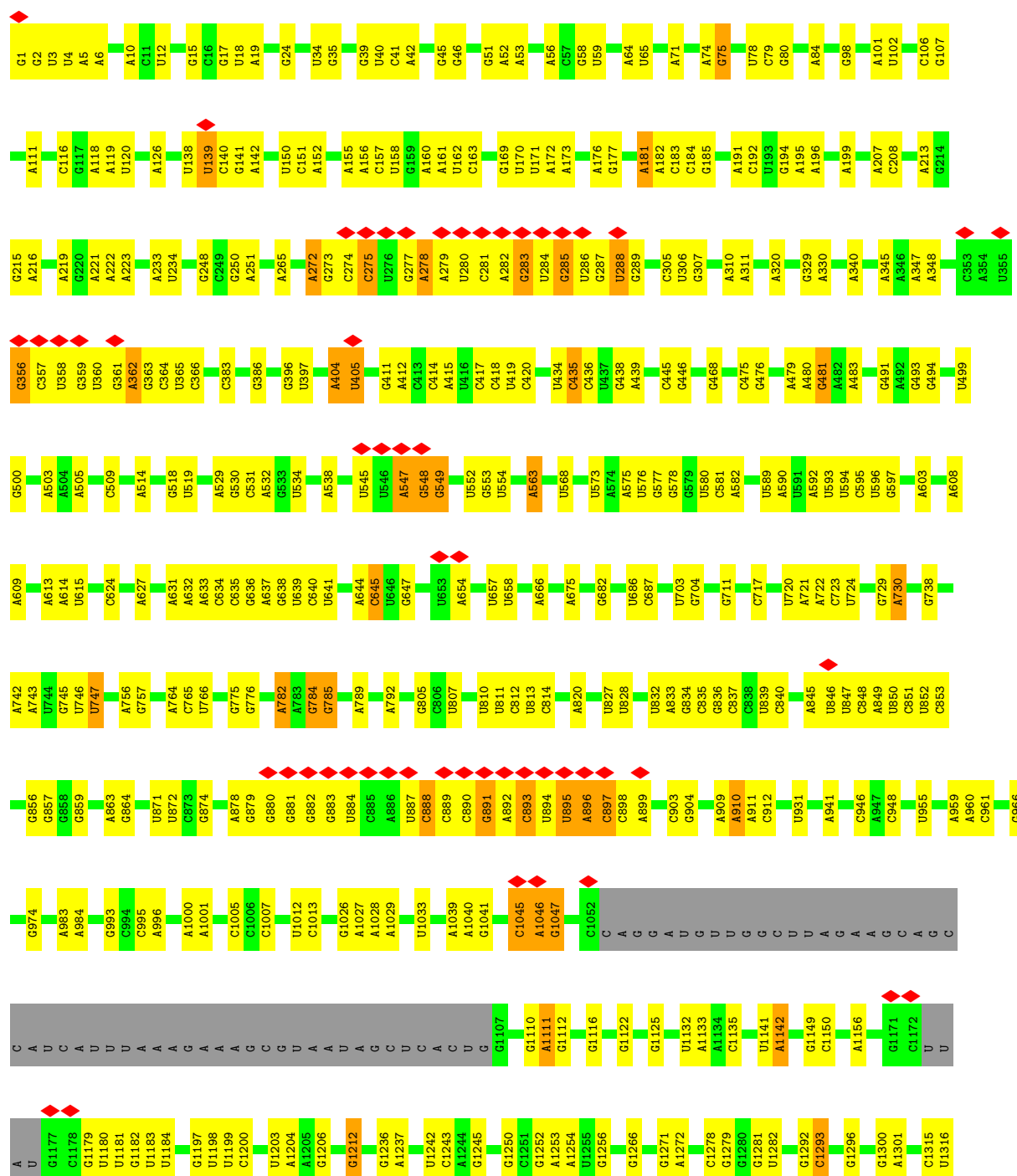
- Molecule 20: Small ribosomal subunit protein bS20



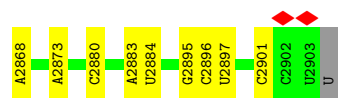
- Molecule 21: Small ribosomal subunit protein bS21



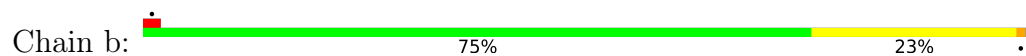
• Molecule 22: 23S rRNA



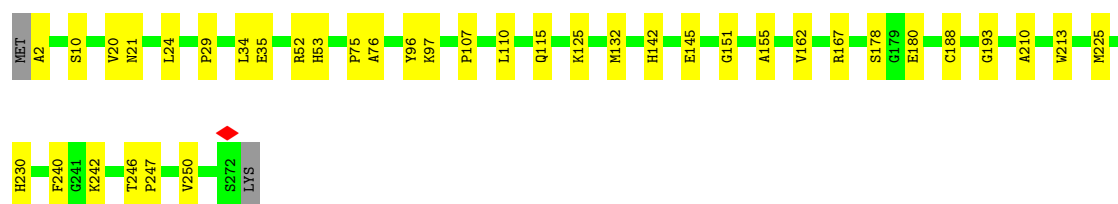
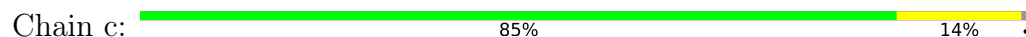
A2748	G2625	C2499	G2383	A2287	C	A	C2023	G1873	C1764	A1614	G1527	A1431	C1319
G2626	C2626	G2502	U2384	A2288	C	G	G2024	C1874	A1773	A1618	A1528	G1432	C1320
G2627	G2627	A2503	C2385	A2289	C	A	U2025	G1875	C1774	A1618	G1529	A1433	A1434
U2629	G2630	G2504	C2386	U2290	C	U	G2026	A1889	U1782	G1622	C1531	G1435	U1329
G2630	A2635	G2505	U2392	U2291	C	A	A2030	A1890	A1786	A1626	A1532	G1436	U1340
U2635	C2636	U2514	C2394	G2298	U	G	A2031	C1902	A1786	A1626	G1533	C1437	U1341
G2636	U2637	C2515	C2395	U2299	U	U	G2032	C1905	C1790	U1636	U1534	U1438	G1342
G2638	G2638	A2516	G2396	C2301	A	G	A2033	G1906	A1791	A1637	A1535	U1439	U1343
U2646	U2647	A2518	U2402	C2302	A	G	G2038	U1911	U1794	C1646	C1536	U1442	U1344
G2648	G2649	U2522	C2403	U2302	U	A	U2039	A1912	C1795	U1647	G1537	U1443	C1349
U2650	U2650	G2529	A2406	U2305	G	G	C2043	A1913	U1796	G1648	G1538	G1444	C1350
A2657	A2657	G2532	G2410	G2308	U	U	A2052	C1914	U1797	G1649	U1539	U1445	U1351
G2661	G2662	U2537	U2419	U2312	U	A	U2055	A1915	U1798	A1654	G1540	C1447	C1352
G2663	G2663	U2538	C2420	C2313	U	G	G2056	U1916	G1799	A1654	C1541	G1448	A1354
U2680	C2681	A2547	A2425	G2316	U	U	C2060	U1917	C1800	G1687	A1544	G1482	G1355
U2687	U2687	U2548	G2429	A2317	G	A	A2061	G1929	A1801	G1674	A1545	A1483	G1361
G2688	G2689	U2552	A2430	G2322	A	A	G2062	U1930	A1802	A1677	G1546	U1460	C1362
U2690	U2690	C2326	A2435	A2322	U	U	U2065	U1931	A1803	A1678	G1547	A1469	C1363
U2698	U2699	A2327	U2441	G2325	G	G	C2069	A1932	G1807	U1683	A1548	U1470	G1370
G2700	U2701	U2328	G2444	A2326	C	A	A2070	U1933	A1808	G1684	A1549	G1473	C1371
G2709	G2714	G2233	G2445	A2333	U	U	U2075	G1937	A1809	A1705	U1554	U1474	A1378
C2715	C2716	G2234	U2446	A2336	C	C	G2087	C1962	C1824	C1704	U1563	U1475	U1379
U2723	U2724	G2238	U2447	A2340	G	A	U2086	C1967	A1829	G1710	C1564	U1476	G1380
A2725	A2726	G2239	U2448	A2343	U	U	C2087	G1968	C1830	A1711	C1565	U1481	A1383
G2727	G2728	U2240	U2449	A2344	C	C	G2093	A1969	G1831	G1715	A1569	G1482	C1386
U2729	U2729	U2241	G2455	A2345	U	U	A2095	U1970	C1835	U1720	A1570	U1484	A1387
G2732	G2733	U2242	C2456	A2346	C	C	U2096	U1971	G1842	G1721	A1571	U1485	A1392
U2845	U2846	U2243	U2457	A2347	G	A	A2097	G1972	C1843	U1725	A1572	C1493	U1393
G2847	G2848	U2244	U2469	A2347	U	U	U2098	U1980	A1847	C1728	C1575	A1494	U1394
U2849	U2849	U2245	G2475	A2350	C	C	U2099	A1981	A1853	U1729	U1576	A1495	U1395
C2858	C2859	G2246	A2476	A2351	G	G	G2100	G1982	U1855	C1730	C1577	A1496	U1396
U2861	U2861	A2247	U2477	A2352	C	C	A2101	U1983	G1857	G1731	U1578	C1498	U1397
G2867	G2867	G2248	A2478	A2353	G	A	G2102	C1987	A1858	U1736	A1583	U1405	C1398
U2874	U2874	U2249	G2481	A2354	A	C	C	C2000	U1862	G1737	C1584	U1411	U1406
U2875	U2875	U2250	A2482	A2355	C	C	U	G2001	G1863	G1738	A1585	U1412	U1413
U2876	U2876	U2251	U2483	A2356	U	U	G	G2002	U1864	A1744	G1510	G1416	C1417
U2877	U2877	U2252	G2486	A2357	G	A	A	A2013	U1869	A1745	G1515	C1427	A1427
U2878	U2878	U2253	U2491	A2358	A	A	U	A2014	C1870	U1747	G1519	C1428	C1428
U2879	U2879	U2254	G2498	A2359	U	U	G	A2015	A1871	C1760	G1524	G1429	U1398
U2880	U2880	U2255	C2499	A2360	U	U	U	A2020	A1872	C1760	A1525	G1430	C1430
U2881	U2881	U2256	C2499	A2360	A	A	U						
U2882	U2882	U2257	C2499	A2360	C	C							
U2883	U2883	U2258	C2499	A2360	U	U							
U2884	U2884	U2259	C2499	A2360	G	G							
U2885	U2885	U2260	C2499	A2360	A	A							
U2886	U2886	U2261	C2499	A2360	U	U							
U2887	U2887	U2262	C2499	A2360	C	C							
U2888	U2888	U2263	C2499	A2360	U	U							
U2889	U2889	U2264	C2499	A2360	G	G							
U2890	U2890	U2265	C2499	A2360	A	A							
U2891	U2891	U2266	C2499	A2360	U	U							
U2892	U2892	U2267	C2499	A2360	C	C							
U2893	U2893	U2268	C2499	A2360	U	U							
U2894	U2894	U2269	C2499	A2360	G	G							
U2895	U2895	U2270	C2499	A2360	A	A							
U2896	U2896	U2271	C2499	A2360	U	U							
U2897	U2897	U2272	C2499	A2360	C	C							
U2898	U2898	U2273	C2499	A2360	U	U							
U2899	U2899	U2274	C2499	A2360	G	G							
U2900	U2900	U2275	C2499	A2360	A	A							
U2901	U2901	U2276	C2499	A2360	U	U							
U2902	U2902	U2277	C2499	A2360	C	C							
U2903	U2903	U2278	C2499	A2360	U	U							
U2904	U2904	U2279	C2499	A2360	G	G							
U2905	U2905	U2280	C2499	A2360	A	A							
U2906	U2906	U2281	C2499	A2360	U	U							
U2907	U2907	U2282	C2499	A2360	C	C							
U2908	U2908	U2283	C2499	A2360	U	U							
U2909	U2909	U2284	C2499	A2360	G	G							
U2910	U2910	U2285	C2499	A2360	A	A							
U2911	U2911	U2286	C2499	A2360	U	U							
U2912	U2912	U2287	C2499	A2360	C	C							
U2913	U2913	U2288	C2499	A2360	U	U							
U2914	U2914	U2289	C2499	A2360	G	G							
U2915	U2915	U2290	C2499	A2360	A	A							
U2916	U2916	U2291	C2499	A2360	U	U							
U2917	U2917	U2292	C2499	A2360	C	C							
U2918	U2918	U2293	C2499	A2360	U	U							
U2919	U2919	U2294	C2499	A2360	G	G							
U2920	U2920	U2295	C2499	A2360	A	A							
U2921	U2921	U2296	C2499	A2360	U	U							
U2922	U2922	U2297	C2499	A2360	C	C							
U2923	U2923	U2298	C2499	A2360	U	U							
U2924	U2924	U2299	C2499	A2360	G	G							
U2925	U2925	U2300	C2499	A2360	A	A							
U2926	U2926	U2301	C2499	A2360	U	U							
U2927	U2927	U2302	C2499	A2360	C	C							
U2928	U2928	U2303	C2499	A2360	U	U							
U2929	U2929	U2304	C2499	A2360	G	G							
U2930	U2930	U2305	C2499	A2360	A	A							
U2931	U2931	U2306	C2499	A2360	U	U							
U2932	U2932	U2307	C2499	A2360	C	C							
U2933	U2933	U2308	C2499	A2360	U	U							
U2934	U2934	U2309	C2499	A2360	G	G							
U2935	U2935	U2310	C2499	A2360	A	A							
U2936	U2936	U2311	C2499	A2360	U	U							
U2937	U2937	U2312	C2499	A2360	C	C							
U2938	U2938	U2313	C2499	A2360	U	U							
U2939	U2939	U2314	C2499	A2360	G	G							
U2940	U2940	U2315	C2499	A2360	A	A							
U2941	U2941	U2316	C2499	A2360	U	U							
U2942	U2942	U2317	C2499	A2360	C	C							
U2943	U2943	U2318	C2499	A2360	U	U							
U2944	U2944	U2319	C2499	A2360	G	G							
U2945	U2945	U2320	C2499	A2360	A	A							
U2946	U2946	U2321	C2499	A2360	U	U							
U2947	U2947	U2322	C2499	A2360	C	C							
U2948	U2948	U2323	C2499	A2360	U	U							
U2949	U2949	U2324	C2499	A2360	G	G							
U2950	U2950	U2325	C2499	A2360	A	A							
U2951	U2951	U2326	C2499	A2360	U	U							
U2952	U2952	U2327	C2499	A2360	C	C							
U2953	U2953	U2328	C2499	A2360	U	U							
U2954	U2954	U2329	C2499	A2360	G	G							
U2955	U2955	U2330	C2499	A2360	A	A							
U2956	U2956	U2331	C2499	A2360	U	U							
U2957	U2957	U2332	C2499	A2360	C	C							
U2958	U2958	U2333	C2499	A2360	U	U							
U2959	U2959	U2334	C2499	A2360	G	G							
U2960	U2960	U2335	C2499										



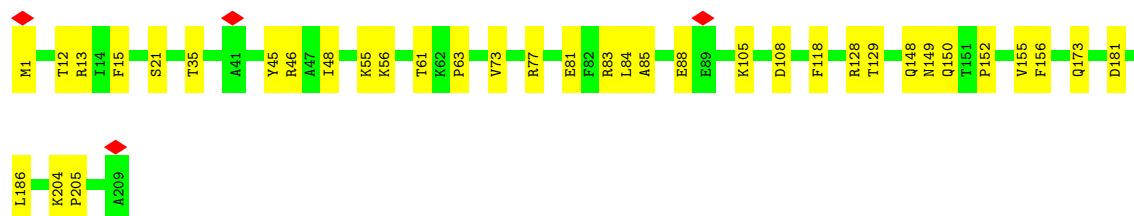
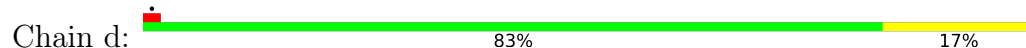
• Molecule 23: 5S rRNA



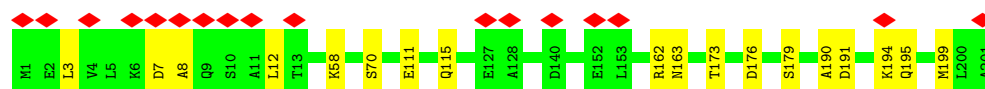
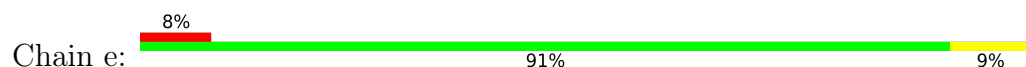
• Molecule 24: Large ribosomal subunit protein uL2



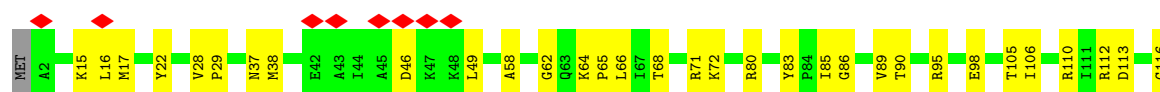
• Molecule 25: Large ribosomal subunit protein uL3

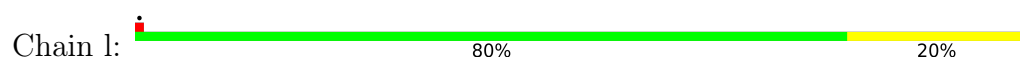


• Molecule 26: Large ribosomal subunit protein uL4

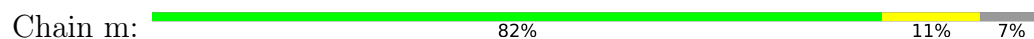


• Molecule 27: Large ribosomal subunit protein uL5

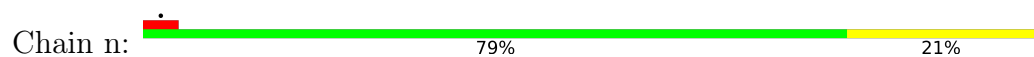




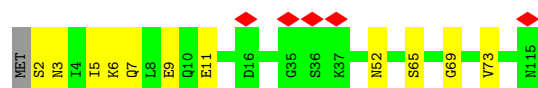
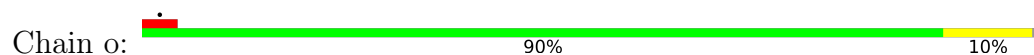
- Molecule 34: Large ribosomal subunit protein bL17



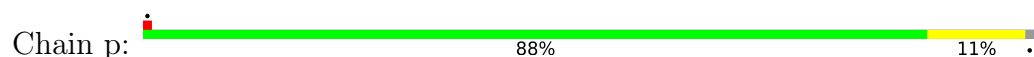
- Molecule 35: Large ribosomal subunit protein uL18



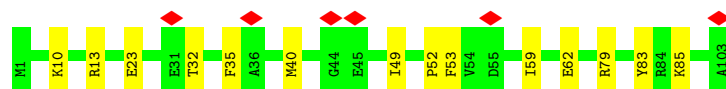
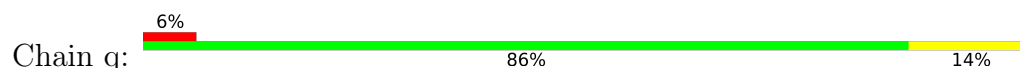
- Molecule 36: Large ribosomal subunit protein bL19



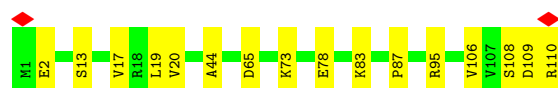
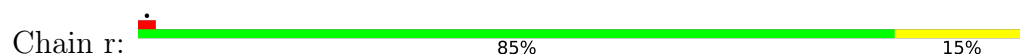
- Molecule 37: Large ribosomal subunit protein bL20



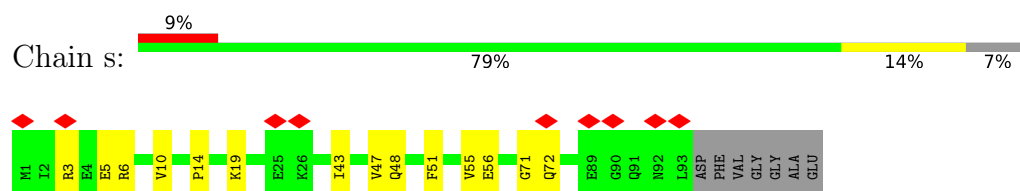
- Molecule 38: Large ribosomal subunit protein bL21



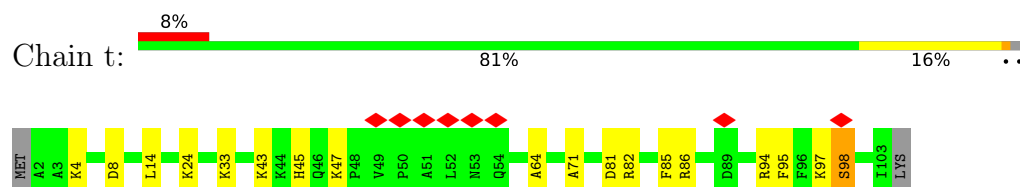
- Molecule 39: Large ribosomal subunit protein uL22



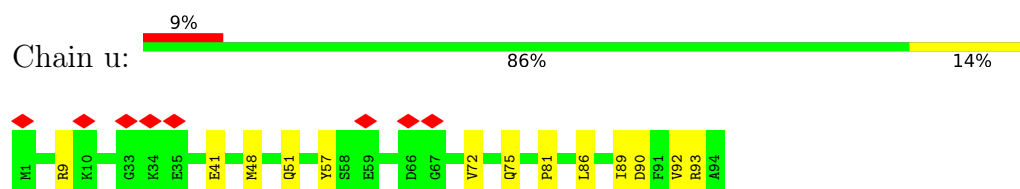
- Molecule 40: Large ribosomal subunit protein uL23



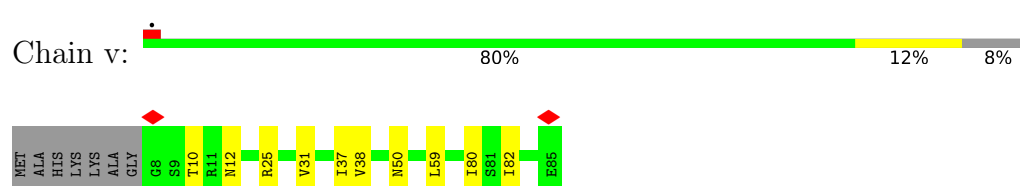
- Molecule 41: Large ribosomal subunit protein uL24



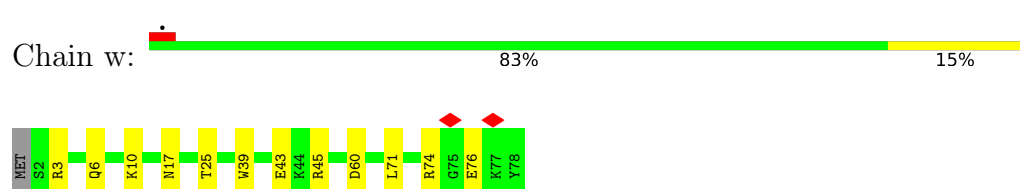
- Molecule 42: Large ribosomal subunit protein bL25



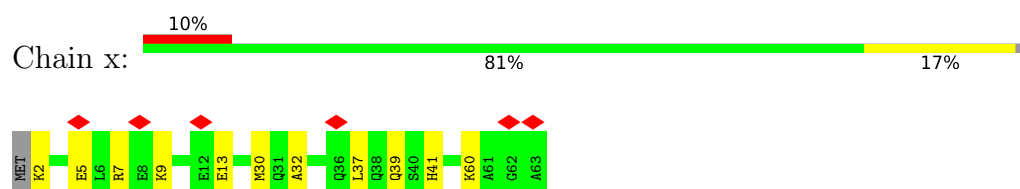
- Molecule 43: Large ribosomal subunit protein bL27



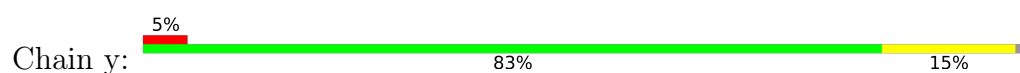
- Molecule 44: Large ribosomal subunit protein bL28



- Molecule 45: Large ribosomal subunit protein uL29

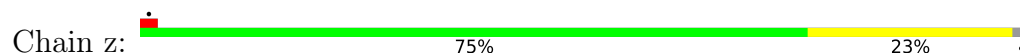


- Molecule 46: Large ribosomal subunit protein uL30





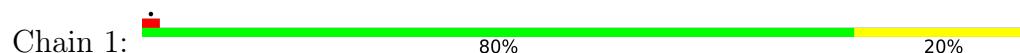
- Molecule 47: Large ribosomal subunit protein bL32



- Molecule 48: Large ribosomal subunit protein bL33



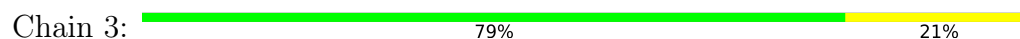
- Molecule 49: Large ribosomal subunit protein bL34



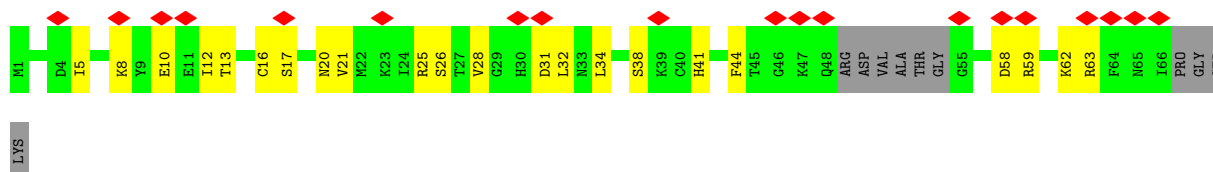
- Molecule 50: Large ribosomal subunit protein bL35



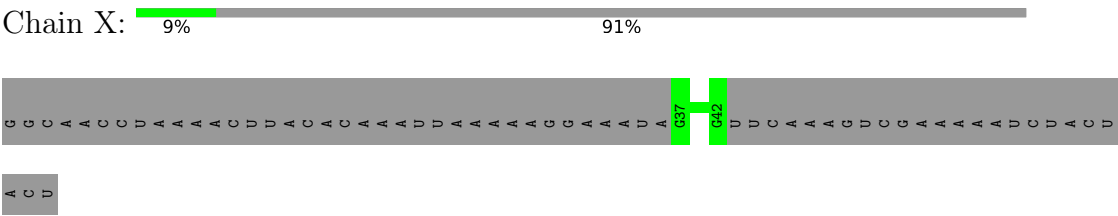
- Molecule 51: Large ribosomal subunit protein bL36A



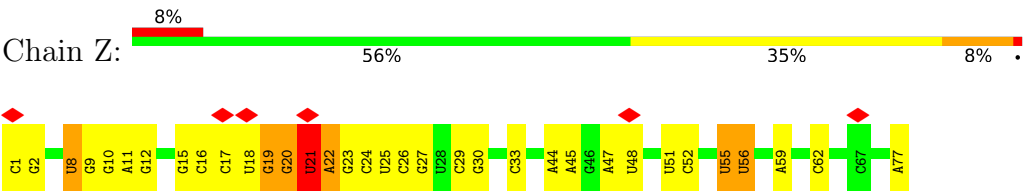
- Molecule 52: Large ribosomal subunit protein bL31



● Molecule 53: mRNA



● Molecule 54: P-site tRNA-fMet



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	244856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.239	Depositor
Minimum map value	-0.122	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.024	Depositor
Map size ($\text{\AA}$)	439.9, 439.9, 439.9	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, 4D4, MG, MEQ, IAS, 4SU, 5MU, 4OC, 6MZ, OMU, MS6, OMG, 3TD, UR3, PSU, MA6, D2T, OMC, G7M, 2MG, 2MA, 5MC, H2U

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	A	0.35	0/36073	0.30	0/56264
2	B	0.21	0/1784	0.32	0/2403
3	C	0.26	0/1651	0.36	0/2225
4	D	0.27	0/1665	0.37	0/2227
5	E	0.30	0/1165	0.37	0/1568
6	F	0.26	0/858	0.42	0/1160
7	G	0.22	0/1219	0.36	0/1635
8	H	0.31	0/989	0.38	0/1326
9	I	0.27	0/1034	0.42	0/1375
10	J	0.27	0/796	0.43	0/1077
11	K	0.27	0/884	0.35	0/1191
12	L	0.31	0/960	0.40	0/1286
13	M	0.27	0/900	0.45	0/1204
14	N	0.28	0/817	0.43	0/1088
15	O	0.29	0/722	0.38	0/964
16	P	0.31	0/653	0.39	0/877
17	Q	0.28	0/650	0.36	0/871
18	R	0.28	0/553	0.38	0/742
19	S	0.24	0/685	0.39	0/922
20	T	0.29	0/676	0.35	0/895
21	U	0.19	0/597	0.35	0/792
22	a	0.40	0/65842	0.31	0/102711
23	b	0.33	0/2850	0.27	0/4444
24	c	0.36	0/2121	0.39	0/2852
25	d	0.36	0/1576	0.35	0/2119
26	e	0.31	0/1571	0.35	0/2113
27	f	0.27	0/1434	0.36	0/1926
28	g	0.25	0/1343	0.42	0/1816
29	h	0.23	0/306	0.40	0/413
30	i	0.34	0/1152	0.35	0/1551
31	j	0.35	0/955	0.36	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.34	0/1062	0.39	0/1413
33	l	0.34	0/1073	0.37	0/1433
34	m	0.37	0/958	0.42	0/1281
35	n	0.29	0/902	0.39	0/1209
36	o	0.34	0/929	0.34	0/1242
37	p	0.38	0/960	0.37	0/1278
38	q	0.35	0/829	0.38	0/1107
39	r	0.34	0/864	0.39	0/1156
40	s	0.30	0/744	0.45	0/994
41	t	0.28	0/787	0.49	2/1051 (0.2%)
42	u	0.29	0/766	0.36	0/1025
43	v	0.35	0/599	0.36	0/792
44	w	0.34	0/635	0.40	0/848
45	x	0.25	0/502	0.38	0/667
46	y	0.33	0/453	0.36	0/605
47	z	0.34	0/450	0.36	0/599
48	0	0.28	0/424	0.31	0/565
49	1	0.38	0/380	0.43	0/498
50	2	0.37	0/513	0.42	0/676
51	3	0.36	0/303	0.38	0/397
52	4	0.21	0/488	0.41	0/649
53	X	0.29	0/145	0.26	0/224
54	Z	0.28	0/1725	0.26	0/2687
All	All	0.36	0/150972	0.33	2/225712 (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	M	0	1
50	2	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	t	98	SER	CA-C-N	5.71	132.44	121.54
41	t	98	SER	C-N-CA	5.71	132.44	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
13	M	104	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32466	0	16359	351	0
2	B	1753	0	1780	19	0
3	C	1624	0	1696	19	0
4	D	1643	0	1707	36	0
5	E	1152	0	1196	17	0
6	F	839	0	833	24	0
7	G	1203	0	1254	22	0
8	H	979	0	1031	17	0
9	I	1022	0	1070	30	0
10	J	786	0	828	19	0
11	K	877	0	884	16	0
12	L	957	0	1017	17	0
13	M	891	0	952	31	0
14	N	805	0	844	12	0
15	O	714	0	734	7	0
16	P	643	0	661	11	0
17	Q	641	0	682	9	0
18	R	544	0	565	9	0
19	S	668	0	693	15	0
20	T	670	0	719	5	0
21	U	589	0	629	10	0
22	a	59301	0	29850	524	0
23	b	2549	0	1291	15	0
24	c	2082	0	2154	26	0
25	d	1566	0	1618	26	0
26	e	1552	0	1619	10	0
27	f	1410	0	1444	37	0
28	g	1323	0	1371	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	h	303	0	327	15	0
30	i	1129	0	1162	19	0
31	j	946	0	1023	11	0
32	k	1053	0	1129	21	0
33	l	1075	0	1145	16	0
34	m	945	0	989	9	0
35	n	892	0	923	14	0
36	o	917	0	962	8	0
37	p	947	0	1019	12	0
38	q	816	0	839	10	0
39	r	857	0	922	10	0
40	s	738	0	807	9	0
41	t	779	0	831	14	0
42	u	753	0	780	10	0
43	v	592	0	607	6	0
44	w	625	0	652	8	0
45	x	501	0	531	7	0
46	y	449	0	488	5	0
47	z	444	0	458	9	0
48	0	417	0	451	8	0
49	1	377	0	418	9	0
50	2	504	0	572	7	0
51	3	302	0	343	6	0
52	4	480	0	482	18	0
53	X	130	0	66	0	0
54	Z	1645	0	842	16	0
55	A	119	0	0	0	0
55	Z	1	0	0	0	0
55	a	328	0	0	0	0
55	b	6	0	0	0	0
55	c	1	0	0	0	0
55	d	1	0	0	0	0
55	z	1	0	0	0	0
All	All	140322	0	94249	1465	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:A:HO2'	1:A:415:A:H8	0.99	0.97
22:a:1047:G:HO2'	22:a:1110:G:H1	1.13	0.97
1:A:76:G:H1	1:A:93:U:H3	1.11	0.97
22:a:1870:C:HO2'	22:a:1871:A:H8	0.99	0.95
22:a:2100:G:H1	22:a:2189:U:H3	0.95	0.93
22:a:1534:U:H3	22:a:1537:G:H1	1.14	0.91
25:d:61:THR:HG22	25:d:63:PRO:HD2	1.55	0.89
1:A:42:G:H21	1:A:622:A:H8	1.21	0.87
1:A:664:G:H22	1:A:741:G:H1	1.25	0.83
1:A:437:U:HO2'	4:D:120:HIS:HD1	1.22	0.83
28:g:38:ASN:ND2	28:g:64:GLN:OE1	2.12	0.81
52:4:59:ARG:HA	52:4:62:LYS:HE2	1.61	0.81
22:a:545:U:O2	22:a:548:G:O6	1.99	0.80
1:A:509:A:H8	1:A:543:U:HO2'	1.30	0.79
1:A:509:A:H8	1:A:543:U:O2'	1.65	0.79
3:C:35:SER:OG	3:C:59:ARG:NH2	2.16	0.78
1:A:677:U:H3	1:A:713:G:H22	1.32	0.78
35:n:76:LYS:NZ	35:n:80:GLU:OE1	2.15	0.78
1:A:8:A:N6	4:D:202:GLU:O	2.17	0.78
22:a:1417:C:HO2'	22:a:1587:G:HO2'	1.22	0.77
27:f:158:THR:HG22	27:f:160:ALA:H	1.49	0.77
13:M:12:HIS:O	13:M:44:LYS:NZ	2.17	0.77
1:A:428:G:H1'	1:A:430:A:C8	2.19	0.77
24:c:142:HIS:ND1	24:c:193:GLY:O	2.17	0.76
16:P:14:ARG:HG3	16:P:42:ILE:HD11	1.67	0.76
1:A:673:A:H2'	1:A:674:G:C8	2.21	0.75
4:D:172:GLU:HG2	4:D:183:LYS:HD2	1.68	0.74
7:G:68:ASN:ND2	7:G:130:ASN:OD1	2.21	0.74
29:h:1:MET:N	29:h:21:VAL:O	2.21	0.74
1:A:537:G:OP1	12:L:110:ARG:NH2	2.22	0.73
26:e:173:THR:HA	26:e:199:MET:HE1	1.70	0.72
9:I:106:ARG:NH1	9:I:107:ASP:O	2.23	0.72
22:a:2100:G:O6	22:a:2189:U:O4	2.06	0.72
32:k:91:ASP:OD1	32:k:92:LEU:N	2.21	0.71
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.73	0.71
22:a:2102:G:H1	22:a:2187:U:H3	0.79	0.71
22:a:881:G:N1	22:a:895:U:N3	2.36	0.71
3:C:110:GLU:HB2	3:C:144:LEU:HD22	1.71	0.71
1:A:407:U:O2'	4:D:113:GLU:OE1	2.10	0.70
22:a:881:G:H1	22:a:895:U:H3	1.35	0.70
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.24	0.70
12:L:71:GLY:O	12:L:99:ARG:NH2	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:881:G:O6	22:a:895:U:O4	2.10	0.69
35:n:99:TYR:OH	35:n:111:ARG:NH1	2.26	0.69
1:A:1086:U:H3	1:A:1099:G:H22	1.39	0.69
11:K:13:ARG:N	11:K:76:GLU:OE2	2.26	0.69
28:g:39:ASP:O	28:g:55:ARG:NH1	2.25	0.68
43:v:10:THR:HG22	43:v:12:ASN:H	1.56	0.68
28:g:2:SER:OG	28:g:3:ARG:N	2.23	0.68
3:C:128:VAL:HG13	3:C:132:ARG:HH21	1.59	0.68
10:J:9:ARG:HB2	10:J:99:GLN:HB2	1.76	0.68
10:J:10:LEU:HD13	10:J:22:THR:HG22	1.75	0.68
22:a:1434:A:H2'	22:a:1435:G:C8	2.28	0.68
13:M:23:TYR:HB3	13:M:66:GLU:HG3	1.76	0.68
22:a:1434:A:H2'	22:a:1435:G:H8	1.58	0.68
9:I:12:ARG:HG3	9:I:13:LYS:H	1.59	0.68
4:D:124:MET:HG2	4:D:146:ARG:HG2	1.74	0.67
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.75	0.67
5:E:164:ILE:O	8:H:114:ARG:NH2	2.27	0.67
24:c:2:ALA:N	24:c:20:VAL:O	2.28	0.67
13:M:59:GLU:HA	13:M:62:LYS:HZ3	1.59	0.67
48:0:7:GLU:OE2	48:0:27:LYS:NZ	2.23	0.67
1:A:1026:G:O6	1:A:1035:A:N1	2.28	0.67
22:a:1607:C:N4	22:a:1622:G:OP2	2.22	0.67
22:a:639:U:H2'	22:a:640:C:C6	2.29	0.67
11:K:37:ARG:NH1	11:K:83:GLU:OE2	2.28	0.67
22:a:1007:C:OP1	30:i:37:ARG:NH2	2.28	0.66
1:A:946:A:H2'	1:A:947:G:C8	2.30	0.66
1:A:1356:G:H2'	1:A:1357:A:C8	2.30	0.66
23:b:1:U:H2'	23:b:2:G:H8	1.60	0.66
1:A:405:U:OP2	4:D:3:ARG:NH1	2.28	0.66
1:A:544:G:OP1	4:D:56:ARG:NH2	2.27	0.66
10:J:6:ILE:HB	10:J:76:ILE:HB	1.77	0.66
22:a:1026:G:H2'	22:a:1027:A:H8	1.61	0.66
4:D:98:LEU:HB2	4:D:135:TYR:HB3	1.77	0.66
1:A:1137:C:O2	1:A:1138:G:N2	2.30	0.65
19:S:29:LYS:HA	19:S:29:LYS:HE3	1.78	0.65
7:G:113:ASP:OD2	7:G:122:ASN:ND2	2.29	0.65
22:a:1534:U:O2	22:a:1537:G:O6	2.13	0.65
1:A:1009:U:O2	1:A:1020:G:N2	2.19	0.65
22:a:2102:G:N2	22:a:2187:U:O2	2.22	0.65
22:a:2305:U:H5''	27:f:131:GLY:HA3	1.79	0.65
22:a:2394:C:H5''	32:k:63:LYS:HE2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:ARG:NH1	6:F:68:GLN:OE1	2.30	0.65
38:q:10:LYS:NZ	38:q:23:GLU:OE1	2.27	0.65
1:A:714:G:H2'	1:A:715:A:C8	2.32	0.64
22:a:2299:U:OP1	27:f:72:LYS:NZ	2.30	0.64
1:A:1006:G:O6	1:A:1023:U:O2	2.15	0.64
22:a:139:U:H5''	22:a:140:C:H5	1.63	0.64
22:a:1245:G:OP1	32:k:13:LYS:NZ	2.27	0.64
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.79	0.64
52:4:58:ASP:OD1	52:4:59:ARG:N	2.31	0.64
1:A:147:G:H2'	1:A:148:G:C8	2.33	0.64
18:R:16:GLU:HG3	18:R:18:VAL:HG23	1.78	0.64
34:m:56:LYS:NZ	34:m:90:ARG:O	2.31	0.64
22:a:1365:A:OP1	44:w:3:ARG:NH2	2.29	0.64
22:a:782:A:N1	24:c:225:MET:HE2	2.13	0.63
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.31	0.63
14:N:37:SER:OG	14:N:40:ASP:OD2	2.16	0.63
31:j:43:ILE:HD12	31:j:56:ASP:HB2	1.80	0.63
36:o:2:SER:OG	36:o:3:ASN:N	2.24	0.63
1:A:427:U:H3'	1:A:428:G:H5''	1.80	0.63
22:a:2328:A:H2'	22:a:2329:U:C6	2.34	0.63
22:a:2313:C:O4'	27:f:37:ASN:ND2	2.31	0.63
1:A:613:C:OP1	4:D:81:ARG:NH2	2.28	0.63
18:R:37:GLY:O	18:R:63:ARG:NH2	2.29	0.63
13:M:27:LYS:O	13:M:31:LYS:HG3	1.98	0.63
22:a:284:U:O2	22:a:356:G:O6	2.16	0.63
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.79	0.63
16:P:36:VAL:HG11	16:P:57:ILE:HG13	1.80	0.62
1:A:1311:A:OP1	52:4:59:ARG:NH1	2.32	0.62
1:A:1378:C:OP1	7:G:5:ARG:NH1	2.32	0.62
2:B:217:VAL:O	2:B:221:VAL:HG12	1.99	0.62
13:M:11:ASP:OD2	13:M:46:SER:OG	2.15	0.62
28:g:60:ASP:OD1	28:g:61:GLY:N	2.30	0.62
22:a:1649:G:O2'	34:m:106:ASP:OD2	2.14	0.62
22:a:2102:G:O6	22:a:2187:U:O4	2.18	0.62
51:3:18:LYS:HE2	51:3:21:GLY:HA2	1.81	0.62
22:a:2635:A:O2'	25:d:81:GLU:OE1	2.13	0.62
43:v:59:LEU:HD12	43:v:80:ILE:HD12	1.82	0.62
9:I:28:ILE:HG21	9:I:35:LEU:HD12	1.80	0.62
1:A:1009:U:H3	1:A:1020:G:H1	0.72	0.62
22:a:278:A:N1	22:a:361:G:O2'	2.32	0.62
22:a:2298:A:OP1	27:f:71:ARG:NH2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:GLU:OE1	5:E:112:ARG:NH2	2.31	0.61
1:A:1119:C:OP1	9:I:85:ARG:NH1	2.31	0.61
1:A:398:U:H2'	1:A:399:G:H8	1.65	0.61
2:B:117:LEU:HB3	2:B:141:LEU:HD12	1.82	0.61
40:s:47:VAL:HG23	40:s:51:PHE:HD2	1.65	0.61
1:A:413:G:H21	1:A:428:G:H2'	1.62	0.61
1:A:1280:A:OP2	10:J:9:ARG:NH2	2.32	0.61
1:A:413:G:N2	1:A:428:G:H2'	2.15	0.61
1:A:76:G:O6	1:A:93:U:O4	2.18	0.61
1:A:1130:A:H2'	1:A:1131:G:H8	1.64	0.61
1:A:337:G:H2'	1:A:338:A:C8	2.36	0.61
22:a:2547:A:H2'	22:a:2548:U:C6	2.35	0.61
1:A:215:C:H1'	1:A:465:A:N6	2.16	0.61
16:P:45:GLU:O	16:P:46:LYS:HG2	2.00	0.61
22:a:320:A:N3	26:e:163:ASN:ND2	2.46	0.61
1:A:1516:2MG:N1	1:A:1519:MA6:OP2	2.34	0.61
47:z:54:VAL:HG23	47:z:55:ILE:HG12	1.83	0.61
22:a:534:U:O2'	37:p:49:ASP:OD2	2.14	0.60
22:a:1469:A:H2'	22:a:1470:A:C8	2.36	0.60
22:a:2788:C:H2'	22:a:2789:C:C6	2.36	0.60
1:A:492:C:H2'	1:A:493:A:C8	2.36	0.60
3:C:46:GLU:HG2	3:C:87:LEU:HD21	1.84	0.60
6:F:88:MET:HE2	6:F:90:MET:HE2	1.83	0.60
14:N:3:LYS:HB2	14:N:6:MET:HG2	1.83	0.60
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.83	0.60
22:a:1197:G:H2'	22:a:1198:U:H6	1.65	0.60
33:l:53:MET:HG3	33:l:120:ALA:HB2	1.83	0.60
26:e:176:ASP:OD1	26:e:179:SER:OG	2.18	0.60
1:A:555:U:H2'	1:A:556:C:C6	2.36	0.60
1:A:823:C:HO2'	8:H:2:SER:N	2.00	0.60
1:A:1038:C:H2'	1:A:1039:G:H8	1.67	0.60
1:A:1166:G:N1	1:A:1169:A:OP2	2.34	0.60
22:a:1704:C:H2'	22:a:1705:A:H8	1.65	0.60
1:A:202:G:H21	1:A:466:A:H61	1.48	0.60
1:A:746:A:H2'	1:A:747:A:C8	2.37	0.60
1:A:1009:U:O4	1:A:1020:G:O6	2.20	0.60
26:e:111:GLU:OE2	26:e:115:GLN:NE2	2.35	0.60
22:a:545:U:O2	22:a:548:G:C6	2.53	0.60
30:i:13:ARG:NH1	30:i:49:ASP:O	2.34	0.60
1:A:423:G:O2'	1:A:424:G:O4'	2.18	0.60
19:S:11:ILE:HG13	19:S:38:SER:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1799:G:N7	24:c:178:SER:OG	2.31	0.60
7:G:26:PHE:HD1	7:G:101:MET:HG2	1.66	0.59
7:G:140:ASP:OD1	7:G:143:ARG:NH1	2.33	0.59
1:A:1098:C:O2'	21:U:71:TYR:O	2.20	0.59
1:A:1314:C:OP2	19:S:4:SER:OG	2.14	0.59
13:M:104:THR:HG22	13:M:105:ASN:H	1.65	0.59
22:a:1667:G:O2'	22:a:1991:U:O4	2.19	0.59
33:l:53:MET:HE1	33:l:103:TYR:CD1	2.37	0.59
1:A:1030:U:O2'	1:A:1031:C:O5'	2.18	0.59
3:C:105:GLU:OE2	3:C:107:ARG:NH2	2.36	0.59
7:G:93:PRO:HA	7:G:96:ARG:HD3	1.84	0.59
22:a:1794:A:H2'	22:a:1795:C:C6	2.37	0.59
27:f:29:PRO:HB2	27:f:169:LEU:HD22	1.84	0.59
35:n:88:LYS:HE2	35:n:116:GLN:HE22	1.66	0.59
27:f:106:ILE:HD12	52:4:34:LEU:HD21	1.84	0.59
1:A:1218:C:H2'	1:A:1219:A:C8	2.38	0.59
25:d:46:ARG:NH1	25:d:85:ALA:O	2.25	0.59
21:U:31:GLU:OE2	21:U:35:ARG:NE	2.34	0.59
22:a:284:U:H2'	22:a:285:G:H8	1.67	0.59
22:a:2095:A:O5'	29:h:11:ASN:ND2	2.36	0.59
42:u:9:ARG:HG2	42:u:41:GLU:HG3	1.84	0.59
22:a:307:G:N1	22:a:310:A:OP2	2.31	0.59
22:a:993:G:OP2	37:p:51:ARG:NH2	2.36	0.59
22:a:1315:C:O2'	22:a:1392:A:N3	2.34	0.58
33:l:41:LEU:HG	33:l:96:ILE:HG13	1.85	0.58
15:O:18:ASP:OD2	15:O:20:ASN:N	2.29	0.58
34:m:86:ARG:NE	34:m:117:ASP:OD2	2.33	0.58
24:c:75:PRO:HG2	24:c:97:LYS:HG3	1.85	0.58
33:l:105:MET:HE3	33:l:108:VAL:HG21	1.84	0.58
1:A:545:C:H2'	1:A:546:A:H5'	1.86	0.58
18:R:71:THR:HG23	18:R:73:ARG:H	1.68	0.58
22:a:742:A:H2'	22:a:743:A:C8	2.38	0.58
22:a:1548:A:H2'	22:a:1549:A:C8	2.38	0.58
22:a:347:A:H2'	22:a:348:A:C8	2.39	0.58
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.37	0.58
1:A:950:U:O4	13:M:104:THR:HG21	2.04	0.58
2:B:120:GLN:OE1	2:B:137:ARG:NH1	2.37	0.58
1:A:539:A:H2'	1:A:540:G:C8	2.38	0.57
22:a:499:U:H5''	41:t:43:LYS:HE2	1.86	0.57
22:a:1636:U:H2'	22:a:1637:A:H8	1.68	0.57
1:A:64:G:OP1	1:A:382:A:N6	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:G:O2'	1:A:469:C:O2'	2.20	0.57
22:a:1047:G:O2'	22:a:1110:G:N1	2.22	0.57
1:A:423:G:O2'	1:A:424:G:O5'	2.22	0.57
22:a:2845:U:H5''	36:o:52:ASN:O	2.04	0.57
22:a:414:C:H2'	22:a:415:A:C8	2.40	0.57
27:f:80:ARG:HB2	27:f:83:TYR:HE2	1.70	0.57
1:A:28:A:O2'	1:A:296:U:OP1	2.16	0.57
22:a:631:A:OP2	50:2:23:LYS:NZ	2.37	0.57
22:a:1386:C:H2'	22:a:1387:A:C8	2.39	0.57
1:A:653:U:OP1	8:H:56:LYS:NZ	2.26	0.57
12:L:99:ARG:NH1	12:L:104:CYS:SG	2.77	0.57
32:k:132:ARG:HG3	32:k:142:ILE:HD12	1.86	0.57
37:p:97:ASP:OD2	38:q:13:ARG:NH1	2.38	0.57
22:a:2566:A:N1	31:j:28:SER:OG	2.35	0.57
22:a:2799:A:O2'	22:a:2800:A:H5''	2.05	0.57
10:J:26:VAL:HG23	10:J:36:VAL:HG21	1.85	0.56
22:a:414:C:H2'	22:a:415:A:H8	1.71	0.56
22:a:1720:U:H2'	22:a:1721:G:O4'	2.05	0.56
1:A:131:A:H2'	1:A:132:C:C6	2.40	0.56
1:A:1152:A:OP1	10:J:70:HIS:ND1	2.33	0.56
4:D:11:LEU:HD13	4:D:63:ARG:HG2	1.88	0.56
22:a:475:C:O2	22:a:479:A:N6	2.36	0.56
22:a:639:U:H2'	22:a:640:C:H6	1.70	0.56
22:a:1405:U:H2'	22:a:1406:U:C6	2.40	0.56
22:a:1796:U:H2'	22:a:1797:G:H8	1.70	0.56
29:h:6:LEU:HD11	29:h:37:VAL:HG13	1.85	0.56
41:t:8:ASP:O	41:t:24:LYS:NZ	2.34	0.56
13:M:10:PRO:HB2	13:M:13:LYS:HG3	1.87	0.56
15:O:6:GLU:OE1	15:O:6:GLU:N	2.28	0.56
7:G:113:ASP:HB2	7:G:119:ARG:HG3	1.87	0.56
44:w:43:GLU:OE2	44:w:45:ARG:NH2	2.38	0.56
48:0:9:ILE:HD12	48:0:51:GLU:HG3	1.87	0.56
22:a:856:G:H2'	22:a:857:G:C8	2.41	0.56
22:a:910:A:H2'	22:a:911:A:C8	2.40	0.56
22:a:2316:G:H2'	22:a:2317:A:H8	1.70	0.56
37:p:109:LEU:HD11	38:q:40:MET:HE1	1.86	0.56
6:F:44:ARG:HG3	6:F:44:ARG:HH11	1.71	0.56
13:M:59:GLU:HA	13:M:62:LYS:NZ	2.20	0.56
19:S:19:VAL:HG21	19:S:44:MET:HG2	1.86	0.56
30:i:88:THR:N	30:i:91:GLU:OE1	2.25	0.56
34:m:22:ARG:HG3	34:m:70:THR:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:U:H2'	1:A:391:G:C8	2.41	0.56
22:a:1340:U:OP1	40:s:19:LYS:NZ	2.38	0.56
1:A:390:U:H2'	1:A:391:G:H8	1.70	0.56
1:A:713:G:H2'	1:A:714:G:C8	2.40	0.56
3:C:19:ASN:O	3:C:40:ARG:NH2	2.38	0.56
5:E:149:SER:OG	5:E:152:MET:HE3	2.05	0.56
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.88	0.56
22:a:1636:U:H2'	22:a:1637:A:C8	2.41	0.56
35:n:56:LYS:O	35:n:60:GLU:HG3	2.06	0.56
13:M:104:THR:HG22	13:M:105:ASN:N	2.21	0.55
1:A:546:A:H2'	4:D:68:LEU:HD21	1.87	0.55
22:a:359:G:H2'	22:a:360:U:H6	1.71	0.55
22:a:2883:A:OP2	47:z:50:ARG:NH1	2.39	0.55
39:r:83:LYS:HG2	39:r:95:ARG:HD3	1.87	0.55
1:A:399:G:H2'	1:A:400:C:C6	2.41	0.55
1:A:414:A:O2'	1:A:415:A:O5'	2.24	0.55
1:A:715:A:H2'	1:A:716:A:C8	2.41	0.55
1:A:1144:G:N2	1:A:1146:A:H62	2.04	0.55
6:F:88:MET:HE1	18:R:61:ARG:HG2	1.87	0.55
22:a:284:U:H2'	22:a:285:G:C8	2.41	0.55
22:a:360:U:H2'	22:a:361:G:O4'	2.07	0.55
1:A:411:A:OP1	4:D:26:ARG:NH1	2.32	0.55
1:A:1273:C:H2'	1:A:1274:A:O4'	2.07	0.55
1:A:1356:G:H2'	1:A:1357:A:H8	1.70	0.55
2:B:61:ALA:HB2	2:B:221:VAL:HG23	1.89	0.55
22:a:2343:U:HO2'	22:a:2373:G:HO2'	1.52	0.55
1:A:1391:U:H2'	1:A:1392:G:C8	2.42	0.55
1:A:744:C:H2'	1:A:745:G:H8	1.71	0.55
22:a:84:A:N1	22:a:98:G:O2'	2.35	0.55
22:a:2329:U:H2'	22:a:2330:G:C8	2.42	0.55
1:A:1130:A:H2'	1:A:1131:G:C8	2.42	0.55
5:E:13:GLU:OE2	5:E:68:ARG:NH1	2.39	0.55
22:a:64:A:H2'	22:a:65:U:C6	2.42	0.55
22:a:1252:G:OP2	37:p:13:ARG:NH1	2.31	0.55
22:a:2291:U:H2'	22:a:2292:U:C6	2.42	0.55
35:n:27:VAL:HG21	35:n:40:ILE:HD12	1.88	0.55
22:a:191:A:H2'	22:a:192:C:C6	2.41	0.55
22:a:1864:U:OP1	22:a:2410:G:O2'	2.19	0.55
22:a:1869:G:N2	22:a:1872:A:OP2	2.38	0.55
10:J:52:LEU:HD11	10:J:59:LYS:HD2	1.88	0.55
27:f:116:GLY:HA3	27:f:178:ARG:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:m:28:LEU:HD23	34:m:48:VAL:HG21	1.89	0.55
1:A:78:A:H2'	1:A:79:G:H8	1.72	0.54
22:a:365:U:H2'	22:a:366:C:C6	2.43	0.54
22:a:1794:A:H2'	22:a:1795:C:H6	1.72	0.54
1:A:1151:A:HO2'	1:A:1152:A:H8	1.53	0.54
1:A:1323:G:H2'	1:A:1324:A:C8	2.41	0.54
22:a:1816:C:N4	24:c:35:GLU:OE2	2.36	0.54
23:b:66:A:N6	23:b:107:G:H2'	2.22	0.54
21:U:39:GLU:OE1	21:U:47:ARG:NH1	2.41	0.54
23:b:52:A:N7	35:n:64:TYR:OH	2.26	0.54
1:A:1033:G:H2'	1:A:1034:G:C8	2.43	0.54
16:P:36:VAL:HG13	16:P:53:ASP:HB3	1.90	0.54
22:a:1156:A:C8	37:p:51:ARG:HG2	2.42	0.54
22:a:2419:U:H4'	48:0:22:THR:HG21	1.90	0.54
1:A:216:U:H2'	1:A:217:C:C6	2.42	0.54
1:A:683:G:N2	11:K:39:GLY:O	2.40	0.54
19:S:12:ASP:OD2	19:S:35:SER:OG	2.19	0.54
22:a:172:A:H2'	22:a:173:A:C8	2.42	0.54
22:a:1746:A:H2'	22:a:1747:U:C6	2.42	0.54
32:k:77:ILE:HD11	32:k:108:ALA:HB1	1.90	0.54
42:u:51:GLN:OE1	42:u:57:TYR:OH	2.23	0.54
1:A:89:U:H2'	1:A:90:C:C6	2.43	0.54
22:a:1266:G:O2'	22:a:2012:G:O6	2.25	0.54
1:A:575:G:O2'	1:A:821:G:OP2	2.20	0.54
9:I:88:MET:HE3	9:I:98:LEU:HD12	1.88	0.54
22:a:126:A:OP1	49:1:45:SER:OG	2.26	0.54
22:a:851:C:H2'	22:a:852:U:H6	1.73	0.54
35:n:34:HIS:O	35:n:102:ARG:NH1	2.40	0.54
1:A:78:A:H2'	1:A:79:G:C8	2.43	0.54
27:f:80:ARG:HB2	27:f:83:TYR:CE2	2.42	0.54
12:L:4:VAL:HG23	17:Q:34:TYR:HB3	1.90	0.54
16:P:48:GLU:OE2	16:P:51:ARG:HB2	2.08	0.54
33:l:1:MET:HE2	33:l:1:MET:HA	1.89	0.54
1:A:1040:U:H2'	1:A:1041:G:C8	2.44	0.53
6:F:37:HIS:HB3	6:F:97:THR:HG22	1.88	0.53
10:J:24:GLU:HG3	10:J:90:LEU:HD21	1.90	0.53
15:O:18:ASP:HB3	15:O:21:ASP:HB2	1.89	0.53
22:a:721:A:H2'	22:a:722:A:C8	2.43	0.53
22:a:1278:C:H2'	22:a:1279:G:H8	1.73	0.53
23:b:1:U:H2'	23:b:2:G:C8	2.41	0.53
1:A:45:G:H2'	1:A:46:G:H8	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.90	0.53
22:a:636:G:OP1	32:k:129:LYS:NZ	2.41	0.53
22:a:881:G:N2	22:a:895:U:O2	2.39	0.53
25:d:1:MET:SD	25:d:205:PRO:HG2	2.47	0.53
1:A:499:A:H61	1:A:547:A:H5''	1.73	0.53
1:A:1120:C:H2'	1:A:1121:U:H6	1.73	0.53
8:H:50:LYS:HG3	8:H:52:GLU:OE2	2.09	0.53
14:N:29:ALA:O	14:N:33:ASP:HB2	2.08	0.53
22:a:729:G:H5''	22:a:730:A:H5''	1.89	0.53
22:a:1796:U:H2'	22:a:1797:G:C8	2.44	0.53
22:a:2243:U:H2'	22:a:2244:U:C6	2.44	0.53
1:A:1040:U:H2'	1:A:1041:G:H8	1.72	0.53
3:C:123:GLN:OE1	3:C:136:ARG:NH2	2.42	0.53
22:a:807:U:OP2	32:k:41:ARG:NH1	2.42	0.53
22:a:1509:A:HO2'	22:a:1510:G:H8	1.55	0.53
41:t:4:LYS:O	41:t:94:ARG:NH2	2.41	0.53
22:a:851:C:H2'	22:a:852:U:C6	2.44	0.53
22:a:2848:G:O2'	22:a:2867:G:N2	2.33	0.53
25:d:13:ARG:HD3	25:d:21:SER:OG	2.07	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.43	0.53
1:A:201:G:HO2'	1:A:469:C:HO2'	1.55	0.53
22:a:1570:A:H2'	22:a:1571:A:C8	2.42	0.53
22:a:2430:A:N3	22:a:2430:A:H2'	2.23	0.53
1:A:382:A:H2'	1:A:383:A:C8	2.44	0.53
1:A:636:U:O2'	1:A:637:C:H5'	2.08	0.53
6:F:96:VAL:HG12	6:F:96:VAL:O	2.09	0.53
22:a:468:G:OP2	49:l:37:LYS:NZ	2.42	0.53
23:b:66:A:H61	23:b:107:G:H2'	1.74	0.53
1:A:148:G:O2'	1:A:1446:A:N3	2.40	0.53
1:A:524:G:H2'	1:A:525:C:C6	2.44	0.53
24:c:21:ASN:HB3	24:c:24:LEU:HG	1.89	0.53
1:A:508:U:H1'	1:A:509:A:H2	1.74	0.53
1:A:1010:U:H2'	1:A:1011:C:C6	2.43	0.53
10:J:18:ILE:O	10:J:22:THR:HG23	2.07	0.53
13:M:70:ARG:HE	27:f:112:ARG:HH12	1.57	0.53
22:a:138:U:O2'	22:a:141:G:O6	2.26	0.53
22:a:221:A:N1	22:a:265:A:O2'	2.41	0.53
22:a:1141:U:H4'	22:a:1142:A:O4'	2.09	0.53
25:d:181:ASP:HB3	25:d:186:LEU:HB2	1.91	0.53
1:A:754:C:O5'	15:O:72:ARG:NH2	2.42	0.52
22:a:1028:A:H2'	22:a:1029:A:C8	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:6:GLN:O	44:w:74:ARG:NH1	2.42	0.52
1:A:202:G:O2'	1:A:468:A:N3	2.40	0.52
1:A:362:G:N2	1:A:365:U:OP2	2.39	0.52
22:a:892:A:H2'	22:a:893:C:C6	2.44	0.52
22:a:1292:G:H2'	22:a:1293:C:C6	2.45	0.52
22:a:1856:U:H2'	22:a:1857:G:O4'	2.09	0.52
1:A:530:G:H2'	1:A:530:G:N3	2.24	0.52
22:a:2591:C:H2'	22:a:2592:G:C8	2.43	0.52
22:a:476:G:N1	22:a:479:A:OP2	2.37	0.52
11:K:75:LYS:HZ3	11:K:75:LYS:HB2	1.73	0.52
22:a:359:G:H2'	22:a:360:U:C6	2.44	0.52
22:a:640:C:H2'	22:a:641:U:C6	2.44	0.52
22:a:742:A:H2'	22:a:743:A:H8	1.75	0.52
22:a:363:G:H2'	22:a:364:C:H6	1.75	0.52
22:a:879:G:H2'	22:a:880:G:C8	2.45	0.52
37:p:86:ALA:HB2	37:p:116:ALA:HB2	1.92	0.52
54:Z:22:A:H61	54:Z:47:A:H2'	1.73	0.52
1:A:415:A:H2'	1:A:416:G:H8	1.75	0.52
1:A:459:A:H2'	1:A:460:A:C8	2.45	0.52
22:a:720:U:H2'	22:a:721:A:C8	2.45	0.52
22:a:1149:G:H2'	22:a:1150:C:C6	2.45	0.52
22:a:1548:A:H2'	22:a:1549:A:H8	1.75	0.52
22:a:2327:A:H2'	22:a:2328:A:C8	2.44	0.52
27:f:98:GLU:OE2	52:4:25:ARG:NE	2.37	0.52
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.91	0.52
32:k:81:ASP:HA	32:k:84:LYS:HD2	1.91	0.52
35:n:83:LEU:HD11	35:n:114:GLY:HA3	1.92	0.52
1:A:151:A:OP2	1:A:169:C:N4	2.42	0.52
22:a:3:U:H2'	22:a:4:U:C6	2.45	0.52
22:a:2101:A:H2'	22:a:2102:G:H8	1.75	0.52
54:Z:24:C:H2'	54:Z:25:U:C6	2.45	0.52
1:A:517:G:O2'	1:A:518:C:O5'	2.27	0.52
5:E:151:GLU:OE2	5:E:151:GLU:N	2.41	0.52
22:a:1:G:H2'	22:a:2:G:H8	1.75	0.52
22:a:1484:U:H2'	22:a:1485:U:C6	2.45	0.52
22:a:2483:C:N3	33:l:123:LYS:NZ	2.58	0.52
27:f:140:GLU:HA	52:4:28:VAL:HG22	1.92	0.52
51:3:16:ILE:HD13	51:3:25:VAL:HG22	1.92	0.52
1:A:601:G:OP1	8:H:89:LYS:NZ	2.31	0.52
1:A:769:G:H4'	1:A:1513:A:H4'	1.92	0.52
16:P:40:ASN:HB3	16:P:43:ALA:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:903:C:H2'	22:a:904:G:H8	1.74	0.52
22:a:1802:A:H2'	22:a:1803:A:C8	2.44	0.52
28:g:107:LEU:HB3	28:g:152:ARG:HG3	1.92	0.52
29:h:4:ILE:HG22	29:h:18:GLN:HG2	1.92	0.52
29:h:6:LEU:HD21	29:h:37:VAL:HG22	1.92	0.52
1:A:696:A:H2'	1:A:697:U:H6	1.75	0.51
2:B:104:TRP:HA	2:B:107:VAL:HG22	1.92	0.51
22:a:1386:C:H2'	22:a:1387:A:H8	1.75	0.51
33:l:77:PRO:HG2	33:l:80:VAL:HG21	1.91	0.51
1:A:224:U:H2'	1:A:225:C:C6	2.45	0.51
1:A:451:A:N6	1:A:480:U:O2'	2.41	0.51
4:D:58:LYS:HD3	4:D:203:LEU:HD11	1.91	0.51
22:a:1902:C:H4'	24:c:242:LYS:O	2.11	0.51
22:a:2266:A:H4'	22:a:2267:A:N3	2.25	0.51
1:A:1062:U:H2'	1:A:1063:C:C6	2.44	0.51
1:A:1314:C:H2'	1:A:1315:U:C6	2.45	0.51
22:a:288:U:H2'	22:a:289:G:C8	2.45	0.51
22:a:1597:A:H5''	22:a:1598:A:H5'	1.93	0.51
25:d:108:ASP:OD2	25:d:173:GLN:HA	2.11	0.51
45:x:39:GLN:OE1	45:x:41:HIS:HE1	1.94	0.51
7:G:15:ASP:OD2	7:G:19:GLY:N	2.43	0.51
9:I:7:TYR:HH	9:I:9:THR:HG1	1.58	0.51
22:a:552:U:H2'	22:a:553:G:H8	1.76	0.51
22:a:644:A:H2'	22:a:645:C:O4'	2.10	0.51
22:a:1526:C:H2'	22:a:1527:G:O4'	2.10	0.51
4:D:99:ASP:OD2	4:D:100:ASN:N	2.44	0.51
22:a:2618:G:H21	25:d:155:VAL:HG21	1.75	0.51
22:a:2698:U:H2'	22:a:2699:C:C6	2.46	0.51
1:A:945:G:C2	1:A:946:A:C8	2.98	0.51
13:M:86:TYR:O	13:M:90:ARG:HG2	2.10	0.51
22:a:277:G:H4'	22:a:278:A:O5'	2.11	0.51
22:a:347:A:H2'	22:a:348:A:H8	1.75	0.51
1:A:269:C:H2'	1:A:270:A:C8	2.45	0.51
1:A:464:U:N3	1:A:467:U:OP2	2.30	0.51
1:A:900:A:H2'	1:A:901:A:C8	2.45	0.51
4:D:101:VAL:HG12	4:D:105:MET:HE2	1.91	0.51
22:a:2246:G:H2'	22:a:2247:A:C8	2.46	0.51
41:t:86:ARG:HG3	41:t:95:PHE:CE1	2.46	0.51
1:A:2:A:H4'	4:D:83:LYS:NZ	2.26	0.51
10:J:24:GLU:OE2	10:J:92:LEU:HD13	2.11	0.51
13:M:59:GLU:OE2	13:M:62:LYS:NZ	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:183:C:H42	22:a:213:A:H61	1.59	0.51
38:q:40:MET:HE2	38:q:49:ILE:HG12	1.92	0.51
41:t:33:LYS:HB3	41:t:64:ALA:HB1	1.93	0.51
3:C:164:ARG:NH1	3:C:166:GLU:OE2	2.44	0.51
13:M:92:ARG:HD3	22:a:888:C:C5	2.46	0.51
22:a:581:C:H2'	22:a:582:A:C8	2.46	0.51
22:a:703:U:H2'	22:a:704:G:O4'	2.11	0.51
22:a:879:G:H2'	22:a:880:G:H8	1.76	0.51
22:a:995:C:OP2	37:p:54:LYS:NZ	2.39	0.51
25:d:55:LYS:HE2	25:d:77:ARG:HA	1.92	0.51
29:h:34:GLY:O	29:h:36:ALA:N	2.44	0.51
7:G:16:PRO:HB2	9:I:42:GLU:HG3	1.93	0.50
7:G:68:ASN:HD22	7:G:130:ASN:CG	2.18	0.50
8:H:22:LYS:O	8:H:65:TYR:OH	2.26	0.50
13:M:89:LEU:HD22	13:M:93:ARG:HH12	1.76	0.50
22:a:306:U:H2'	22:a:307:G:O4'	2.11	0.50
22:a:2273:A:H2'	22:a:2274:A:C8	2.46	0.50
1:A:509:A:O2'	1:A:510:A:N3	2.35	0.50
6:F:1:MET:HG3	6:F:65:GLU:HG2	1.92	0.50
22:a:1197:G:H2'	22:a:1198:U:C6	2.46	0.50
36:o:5:ILE:HG22	36:o:9:GLU:OE1	2.10	0.50
1:A:1229:A:OP2	13:M:113:ARG:NH1	2.44	0.50
3:C:47:LEU:HD21	3:C:87:LEU:HD11	1.93	0.50
10:J:88:MET:HE3	10:J:88:MET:HA	1.94	0.50
22:a:1242:U:H2'	22:a:1243:C:C6	2.47	0.50
22:a:1930:G:O2'	22:a:1968:G:O6	2.28	0.50
48:O:10:LYS:HD2	48:O:20:PHE:CD2	2.46	0.50
9:I:57:MET:HE1	9:I:90:TYR:CE1	2.47	0.50
1:A:1477:U:H2'	1:A:1478:U:C6	2.47	0.50
22:a:849:A:H2'	22:a:850:U:C6	2.47	0.50
22:a:2074:U:H2'	22:a:2075:U:C6	2.47	0.50
22:a:2469:A:N6	22:a:2481:G:O2'	2.39	0.50
1:A:539:A:OP1	12:L:111:LYS:HD2	2.12	0.50
1:A:1010:U:H2'	1:A:1011:C:H6	1.77	0.50
7:G:48:GLU:O	7:G:52:GLN:HG2	2.12	0.50
8:H:10:MET:HG3	8:H:27:MET:SD	2.52	0.50
22:a:24:G:O2'	39:r:78:GLU:O	2.30	0.50
22:a:2680:U:O2'	22:a:2681:C:H5'	2.12	0.50
25:d:13:ARG:HD2	25:d:15:PHE:CZ	2.46	0.50
39:r:2:GLU:HA	39:r:108:SER:HB3	1.92	0.50
2:B:54:LEU:HG	2:B:220:THR:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:72:ILE:HD12	5:E:145:GLU:HG3	1.93	0.50
22:a:721:A:H2'	22:a:722:A:H8	1.77	0.50
22:a:1980:G:O2'	22:a:1982:U:OP2	2.29	0.50
42:u:48:MET:HE3	42:u:51:GLN:NE2	2.27	0.50
1:A:728:A:H2'	1:A:729:A:C8	2.47	0.50
4:D:140:ASN:N	4:D:182:PHE:O	2.40	0.50
7:G:15:ASP:OD1	7:G:23:LEU:HB3	2.12	0.50
22:a:468:G:N7	49:1:39:ARG:NH2	2.56	0.50
22:a:820:A:H4'	22:a:836:G:H22	1.77	0.50
22:a:848:C:H2'	22:a:849:A:C8	2.47	0.50
22:a:898:C:H2'	22:a:899:A:O4'	2.12	0.50
1:A:653:U:H5'	8:H:56:LYS:NZ	2.27	0.50
13:M:3:ARG:HH21	27:f:110:ARG:HG2	1.76	0.50
31:j:63:VAL:HG23	31:j:64:ARG:HG3	1.93	0.50
2:B:96:TRP:CZ2	2:B:100:MET:HB3	2.47	0.49
23:b:42:C:C6	27:f:66:LEU:HB2	2.47	0.49
1:A:486:U:H2'	1:A:487:A:H8	1.78	0.49
1:A:1004:A:C5	1:A:1026:G:H1'	2.46	0.49
20:T:44:LYS:HZ3	20:T:87:ALA:HB2	1.76	0.49
22:a:833:A:H2'	22:a:834:G:C8	2.47	0.49
22:a:1182:G:H2'	22:a:1183:U:O4'	2.11	0.49
1:A:235:C:H2'	1:A:236:A:C8	2.47	0.49
1:A:501:C:H2'	1:A:502:A:C8	2.47	0.49
22:a:397:U:OP2	44:w:10:LYS:NZ	2.33	0.49
22:a:638:G:H2'	22:a:639:U:C6	2.47	0.49
22:a:657:U:H2'	22:a:658:U:C6	2.47	0.49
22:a:1590:A:H2'	22:a:1591:A:C8	2.48	0.49
22:a:1614:A:H8	22:a:1614:A:P	2.35	0.49
22:a:2537:U:H2'	22:a:2538:C:C6	2.47	0.49
28:g:2:SER:O	28:g:6:LYS:HG2	2.13	0.49
28:g:52:PHE:CE2	28:g:72:LEU:HD22	2.48	0.49
52:4:8:LYS:NZ	52:4:10:GLU:HB3	2.27	0.49
4:D:102:VAL:HG13	4:D:107:PHE:HB2	1.94	0.49
22:a:593:U:H2'	22:a:594:U:C6	2.47	0.49
22:a:871:U:H2'	22:a:872:U:C6	2.47	0.49
22:a:1704:C:H2'	22:a:1705:A:C8	2.46	0.49
9:I:58:VAL:HG13	9:I:59:GLU:OE1	2.13	0.49
22:a:894:U:H2'	22:a:895:U:C6	2.46	0.49
22:a:1438:U:H2'	22:a:1439:A:H8	1.78	0.49
22:a:2646:C:OP2	22:a:2732:G:O2'	2.31	0.49
46:y:58:GLU:HG2	46:y:58:GLU:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:C:H2'	1:A:1039:G:C8	2.45	0.49
7:G:30:LEU:HD22	7:G:43:VAL:HG23	1.94	0.49
22:a:594:U:H2'	22:a:595:C:C6	2.48	0.49
22:a:1026:G:H2'	22:a:1027:A:C8	2.45	0.49
22:a:1296:G:OP1	22:a:2709:G:O2'	2.21	0.49
22:a:2395:C:H2'	22:a:2396:G:O4'	2.12	0.49
1:A:1118:U:H2'	1:A:1119:C:H6	1.78	0.49
1:A:1314:C:H2'	1:A:1315:U:H6	1.78	0.49
6:F:88:MET:HG2	6:F:90:MET:HE2	1.93	0.49
10:J:12:ALA:HB2	10:J:96:VAL:HG22	1.94	0.49
12:L:111:LYS:HA	12:L:114:ARG:CG	2.43	0.49
22:a:577:G:O2'	22:a:1254:A:OP1	2.30	0.49
22:a:2637:U:H5''	25:d:83:ARG:HH11	1.78	0.49
22:a:2830:C:O3'	25:d:56:LYS:NZ	2.45	0.49
32:k:77:ILE:CD1	32:k:108:ALA:HB1	2.43	0.49
33:l:66:ARG:NH1	33:l:104:GLU:OE1	2.46	0.49
1:A:389:A:H3'	1:A:390:U:H6	1.76	0.49
1:A:459:A:H2'	1:A:460:A:H8	1.76	0.49
1:A:744:C:H2'	1:A:745:G:C8	2.47	0.49
22:a:2:G:H2'	22:a:3:U:C6	2.48	0.49
22:a:116:C:O2'	22:a:126:A:N3	2.38	0.49
22:a:848:C:H2'	22:a:849:A:H8	1.78	0.49
22:a:1853:A:H2'	22:a:1854:A:C8	2.48	0.49
22:a:2030:6MZ:C2	22:a:2499:C:H5''	2.43	0.49
26:e:58:LYS:NZ	26:e:70:SER:O	2.36	0.49
28:g:94:TYR:HA	28:g:106:SER:O	2.13	0.49
30:i:69:ARG:NH1	30:i:90:GLU:OE2	2.42	0.49
1:A:215:C:H2'	1:A:216:U:C6	2.48	0.49
1:A:600:A:H5''	8:H:89:LYS:HD3	1.94	0.49
1:A:663:A:H5'	1:A:836:G:OP1	2.13	0.49
1:A:868:C:H2'	1:A:869:G:O4'	2.13	0.49
14:N:19:LYS:HD2	14:N:20:TYR:CE1	2.48	0.49
22:a:363:G:H2'	22:a:364:C:C6	2.48	0.49
22:a:500:G:N1	22:a:503:A:OP2	2.42	0.49
22:a:1533:C:O2	22:a:1539:U:N3	2.45	0.49
28:g:153:ARG:HB2	28:g:153:ARG:CZ	2.43	0.49
2:B:60:ILE:HA	2:B:63:ARG:NH1	2.28	0.49
6:F:21:MET:HA	6:F:24:ARG:HG2	1.95	0.49
22:a:5:A:H2'	22:a:6:A:C8	2.48	0.49
22:a:106:C:H2'	22:a:107:G:H8	1.78	0.49
22:a:2312:U:H5'	27:f:85:ILE:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:l:58:LYS:O	33:l:60:GLN:NE2	2.45	0.49
21:U:4:ILE:HG13	21:U:19:PHE:HA	1.94	0.48
22:a:219:A:N3	22:a:234:U:O2'	2.40	0.48
22:a:278:A:C6	22:a:362:A:C8	3.01	0.48
25:d:48:ILE:HG23	25:d:84:LEU:HD11	1.95	0.48
1:A:45:G:H2'	1:A:46:G:C8	2.48	0.48
1:A:415:A:H2'	1:A:416:G:C8	2.48	0.48
3:C:11:ARG:NH2	3:C:175:LEU:O	2.46	0.48
5:E:113:ALA:O	5:E:117:VAL:HG22	2.14	0.48
14:N:49:GLN:OE1	19:S:13:LEU:N	2.29	0.48
22:a:172:A:H2'	22:a:173:A:H8	1.79	0.48
22:a:1342:A:O2'	22:a:1344:U:OP2	2.27	0.48
22:a:1494:A:H2'	22:a:1495:A:C8	2.48	0.48
22:a:2532:G:O2'	22:a:2657:A:N1	2.45	0.48
24:c:145:GLU:HG2	24:c:151:GLY:C	2.38	0.48
25:d:12:THR:OG1	25:d:13:ARG:N	2.46	0.48
27:f:68:THR:N	27:f:86:GLY:O	2.41	0.48
30:i:110:PRO:O	30:i:115:GLY:HA3	2.13	0.48
1:A:518:C:H2'	1:A:530:G:C8	2.48	0.48
1:A:1287:A:H2'	1:A:1288:A:C8	2.48	0.48
2:B:129:LEU:HD23	2:B:133:GLU:HB3	1.95	0.48
22:a:1000:A:H2'	22:a:1001:A:C8	2.48	0.48
22:a:2101:A:H2'	22:a:2102:G:C8	2.48	0.48
33:l:21:ALA:HB2	33:l:97:GLN:HB2	1.96	0.48
1:A:460:A:H2'	1:A:461:A:C8	2.48	0.48
1:A:460:A:H2'	1:A:461:A:H8	1.78	0.48
1:A:1029:U:H2'	1:A:1030:U:O4'	2.12	0.48
9:I:115:LYS:HB2	9:I:118:LEU:HD12	1.95	0.48
1:A:471:U:H2'	1:A:472:U:C6	2.49	0.48
1:A:1004:A:H2'	1:A:1005:A:O4'	2.12	0.48
2:B:130:THR:C	2:B:132:LYS:H	2.21	0.48
22:a:1527:G:N1	22:a:1544:A:OP2	2.38	0.48
22:a:2025:C:H2'	22:a:2026:U:C6	2.48	0.48
1:A:223:A:H2'	1:A:224:U:C6	2.49	0.48
13:M:17:ILE:O	13:M:20:THR:OG1	2.32	0.48
22:a:1932:A:H2'	22:a:1933:G:O4'	2.13	0.48
22:a:2228:G:H2'	22:a:2229:U:C6	2.49	0.48
22:a:2287:A:OP1	48:O:30:LYS:NZ	2.40	0.48
22:a:2392:A:OP2	50:2:31:HIS:NE2	2.47	0.48
28:g:95:ARG:HB2	28:g:95:ARG:NH1	2.28	0.48
33:l:36:VAL:HG21	33:l:129:THR:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:C:H2'	1:A:313:A:C8	2.49	0.48
28:g:47:ASP:N	28:g:47:ASP:OD1	2.46	0.48
1:A:407:U:H2'	1:A:408:A:H8	1.79	0.48
10:J:35:GLN:HG2	10:J:77:VAL:HG23	1.96	0.48
13:M:44:LYS:HB2	13:M:47:GLU:OE1	2.13	0.48
22:a:171:U:H2'	22:a:172:A:H8	1.79	0.48
24:c:115:GLN:O	24:c:125:LYS:NZ	2.44	0.48
39:r:65:ASP:OD2	39:r:65:ASP:N	2.46	0.48
22:a:58:G:H2'	22:a:59:U:C6	2.49	0.48
1:A:324:G:N1	1:A:327:A:OP2	2.44	0.48
22:a:250:G:H2'	22:a:251:A:C8	2.49	0.48
22:a:1534:U:C4	22:a:1535:A:H1'	2.49	0.48
27:f:16:LEU:HD12	27:f:28:VAL:HG13	1.94	0.48
27:f:62:GLY:O	27:f:95:ARG:NH1	2.44	0.48
1:A:35:G:H2'	1:A:36:C:C6	2.49	0.47
1:A:429:U:H5'	4:D:9:LEU:HD12	1.96	0.47
12:L:99:ARG:HD2	12:L:104:CYS:SG	2.54	0.47
22:a:2246:G:H2'	22:a:2247:A:H8	1.79	0.47
22:a:2392:A:C2	32:k:55:MET:HE3	2.48	0.47
27:f:37:ASN:OD1	27:f:38:MET:N	2.48	0.47
29:h:27:ARG:NH1	44:w:60:ASP:OD2	2.36	0.47
40:s:43:ILE:O	40:s:47:VAL:HG12	2.14	0.47
1:A:831:A:H5''	2:B:21:ARG:HE	1.79	0.47
22:a:150:U:H2'	22:a:151:C:C6	2.50	0.47
22:a:2340:A:H5'	23:b:41:G:H21	1.79	0.47
22:a:2740:A:H2'	22:a:2741:A:C8	2.49	0.47
22:a:2773:C:H2'	22:a:2774:C:H6	1.78	0.47
1:A:604:G:H2'	1:A:605:U:O4'	2.15	0.47
17:Q:60:GLU:OE2	17:Q:76:VAL:HB	2.14	0.47
22:a:2377:A:H2'	22:a:2378:A:C8	2.49	0.47
23:b:106:G:H2'	23:b:107:G:O4'	2.14	0.47
1:A:161:A:H2'	1:A:162:A:C8	2.49	0.47
1:A:259:G:OP1	20:T:36:TYR:OH	2.22	0.47
1:A:299:G:H2'	1:A:300:A:C8	2.50	0.47
22:a:563:A:OP2	38:q:79:ARG:NH2	2.39	0.47
22:a:1179:G:H2'	22:a:1180:U:C6	2.50	0.47
22:a:2554:U:H2'	22:a:2555:U:C6	2.50	0.47
28:g:38:ASN:OD1	28:g:39:ASP:N	2.46	0.47
29:h:32:PRO:HA	44:w:39:TRP:CD1	2.49	0.47
1:A:580:C:H2'	1:A:581:G:O4'	2.15	0.47
1:A:1039:G:H2'	1:A:1040:U:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:364:C:H2'	22:a:365:U:C6	2.49	0.47
22:a:547:A:H3'	22:a:548:G:C8	2.50	0.47
22:a:2567:G:H2'	22:a:2568:U:C6	2.49	0.47
1:A:335:C:H2'	1:A:336:A:H8	1.80	0.47
1:A:398:U:H2'	1:A:399:G:C8	2.47	0.47
13:M:50:GLU:HA	13:M:53:ILE:HG22	1.97	0.47
22:a:1428:C:C5	22:a:1569:A:H5''	2.48	0.47
32:k:30:THR:HG21	32:k:34:GLY:O	2.13	0.47
1:A:219:U:H2'	1:A:220:G:H8	1.79	0.47
1:A:393:A:OP2	16:P:12:LYS:NZ	2.37	0.47
1:A:662:U:H2'	1:A:663:A:C8	2.49	0.47
1:A:1071:C:H2'	1:A:1072:G:H8	1.79	0.47
1:A:1140:C:H2'	1:A:1141:C:H6	1.79	0.47
1:A:1268:G:H2'	1:A:1269:A:C8	2.49	0.47
1:A:1527:U:H2'	1:A:1528:U:C6	2.49	0.47
1:A:1533:C:H4'	1:A:1534:A:C8	2.50	0.47
2:B:6:MET:HG3	2:B:43:LEU:HD23	1.97	0.47
9:I:65:ILE:HD13	9:I:79:ILE:HG23	1.97	0.47
9:I:88:MET:CE	9:I:98:LEU:HD12	2.44	0.47
9:I:92:GLU:OE2	9:I:95:ARG:NE	2.35	0.47
22:a:675:A:N3	22:a:2443:C:O2'	2.45	0.47
22:a:720:U:H2'	22:a:721:A:H8	1.80	0.47
22:a:1378:A:O2'	22:a:1380:G:N7	2.47	0.47
22:a:2097:A:H2'	22:a:2098:U:C6	2.49	0.47
23:b:2:G:H2'	23:b:3:C:C6	2.50	0.47
36:o:7:GLN:NE2	36:o:11:GLU:OE2	2.42	0.47
40:s:71:GLY:O	40:s:72:GLN:NE2	2.48	0.47
45:x:5:GLU:O	45:x:9:LYS:NZ	2.48	0.47
50:2:62:LEU:HB3	50:2:65:ALA:HB2	1.97	0.47
1:A:736:C:OP1	18:R:61:ARG:NH1	2.48	0.47
1:A:1238:A:OP1	1:A:1335:U:O2'	2.25	0.47
22:a:580:U:H2'	22:a:581:C:C6	2.50	0.47
22:a:832:U:H2'	22:a:833:A:C8	2.50	0.47
22:a:1536:C:O2	22:a:1537:G:N2	2.48	0.47
22:a:1585:C:H2'	22:a:1586:A:O4'	2.14	0.47
22:a:2233:U:H2'	22:a:2234:G:C8	2.49	0.47
40:s:3:ARG:HB3	40:s:5:GLU:OE1	2.14	0.47
54:Z:16:C:OP1	54:Z:17:C:N4	2.42	0.47
1:A:470:C:H2'	1:A:471:U:H6	1.80	0.47
1:A:918:A:H2'	1:A:919:A:C8	2.50	0.47
1:A:1302:C:C5	13:M:17:ILE:HG13	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:46:LEU:HD22	19:S:13:LEU:HD13	1.97	0.47
19:S:45:ILE:HD12	19:S:45:ILE:H	1.79	0.47
22:a:2086:U:H2'	22:a:2087:G:C8	2.50	0.47
24:c:155:ALA:HB2	24:c:162:VAL:HG23	1.97	0.47
28:g:78:GLY:HA2	28:g:82:GLY:HA2	1.97	0.47
31:j:76:VAL:HG12	36:o:73:VAL:HB	1.97	0.47
1:A:107:G:N1	20:T:6:SER:OG	2.36	0.47
1:A:337:G:H2'	1:A:338:A:H8	1.77	0.47
1:A:500:G:H2'	1:A:501:C:C6	2.50	0.47
1:A:652:U:O4	1:A:752:G:O2'	2.33	0.47
22:a:272:A:H2'	22:a:273:G:C8	2.50	0.47
22:a:2780:G:OP2	30:i:120:ARG:HD3	2.15	0.47
22:a:2809:A:H2'	22:a:2810:A:C8	2.50	0.47
31:j:79:PHE:HE2	31:j:102:PRO:HG2	1.79	0.47
1:A:235:C:H2'	1:A:236:A:H8	1.81	0.46
7:G:79:ARG:HA	7:G:84:THR:HA	1.97	0.46
9:I:28:ILE:HA	9:I:63:LEU:HB2	1.98	0.46
11:K:23:ILE:HG21	11:K:96:THR:HG21	1.96	0.46
12:L:36:ARG:HG2	12:L:38:TYR:CD1	2.49	0.46
22:a:2052:A:H4'	25:d:148:GLN:O	2.15	0.46
1:A:140:U:H2'	1:A:141:G:O4'	2.15	0.46
1:A:1011:C:H2'	1:A:1012:A:C8	2.51	0.46
4:D:99:ASP:OD1	4:D:133:ALA:HB1	2.15	0.46
8:H:7:ILE:O	8:H:11:LEU:HG	2.15	0.46
10:J:59:LYS:HE2	10:J:62:ARG:HH22	1.80	0.46
19:S:41:PHE:H	19:S:44:MET:HE2	1.80	0.46
22:a:1203:U:OP2	22:a:1204:A:O2'	2.27	0.46
22:a:2014:A:H2'	22:a:2015:A:C8	2.50	0.46
1:A:428:G:O2'	1:A:429:U:O5'	2.27	0.46
1:A:1036:A:H2'	1:A:1037:C:O4'	2.15	0.46
1:A:1120:C:H2'	1:A:1121:U:C6	2.49	0.46
22:a:837:C:N3	22:a:941:A:N6	2.61	0.46
22:a:2071:A:H2'	22:a:2072:C:C6	2.50	0.46
41:t:85:PHE:HE1	41:t:94:ARG:HG2	1.80	0.46
1:A:126:G:OP1	1:A:605:U:O2'	2.24	0.46
1:A:999:C:N3	1:A:1042:A:N6	2.64	0.46
2:B:6:MET:HE3	2:B:43:LEU:HB3	1.98	0.46
5:E:61:GLN:O	5:E:65:GLU:HG2	2.15	0.46
22:a:3:U:H2'	22:a:4:U:H6	1.81	0.46
22:a:274:C:C4	22:a:275:C:N3	2.84	0.46
41:t:86:ARG:HG3	41:t:95:PHE:CD1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:32:ALA:HB2	45:x:37:LEU:HD23	1.97	0.46
52:4:20:ASN:OD1	52:4:21:VAL:N	2.48	0.46
54:Z:22:A:N6	54:Z:47:A:H2'	2.31	0.46
1:A:834:U:H2'	1:A:835:U:C6	2.51	0.46
17:Q:77:ARG:HH12	17:Q:79:VAL:HA	1.80	0.46
22:a:613:A:H2'	22:a:614:A:O4'	2.15	0.46
22:a:881:G:O6	22:a:895:U:C4	2.69	0.46
22:a:1842:G:H2'	22:a:1843:C:C6	2.51	0.46
22:a:2100:G:N2	22:a:2189:U:O2	2.36	0.46
52:4:16:CYS:HA	52:4:34:LEU:HB2	1.97	0.46
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.46
1:A:1225:A:H2'	1:A:1226:C:C5	2.51	0.46
9:I:28:ILE:HG12	9:I:63:LEU:HB2	1.98	0.46
10:J:36:VAL:HG12	10:J:76:ILE:HD13	1.96	0.46
22:a:897:C:H2'	22:a:898:C:C6	2.51	0.46
22:a:1199:U:H2'	22:a:1200:C:C6	2.51	0.46
22:a:1684:G:H2'	22:a:1685:C:C6	2.51	0.46
22:a:2477:U:O2	51:3:4:ARG:NH2	2.48	0.46
22:a:2522:U:O2'	22:a:2647:U:OP1	2.22	0.46
22:a:2557:G:H2'	22:a:2558:C:C6	2.50	0.46
40:s:6:ARG:O	40:s:10:VAL:HG13	2.15	0.46
43:v:50:ASN:HB2	43:v:82:ILE:HB	1.98	0.46
1:A:579:A:H2'	1:A:580:C:C6	2.51	0.46
1:A:946:A:H2'	1:A:947:G:H8	1.75	0.46
1:A:1410:A:H2'	1:A:1411:C:C6	2.51	0.46
7:G:14:PRO:HB2	7:G:19:GLY:HA2	1.97	0.46
32:k:29:LYS:O	32:k:29:LYS:HG2	2.15	0.46
1:A:309:A:H2'	1:A:310:G:H8	1.81	0.46
1:A:323:U:H2'	1:A:324:G:O4'	2.15	0.46
11:K:52:PHE:O	11:K:53:ARG:HD2	2.16	0.46
11:K:64:GLN:HB2	11:K:99:ALA:HB2	1.98	0.46
22:a:581:C:H2'	22:a:582:A:H8	1.81	0.46
22:a:613:A:H8	22:a:613:A:OP1	1.98	0.46
22:a:836:G:C5	22:a:837:C:C5	3.03	0.46
22:a:888:C:H2'	22:a:889:C:C6	2.51	0.46
26:e:191:ASP:O	26:e:195:GLN:HG3	2.15	0.46
44:w:17:ASN:HB2	44:w:25:THR:OG1	2.16	0.46
1:A:405:U:C5	4:D:5:LEU:HD11	2.50	0.46
1:A:501:C:H2'	1:A:502:A:H8	1.81	0.46
1:A:1030:U:O2'	1:A:1031:C:O2	2.33	0.46
22:a:279:A:N6	22:a:361:G:H1'	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1039:A:H2'	22:a:1040:A:O4'	2.16	0.46
22:a:1563:U:H2'	22:a:1564:C:C6	2.51	0.46
27:f:58:ALA:HB2	27:f:65:PRO:HD3	1.98	0.46
54:Z:29:C:H2'	54:Z:30:G:H8	1.81	0.46
1:A:90:C:H2'	1:A:91:U:C6	2.50	0.46
1:A:371:A:H2'	1:A:372:C:O4'	2.16	0.46
1:A:470:C:H2'	1:A:471:U:C6	2.50	0.46
2:B:188:ASP:OD1	2:B:189:THR:N	2.46	0.46
22:a:1363:C:O2'	22:a:1809:A:N3	2.44	0.46
22:a:2532:G:N2	22:a:2663:G:O2'	2.49	0.46
42:u:75:GLN:HB3	42:u:90:ASP:HB3	1.98	0.46
1:A:864:A:H4'	5:E:90:THR:HG23	1.97	0.45
22:a:160:A:N3	22:a:2208:C:O2'	2.44	0.45
22:a:184:C:H2'	22:a:185:G:H8	1.80	0.45
22:a:1394:U:H2'	22:a:1395:A:O4'	2.17	0.45
22:a:2064:C:H2'	22:a:2065:C:C6	2.51	0.45
22:a:2294:G:P	35:n:94:ARG:HH12	2.38	0.45
22:a:2515:C:H2'	22:a:2516:A:H8	1.81	0.45
22:a:2849:U:H4'	22:a:2868:A:C2	2.50	0.45
1:A:269:C:H2'	1:A:270:A:H8	1.81	0.45
21:U:51:SER:O	21:U:55:ARG:HG3	2.16	0.45
22:a:419:U:H2'	22:a:420:C:C6	2.50	0.45
22:a:518:G:H2'	22:a:519:U:C6	2.51	0.45
22:a:1412:U:H2'	22:a:1413:A:C8	2.50	0.45
27:f:147:ASP:OD1	27:f:150:ARG:NH1	2.49	0.45
28:g:17:VAL:HG11	28:g:50:LEU:HD11	1.97	0.45
39:r:109:ASP:OD2	39:r:110:ARG:HG2	2.17	0.45
1:A:539:A:P	12:L:111:LYS:HD2	2.56	0.45
22:a:39:G:H2'	22:a:40:U:C6	2.52	0.45
22:a:56:A:H5''	49:1:46:LYS:HE3	1.97	0.45
22:a:641:U:O2'	22:a:2350:C:OP1	2.32	0.45
22:a:1842:G:H2'	22:a:1843:C:H6	1.81	0.45
22:a:2514:U:H2'	22:a:2515:C:C6	2.52	0.45
1:A:1014:A:C2	1:A:1219:A:H1'	2.51	0.45
1:A:1033:G:H2'	1:A:1034:G:H8	1.81	0.45
19:S:21:LYS:O	19:S:24:GLU:HG3	2.16	0.45
22:a:279:A:H61	22:a:361:G:H1'	1.81	0.45
22:a:1496:A:H2'	22:a:1498:C:C5	2.52	0.45
27:f:144:ASP:OD1	27:f:144:ASP:N	2.44	0.45
1:A:414:A:C4	1:A:415:A:C8	3.05	0.45
1:A:1169:A:H2'	1:A:1170:A:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1463:U:H2'	1:A:1464:U:C6	2.51	0.45
22:a:277:G:OP2	22:a:277:G:H8	1.99	0.45
22:a:538:A:H5''	30:i:7:LYS:HE3	1.99	0.45
22:a:722:A:H2'	22:a:723:C:C6	2.51	0.45
22:a:1447:C:H2'	22:a:1448:G:H8	1.82	0.45
22:a:1476:U:H2'	22:a:1477:A:H8	1.81	0.45
22:a:2649:C:H2'	22:a:2650:U:C6	2.52	0.45
31:j:58:LEU:HA	31:j:89:ASN:OD1	2.16	0.45
47:z:52:ARG:CZ	47:z:54:VAL:HG12	2.46	0.45
49:1:22:MET:O	49:1:28:ARG:NH1	2.49	0.45
1:A:56:U:H2'	1:A:57:G:C8	2.52	0.45
13:M:70:ARG:HE	27:f:112:ARG:NH1	2.15	0.45
22:a:155:A:H2'	22:a:156:A:C8	2.52	0.45
22:a:2615:U:C2	47:z:4:GLN:HA	2.51	0.45
22:a:2812:G:H2'	22:a:2813:A:C8	2.51	0.45
23:b:14:U:OP2	23:b:70:C:O2'	2.35	0.45
24:c:132:MET:O	24:c:167:ARG:NH2	2.50	0.45
27:f:15:LYS:HE2	27:f:15:LYS:HB3	1.84	0.45
27:f:170:LEU:O	27:f:175:PHE:HB2	2.16	0.45
5:E:26:LYS:HB3	5:E:26:LYS:HE2	1.81	0.45
13:M:66:GLU:HB3	27:f:112:ARG:NH1	2.32	0.45
13:M:101:ARG:HE	13:M:104:THR:HB	1.82	0.45
22:a:272:A:H2'	22:a:273:G:H8	1.82	0.45
22:a:687:C:H1'	49:1:4:THR:HG22	1.97	0.45
22:a:874:G:C6	22:a:904:G:C6	3.05	0.45
22:a:1183:U:H2'	22:a:1184:U:C6	2.52	0.45
22:a:1590:A:H2'	22:a:1591:A:H8	1.80	0.45
22:a:1599:U:H2'	22:a:1600:C:C6	2.52	0.45
22:a:2636:C:H2'	22:a:2637:U:C6	2.52	0.45
24:c:240:PHE:O	24:c:242:LYS:NZ	2.45	0.45
35:n:4:LYS:O	35:n:8:ILE:HG12	2.16	0.45
38:q:52:PRO:HG2	38:q:53:PHE:CD2	2.51	0.45
1:A:1071:C:H2'	1:A:1072:G:C8	2.52	0.45
4:D:58:LYS:NZ	4:D:69:GLU:OE1	2.49	0.45
22:a:2:G:H2'	22:a:3:U:H6	1.82	0.45
22:a:784:G:H5'	22:a:785:G:OP1	2.15	0.45
40:s:56:GLU:N	40:s:56:GLU:OE1	2.50	0.45
1:A:73:C:O2'	1:A:74:A:H8	1.99	0.45
1:A:384:G:H2'	1:A:385:C:C6	2.52	0.45
1:A:407:U:H2'	1:A:408:A:C8	2.52	0.45
22:a:483:A:C8	41:t:45:HIS:HD2	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:568:U:OP1	32:k:36:LYS:HE2	2.17	0.45
46:y:3:LYS:HE2	46:y:40:ASP:HB3	1.98	0.45
1:A:592:G:H2'	1:A:593:U:C6	2.52	0.45
1:A:1314:C:OP1	19:S:6:LYS:NZ	2.32	0.45
1:A:1496:C:H2'	1:A:1497:G:O4'	2.17	0.45
22:a:1432:G:H2'	22:a:1433:A:C8	2.52	0.45
28:g:160:LYS:HB3	28:g:160:LYS:HE2	1.77	0.45
35:n:15:ARG:NH2	35:n:95:SER:OG	2.50	0.45
38:q:32:THR:HA	38:q:62:GLU:HA	1.99	0.45
38:q:83:TYR:OH	38:q:85:LYS:HE3	2.17	0.45
1:A:780:A:H5''	11:K:125:LYS:HD3	1.99	0.44
3:C:83:ASP:HA	3:C:86:LYS:HD2	1.98	0.44
7:G:86:GLN:HB2	7:G:148:ASN:OD1	2.16	0.44
16:P:8:ARG:CZ	16:P:15:PRO:HB3	2.47	0.44
22:a:608:A:H2'	22:a:609:A:C8	2.52	0.44
22:a:813:U:H2'	22:a:814:C:C6	2.53	0.44
22:a:1397:U:OP2	22:a:1398:C:N4	2.35	0.44
25:d:108:ASP:N	25:d:204:LYS:O	2.34	0.44
37:p:15:LYS:HB3	37:p:15:LYS:HE2	1.83	0.44
38:q:35:PHE:HB2	38:q:59:ILE:HB	1.99	0.44
41:t:97:LYS:O	41:t:98:SER:OG	2.34	0.44
42:u:48:MET:O	42:u:51:GLN:HG3	2.17	0.44
1:A:381:C:H2'	1:A:382:A:O4'	2.16	0.44
1:A:751:U:H2'	1:A:752:G:O4'	2.16	0.44
9:I:91:ASP:HB3	9:I:94:LEU:HD23	1.99	0.44
17:Q:14:SER:HB2	17:Q:22:VAL:HG12	1.98	0.44
22:a:5:A:H2'	22:a:6:A:H8	1.82	0.44
22:a:577:G:H2'	22:a:578:G:C8	2.52	0.44
22:a:2649:C:H2'	22:a:2650:U:H6	1.82	0.44
33:l:111:GLU:H	33:l:111:GLU:CD	2.26	0.44
46:y:4:THR:HB	46:y:37:GLU:HG2	2.00	0.44
1:A:965:U:H5''	1:A:966:2MG:OP1	2.17	0.44
1:A:1414:U:H2'	1:A:1415:G:H8	1.82	0.44
4:D:170:TRP:CD2	4:D:186:PRO:HB3	2.52	0.44
9:I:52:LEU:HD11	9:I:63:LEU:HD21	2.00	0.44
22:a:1028:A:N3	22:a:2486:C:O2'	2.40	0.44
22:a:1045:C:O2	22:a:1111:A:N6	2.50	0.44
22:a:2420:C:H4'	48:O:54:ILE:HG21	1.99	0.44
22:a:2818:U:H2'	22:a:2819:G:H8	1.81	0.44
24:c:76:ALA:HB2	24:c:96:TYR:CD1	2.52	0.44
25:d:35:THR:HG22	25:d:73:VAL:HG21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:89:LEU:CD2	28:g:162:VAL:HG22	2.48	0.44
41:t:85:PHE:CE1	41:t:94:ARG:HG2	2.52	0.44
1:A:335:C:H2'	1:A:336:A:C8	2.52	0.44
1:A:687:A:C2	1:A:704:A:C5	3.05	0.44
1:A:1025:U:H4'	1:A:1026:G:O4'	2.18	0.44
11:K:83:GLU:HG2	11:K:109:ASN:HD22	1.83	0.44
21:U:39:GLU:HG2	21:U:43:THR:HB	2.00	0.44
22:a:139:U:H5''	22:a:140:C:C5	2.47	0.44
22:a:948:C:H1'	22:a:984:A:C8	2.52	0.44
22:a:1799:G:O2'	24:c:180:GLU:OE2	2.17	0.44
22:a:1937:A:O2'	22:a:1939:5MU:OP2	2.33	0.44
22:a:2455:G:H2'	22:a:2456:C:C6	2.53	0.44
37:p:49:ASP:HA	37:p:52:GLN:HB2	1.98	0.44
43:v:25:ARG:HH11	43:v:31:VAL:HG12	1.83	0.44
1:A:275:G:H5'	17:Q:16:LYS:HE2	1.98	0.44
5:E:65:GLU:OE1	5:E:68:ARG:NH2	2.51	0.44
11:K:52:PHE:HD1	11:K:56:ARG:HE	1.66	0.44
11:K:84:VAL:HG11	11:K:97:ILE:HG12	1.99	0.44
15:O:17:ARG:H	15:O:17:ARG:HD3	1.81	0.44
22:a:909:A:H2'	22:a:912:C:H5	1.81	0.44
22:a:1199:U:H2'	22:a:1200:C:H6	1.83	0.44
22:a:2038:G:H2'	22:a:2039:U:O4'	2.16	0.44
32:k:62:PRO:HG2	50:2:25:LYS:HB3	1.99	0.44
1:A:1219:A:H2'	1:A:1220:G:C8	2.53	0.44
1:A:1457:G:OP1	20:T:34:LYS:NZ	2.41	0.44
5:E:134:ILE:HD12	5:E:134:ILE:H	1.82	0.44
6:F:88:MET:HE2	6:F:90:MET:CE	2.48	0.44
22:a:183:C:N4	22:a:213:A:H61	2.16	0.44
22:a:624:C:O2'	22:a:657:U:OP1	2.33	0.44
22:a:2591:C:H2'	22:a:2592:G:H8	1.83	0.44
1:A:544:G:OP2	4:D:63:ARG:NH2	2.51	0.44
1:A:883:C:O2'	1:A:884:U:H5'	2.18	0.44
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.52	0.44
18:R:68:LEU:HD23	18:R:68:LEU:HA	1.85	0.44
22:a:364:C:H2'	22:a:365:U:H6	1.81	0.44
22:a:1441:G:H2'	22:a:1442:U:C6	2.52	0.44
22:a:2000:C:OP1	34:m:5:LYS:NZ	2.43	0.44
22:a:2895:G:H2'	22:a:2896:C:C6	2.53	0.44
24:c:145:GLU:HB2	24:c:188:CYS:HB3	1.99	0.44
25:d:46:ARG:NH2	25:d:88:GLU:O	2.49	0.44
30:i:36:LEU:O	30:i:51:GLY:HA3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:m:49:GLU:OE2	34:m:95:THR:OG1	2.35	0.44
52:4:31:ASP:OD1	52:4:32:LEU:N	2.50	0.44
1:A:109:A:H5'	1:A:110:C:C5	2.52	0.44
1:A:826:C:O2	8:H:16:ASN:ND2	2.51	0.44
9:I:12:ARG:O	9:I:13:LYS:C	2.61	0.44
16:P:44:SER:N	16:P:47:GLU:OE1	2.42	0.44
22:a:305:C:H2'	22:a:306:U:C6	2.53	0.44
22:a:548:G:H5''	22:a:549:G:OP2	2.18	0.44
22:a:895:U:H2'	22:a:897:C:C6	2.52	0.44
22:a:1412:U:H2'	22:a:1413:A:H8	1.81	0.44
22:a:1447:C:H2'	22:a:1448:G:C8	2.53	0.44
22:a:2189:U:H1'	22:a:2190:G:H5'	2.00	0.44
22:a:2636:C:O2'	25:d:45:TYR:OH	2.34	0.44
27:f:64:LYS:HD3	52:4:5:ILE:HD12	2.00	0.44
31:j:121:GLU:OE2	36:o:65:SER:OG	2.36	0.44
48:0:10:LYS:O	48:0:52:ALA:N	2.44	0.44
49:1:3:ARG:HA	49:1:3:ARG:HD3	1.77	0.44
1:A:49:U:C2	1:A:361:G:N2	2.86	0.44
1:A:236:A:H2'	1:A:237:G:C8	2.52	0.44
1:A:399:G:H2'	1:A:400:C:H6	1.82	0.44
1:A:461:A:H2'	1:A:462:G:H8	1.82	0.44
1:A:555:U:H2'	1:A:556:C:H6	1.83	0.44
1:A:721:G:H4'	1:A:722:G:O4'	2.18	0.44
1:A:1151:A:O2'	1:A:1152:A:H8	2.01	0.44
4:D:160:GLU:O	4:D:163:GLU:HG2	2.17	0.44
6:F:12:PRO:O	6:F:44:ARG:NH2	2.51	0.44
22:a:279:A:H2'	22:a:280:U:O4'	2.17	0.44
22:a:479:A:N3	22:a:481:G:H5''	2.32	0.44
22:a:576:U:H2'	22:a:577:G:C8	2.52	0.44
22:a:897:C:H2'	22:a:898:C:H6	1.83	0.44
22:a:1370:C:H2'	22:a:1371:G:O4'	2.18	0.44
43:v:38:VAL:HG12	43:v:59:LEU:HB2	1.98	0.44
1:A:674:G:H2'	1:A:675:A:H8	1.83	0.43
6:F:44:ARG:HG3	6:F:44:ARG:NH1	2.30	0.43
8:H:77:ARG:NE	8:H:79:SER:O	2.51	0.43
14:N:22:ALA:O	14:N:26:GLU:OE1	2.36	0.43
21:U:7:ARG:N	21:U:10:GLU:OE2	2.40	0.43
22:a:878:A:N6	22:a:899:A:O2'	2.50	0.43
23:b:45:A:C4	23:b:46:A:C8	3.06	0.43
24:c:132:MET:HG3	24:c:188:CYS:O	2.17	0.43
28:g:37:LEU:HD23	28:g:37:LEU:HA	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:U:H2'	1:A:1119:C:C6	2.53	0.43
22:a:182:A:H2'	22:a:183:C:H6	1.83	0.43
22:a:207:A:H2'	22:a:208:C:O4'	2.19	0.43
22:a:634:C:H2'	22:a:635:C:C6	2.53	0.43
22:a:639:U:C2	22:a:640:C:C5	3.07	0.43
22:a:895:U:H2'	22:a:897:C:H6	1.84	0.43
22:a:1319:C:O2'	22:a:1320:C:H5'	2.18	0.43
22:a:1437:C:H2'	22:a:1438:U:C6	2.53	0.43
22:a:2247:A:H2'	22:a:2248:C:H6	1.83	0.43
24:c:246:THR:HG23	24:c:250:VAL:O	2.18	0.43
29:h:5:LEU:HD21	29:h:12:LEU:HD11	2.00	0.43
46:y:41:THR:HG22	46:y:43:ALA:H	1.83	0.43
1:A:908:A:H2'	1:A:909:A:C8	2.53	0.43
1:A:1236:A:H2'	1:A:1237:C:C6	2.53	0.43
12:L:31:ARG:O	12:L:58:THR:HG23	2.18	0.43
26:e:190:ALA:O	26:e:194:LYS:HG2	2.18	0.43
29:h:17:ASP:N	29:h:17:ASP:OD1	2.50	0.43
39:r:20:VAL:HG11	39:r:44:ALA:HA	2.00	0.43
46:y:45:ARG:HH12	46:y:59:GLU:CD	2.27	0.43
50:2:32:ILE:O	50:2:32:ILE:HG13	2.17	0.43
18:R:12:ARG:O	18:R:16:GLU:HG2	2.18	0.43
22:a:514:A:N3	22:a:581:C:O2'	2.42	0.43
22:a:1683:U:H2'	22:a:1684:G:H8	1.84	0.43
22:a:1869:G:N2	22:a:1871:A:H3'	2.32	0.43
22:a:2820:A:H4'	34:m:3:HIS:CD2	2.54	0.43
27:f:153:ASP:OD1	27:f:153:ASP:N	2.50	0.43
30:i:125:TYR:HH	30:i:132:HIS:CD2	2.34	0.43
36:o:3:ASN:HA	36:o:6:LYS:HG2	2.01	0.43
54:Z:19:G:H1'	54:Z:59:A:C2	2.53	0.43
1:A:34:C:H2'	1:A:35:G:H8	1.82	0.43
1:A:678:U:H2'	1:A:679:C:H6	1.84	0.43
1:A:736:C:H2'	1:A:737:C:C6	2.53	0.43
1:A:977:A:O2'	1:A:979:C:OP2	2.33	0.43
1:A:1144:G:H21	1:A:1146:A:H62	1.66	0.43
6:F:98:GLU:HG2	6:F:99:ALA:N	2.33	0.43
8:H:48:ASP:OD2	8:H:49:PHE:N	2.47	0.43
22:a:1212:G:H1'	22:a:1237:A:N6	2.33	0.43
22:a:2096:C:H2'	22:a:2097:A:H8	1.84	0.43
22:a:2193:G:H2'	22:a:2194:U:C6	2.54	0.43
28:g:60:ASP:O	28:g:62:TRP:N	2.50	0.43
28:g:145:ALA:HB1	28:g:164:TYR:HE1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:h:12:LEU:HD13	29:h:19:VAL:HG11	2.00	0.43
32:k:10:GLU:OE1	32:k:11:GLY:N	2.52	0.43
33:l:20:LEU:HD13	42:u:81:PRO:HG2	2.01	0.43
42:u:72:VAL:HG12	42:u:93:ARG:HA	2.01	0.43
1:A:41:G:H2'	1:A:42:G:C8	2.53	0.43
1:A:613:C:H2'	1:A:614:C:C6	2.54	0.43
3:C:70:THR:HG21	3:C:76:VAL:HG21	1.98	0.43
9:I:98:LEU:HD23	9:I:98:LEU:HA	1.78	0.43
21:U:3:VAL:O	21:U:4:ILE:HD13	2.18	0.43
22:a:17:G:H2'	22:a:18:U:C6	2.53	0.43
22:a:171:U:H2'	22:a:172:A:C8	2.53	0.43
22:a:479:A:H1'	22:a:480:A:H5''	2.01	0.43
22:a:1484:U:H2'	22:a:1485:U:H6	1.82	0.43
22:a:1509:A:O2'	22:a:1510:G:H8	2.01	0.43
22:a:2700:A:H2'	22:a:2701:U:C6	2.54	0.43
23:b:2:G:H2'	23:b:3:C:H6	1.83	0.43
28:g:105:LEU:HB2	28:g:113:VAL:HG13	1.99	0.43
30:i:99:ARG:HA	30:i:99:ARG:HD2	1.78	0.43
1:A:156:C:H2'	1:A:157:U:O4'	2.18	0.43
1:A:1180:A:OP1	9:I:105:THR:OG1	2.24	0.43
4:D:148:LYS:O	4:D:151:LYS:NZ	2.52	0.43
6:F:98:GLU:HG2	6:F:99:ALA:H	1.84	0.43
22:a:589:U:H2'	22:a:590:A:C8	2.54	0.43
34:m:71:ARG:HD2	34:m:71:ARG:HA	1.66	0.43
40:s:48:GLN:HE21	40:s:55:VAL:H	1.67	0.43
1:A:20:U:H2'	1:A:21:G:O4'	2.19	0.43
1:A:649:A:H2'	1:A:650:G:O4'	2.19	0.43
1:A:904:U:H2'	1:A:905:U:C6	2.53	0.43
1:A:1011:C:H2'	1:A:1012:A:H8	1.84	0.43
1:A:1175:G:H2'	1:A:1176:A:H8	1.84	0.43
1:A:1238:A:H2	1:A:1241:G:N3	2.17	0.43
9:I:57:MET:HA	9:I:60:LYS:NZ	2.33	0.43
9:I:94:LEU:HD13	9:I:97:GLU:OE2	2.19	0.43
22:a:891:G:C2	22:a:892:A:N7	2.87	0.43
22:a:1558:C:O4'	22:a:1560:G:C8	2.72	0.43
22:a:2072:C:H2'	22:a:2073:C:H6	1.83	0.43
22:a:2300:C:H2'	22:a:2301:C:H6	1.83	0.43
22:a:2687:U:H2'	22:a:2688:G:O4'	2.18	0.43
1:A:538:G:H2'	1:A:539:A:H8	1.82	0.43
1:A:1004:A:O2'	1:A:1036:A:N6	2.38	0.43
1:A:1251:A:H2'	1:A:1252:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:9:MET:SD	6:F:86:ARG:HB3	2.58	0.43
6:F:42:TRP:HB2	6:F:59:TYR:HB2	2.01	0.43
18:R:21:ILE:HG21	18:R:55:LEU:HD12	2.01	0.43
22:a:666:A:H4'	32:k:48:ARG:HD3	2.01	0.43
22:a:1212:G:O2'	22:a:1236:G:N2	2.42	0.43
22:a:1786:A:H1'	22:a:1938:A:N6	2.34	0.43
22:a:2756:U:H1'	22:a:2757:A:H5''	2.00	0.43
42:u:48:MET:SD	42:u:86:LEU:HD13	2.58	0.43
48:0:5:ILE:HG23	48:0:28:ARG:NH1	2.34	0.43
1:A:193:C:H2'	1:A:194:C:C6	2.53	0.43
1:A:216:U:H2'	1:A:217:C:H6	1.83	0.43
1:A:517:G:HO2'	1:A:518:C:P	2.42	0.43
3:C:118:ASP:HA	3:C:121:THR:OG1	2.19	0.43
9:I:9:THR:O	9:I:85:ARG:HD2	2.18	0.43
22:a:273:G:H2'	22:a:274:C:C6	2.54	0.43
22:a:499:U:H2'	22:a:500:G:O4'	2.19	0.43
22:a:863:A:H2'	22:a:864:G:H8	1.83	0.43
22:a:1586:A:H3'	22:a:1587:G:H8	1.83	0.43
22:a:1914:C:H2'	22:a:1915:3TD:H6	2.01	0.43
22:a:2329:U:H2'	22:a:2330:G:H8	1.84	0.43
22:a:2637:U:C2	22:a:2782:G:N2	2.87	0.43
22:a:2804:U:H2'	22:a:2805:C:C6	2.54	0.43
27:f:17:MET:SD	27:f:22:TYR:HB2	2.59	0.43
39:r:73:LYS:HB3	39:r:106:VAL:HB	2.00	0.43
1:A:62:U:OP1	1:A:385:C:O2'	2.31	0.42
7:G:132:GLY:O	7:G:135:VAL:HG22	2.19	0.42
17:Q:9:GLN:NE2	17:Q:79:VAL:HG21	2.33	0.42
22:a:1198:U:H2'	22:a:1199:U:C6	2.54	0.42
22:a:1774:C:O2	22:a:1774:C:H2'	2.19	0.42
22:a:1782:U:O2	22:a:2608:G:O2'	2.23	0.42
22:a:1790:C:H2'	22:a:1791:A:C8	2.53	0.42
22:a:1824:G:O3'	24:c:247:PRO:HD3	2.19	0.42
22:a:2747:G:O6	22:a:2755:C:H5''	2.18	0.42
40:s:14:PRO:HD3	45:x:30:MET:SD	2.59	0.42
45:x:2:LYS:HA	45:x:5:GLU:OE2	2.19	0.42
47:z:11:SER:O	47:z:15:MET:HG3	2.19	0.42
1:A:89:U:H2'	1:A:90:C:H6	1.84	0.42
1:A:444:G:C6	1:A:491:G:C6	3.07	0.42
1:A:619:U:O2	1:A:619:U:H2'	2.19	0.42
1:A:976:G:OP2	1:A:1358:U:O2'	2.35	0.42
1:A:1030:U:O2'	1:A:1031:C:P	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:C:H2'	1:A:1150:A:C8	2.53	0.42
3:C:47:LEU:HB3	3:C:50:ALA:HB3	2.00	0.42
3:C:153:VAL:HG22	3:C:198:VAL:HG22	2.01	0.42
4:D:139:PRO:HA	4:D:182:PHE:HD2	1.84	0.42
14:N:47:LYS:HD2	14:N:47:LYS:HA	1.85	0.42
22:a:64:A:H2'	22:a:65:U:H6	1.81	0.42
22:a:1181:U:H2'	22:a:1182:G:C8	2.54	0.42
22:a:1599:U:H2'	22:a:1600:C:H6	1.84	0.42
51:3:25:VAL:HB	51:3:35:GLN:HB2	2.01	0.42
1:A:171:A:H2'	1:A:172:A:C8	2.54	0.42
1:A:246:A:C2	1:A:282:A:C5	3.06	0.42
1:A:522:C:H41	12:L:50:ARG:NH2	2.17	0.42
1:A:1318:A:H1'	19:S:37:ARG:HH11	1.84	0.42
2:B:56:GLU:HG3	2:B:198:PHE:CE2	2.54	0.42
6:F:38:ARG:NH2	6:F:63:ASN:OD1	2.49	0.42
7:G:6:VAL:HG12	7:G:6:VAL:O	2.20	0.42
8:H:118:GLN:OE1	8:H:118:GLN:HA	2.19	0.42
22:a:711:G:C6	22:a:721:A:C6	3.06	0.42
22:a:2723:C:H2'	22:a:2724:U:O4'	2.20	0.42
22:a:2847:U:H2'	22:a:2848:G:O4'	2.19	0.42
30:i:34:ARG:HG3	30:i:39:LYS:HB2	2.00	0.42
51:3:18:LYS:HG3	51:3:23:ILE:HD13	2.02	0.42
54:Z:26:C:C2	54:Z:27:G:C8	3.08	0.42
1:A:280:C:N3	17:Q:41:THR:HG22	2.34	0.42
1:A:559:A:H4'	1:A:560:A:H3'	2.02	0.42
1:A:1162:C:H2'	1:A:1163:A:H8	1.83	0.42
1:A:1315:U:H2'	1:A:1316:G:O4'	2.20	0.42
22:a:1773:A:C8	22:a:1829:A:C8	3.07	0.42
22:a:1997:C:OP2	25:d:129:THR:OG1	2.30	0.42
22:a:2461:A:H2'	22:a:2462:C:C6	2.54	0.42
23:b:42:C:N3	27:f:90:THR:HG22	2.34	0.42
27:f:176:PRO:HG3	52:4:44:PHE:CE2	2.54	0.42
32:k:93:ASN:OD1	32:k:94:THR:N	2.53	0.42
35:n:63:LYS:HG3	35:n:64:TYR:N	2.34	0.42
42:u:86:LEU:HD23	42:u:89:ILE:HD11	2.02	0.42
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.42
13:M:83:LEU:HD11	19:S:66:MET:HG2	2.00	0.42
22:a:1281:G:H2'	22:a:1282:U:C6	2.55	0.42
22:a:1349:C:C2	22:a:1350:C:C5	3.08	0.42
22:a:1499:C:C2	22:a:1500:G:C8	3.08	0.42
33:l:110:GLU:O	33:l:114:ARG:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:q:62:GLU:N	38:q:62:GLU:OE1	2.53	0.42
54:Z:55:5MU:H2'	54:Z:56:PSU:O4'	2.20	0.42
1:A:562:U:H1'	12:L:12:ARG:HB3	2.01	0.42
1:A:636:U:OP1	17:Q:6:ARG:NE	2.52	0.42
9:I:5:GLN:OE1	9:I:5:GLN:N	2.53	0.42
22:a:404:A:H1'	22:a:405:U:OP2	2.19	0.42
22:a:538:A:H4'	30:i:7:LYS:HG2	2.02	0.42
27:f:105:THR:HA	52:4:38:SER:HB2	2.01	0.42
28:g:164:TYR:HB2	28:g:167:GLU:HB2	2.02	0.42
30:i:31:GLU:OE1	30:i:34:ARG:NH1	2.52	0.42
42:u:75:GLN:HB2	42:u:92:VAL:HG23	2.00	0.42
54:Z:51:U:H2'	54:Z:52:C:C6	2.55	0.42
1:A:1125:U:OP1	10:J:37:ARG:NE	2.52	0.42
1:A:1312:G:OP2	52:4:63:ARG:NH2	2.49	0.42
13:M:81:MET:HE3	22:a:888:C:C2	2.55	0.42
14:N:24:ARG:NH1	14:N:55:SER:OG	2.53	0.42
14:N:73:PHE:CZ	14:N:78:GLY:HA2	2.55	0.42
15:O:3:LEU:HD23	15:O:3:LEU:HA	1.93	0.42
22:a:18:U:H2'	22:a:19:A:C8	2.55	0.42
22:a:191:A:H2'	22:a:192:C:H6	1.85	0.42
22:a:756:A:H2'	22:a:757:G:O4'	2.20	0.42
22:a:881:G:H2'	22:a:882:G:H8	1.85	0.42
22:a:1039:A:H2	22:a:1116:G:H22	1.68	0.42
22:a:1830:C:H2'	22:a:1831:G:H8	1.85	0.42
22:a:2266:A:H4'	22:a:2267:A:C2	2.55	0.42
22:a:2896:C:H2'	22:a:2897:U:C6	2.54	0.42
43:v:37:ILE:HG21	43:v:80:ILE:HG21	2.01	0.42
44:w:71:LEU:HG	44:w:76:GLU:OE2	2.20	0.42
1:A:62:U:H2'	1:A:63:C:C6	2.54	0.42
1:A:312:C:H2'	1:A:313:A:H8	1.85	0.42
1:A:864:A:H2'	1:A:865:A:C8	2.54	0.42
7:G:79:ARG:HH21	7:G:82:GLY:HA2	1.85	0.42
11:K:87:LYS:HB2	11:K:113:VAL:HG23	2.00	0.42
19:S:80:TYR:CZ	19:S:82:GLY:HA2	2.54	0.42
22:a:75:G:H22	22:a:111:A:H2	1.67	0.42
22:a:2328:A:H2'	22:a:2329:U:H6	1.78	0.42
25:d:128:ARG:HA	25:d:128:ARG:HD3	1.80	0.42
27:f:65:PRO:HA	27:f:89:VAL:HG12	2.01	0.42
35:n:111:ARG:HA	35:n:115:LEU:O	2.20	0.42
1:A:620:C:C2	4:D:132:ILE:HD13	2.55	0.42
1:A:779:C:H2'	1:A:780:A:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1157:A:C2	1:A:1181:G:C4	3.08	0.42
1:A:1244:G:H2'	1:A:1245:C:C6	2.55	0.42
1:A:1250:A:H2'	1:A:1251:A:C8	2.54	0.42
1:A:1286:U:H2'	1:A:1287:A:H5'	2.01	0.42
1:A:1526:G:H2'	1:A:1527:U:C6	2.54	0.42
3:C:16:LYS:HA	3:C:16:LYS:HD3	1.83	0.42
13:M:92:ARG:NH1	22:a:887:U:H5''	2.35	0.42
21:U:58:LYS:HG3	21:U:59:LYS:N	2.35	0.42
22:a:45:G:H5''	22:a:46:G:O5'	2.19	0.42
22:a:445:C:H2'	22:a:446:G:O4'	2.20	0.42
22:a:632:A:H2'	22:a:633:A:C8	2.55	0.42
22:a:1476:U:H2'	22:a:1477:A:C8	2.55	0.42
29:h:34:GLY:C	29:h:36:ALA:H	2.28	0.42
30:i:92:MET:HE3	30:i:92:MET:HB3	1.90	0.42
31:j:105:ARG:HH11	31:j:108:ARG:NH1	2.17	0.42
1:A:678:U:H2'	1:A:679:C:C6	2.55	0.42
10:J:21:ALA:HB1	10:J:92:LEU:HD12	2.01	0.42
22:a:2096:C:H2'	22:a:2097:A:C8	2.55	0.42
27:f:121:SER:HB2	27:f:128:TYR:CE1	2.55	0.42
28:g:127:THR:HB	28:g:130:GLU:OE1	2.19	0.42
52:4:41:HIS:HB3	52:4:44:PHE:CD1	2.55	0.42
1:A:408:A:H2'	1:A:409:U:C6	2.54	0.41
1:A:983:A:H5'	1:A:984:C:OP2	2.20	0.41
1:A:1513:A:H2'	1:A:1514:G:C8	2.55	0.41
1:A:1526:G:H2'	1:A:1527:U:H6	1.85	0.41
4:D:65:TYR:OH	4:D:95:GLU:OE2	2.26	0.41
10:J:15:HIS:HB3	10:J:70:HIS:CE1	2.55	0.41
22:a:723:C:H2'	22:a:724:U:O4'	2.20	0.41
22:a:959:A:H2'	22:a:960:A:C8	2.55	0.41
22:a:966:G:C1'	22:a:2267:A:H62	2.33	0.41
22:a:1545:A:H2'	22:a:1546:G:O4'	2.20	0.41
22:a:1790:C:H2'	22:a:1791:A:C5	2.55	0.41
22:a:1814:G:OP2	22:a:1815:A:O2'	2.23	0.41
22:a:2100:G:H2'	22:a:2101:A:C8	2.54	0.41
22:a:2241:A:H2'	22:a:2242:G:C8	2.55	0.41
22:a:2804:U:H2'	22:a:2805:C:H6	1.84	0.41
28:g:137:ASP:HB3	28:g:140:VAL:HB	2.02	0.41
41:t:81:ASP:OD1	41:t:82:ARG:N	2.52	0.41
54:Z:11:A:H2'	54:Z:12:G:C8	2.54	0.41
1:A:543:U:OP1	4:D:14:ARG:HD2	2.20	0.41
1:A:737:C:H2'	1:A:738:C:H6	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:C:H2'	1:A:986:U:C6	2.54	0.41
3:C:114:LYS:HB2	3:C:185:ASN:HD22	1.85	0.41
10:J:46:LYS:HG2	10:J:68:ARG:HG2	2.02	0.41
14:N:79:LEU:HB2	14:N:84:VAL:HG23	2.02	0.41
22:a:181:A:H1'	22:a:435:C:H5'	2.02	0.41
22:a:434:U:O2	22:a:436:C:N4	2.53	0.41
22:a:1473:G:H2'	22:a:1474:U:C6	2.54	0.41
22:a:1736:U:H2'	22:a:1737:G:O4'	2.20	0.41
22:a:1889:A:H2'	22:a:1890:A:C8	2.55	0.41
22:a:2193:G:H2'	22:a:2194:U:H6	1.85	0.41
22:a:2291:U:OP1	22:a:2380:C:O2'	2.38	0.41
24:c:225:MET:SD	24:c:230:HIS:HB2	2.60	0.41
28:g:105:LEU:HB3	28:g:107:LEU:HG	2.02	0.41
30:i:49:ASP:OD1	30:i:121:LYS:NZ	2.46	0.41
1:A:90:C:H2'	1:A:91:U:H6	1.85	0.41
1:A:1039:G:H2'	1:A:1040:U:H6	1.85	0.41
1:A:1263:C:H2'	1:A:1264:U:H6	1.85	0.41
6:F:39:LEU:HD13	6:F:62:MET:HG2	2.02	0.41
22:a:52:A:H2'	22:a:53:A:C8	2.56	0.41
22:a:2020:A:H5'	47:z:9:THR:CG2	2.50	0.41
22:a:2787:C:H1'	25:d:63:PRO:HG3	2.03	0.41
24:c:210:ALA:HA	24:c:213:TRP:CE3	2.55	0.41
28:g:170:ARG:HH12	51:3:31:PRO:HD3	1.86	0.41
30:i:23:LYS:NZ	30:i:142:ILE:OXT	2.43	0.41
31:j:80:ASP:OD2	36:o:69:GLY:HA3	2.20	0.41
31:j:105:ARG:HH11	31:j:108:ARG:HH12	1.69	0.41
52:4:12:ILE:HG13	52:4:13:THR:N	2.35	0.41
1:A:184:G:H2'	1:A:185:U:C6	2.55	0.41
1:A:508:U:C1'	1:A:509:A:H2	2.33	0.41
1:A:821:G:H2'	1:A:822:U:C6	2.55	0.41
6:F:69:GLU:O	6:F:73:GLU:OE1	2.38	0.41
9:I:94:LEU:HA	9:I:97:GLU:OE2	2.21	0.41
11:K:35:THR:HG1	11:K:40:ASN:C	2.27	0.41
22:a:596:U:H2'	22:a:597:G:H8	1.86	0.41
22:a:1654:A:O2'	25:d:118:PHE:O	2.37	0.41
22:a:2100:G:O6	22:a:2189:U:C4	2.72	0.41
22:a:2773:C:H2'	22:a:2774:C:C6	2.56	0.41
1:A:592:G:H2'	1:A:593:U:H6	1.85	0.41
1:A:695:A:H2'	1:A:696:A:C8	2.56	0.41
1:A:859:G:H2'	1:A:860:A:C8	2.56	0.41
1:A:978:A:C2	1:A:1319:A:C4	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:U:OP1	2:B:174:LYS:NZ	2.30	0.41
1:A:1464:U:H2'	1:A:1465:A:H8	1.85	0.41
4:D:105:MET:HE1	4:D:143:VAL:HB	2.02	0.41
22:a:169:G:H2'	22:a:170:U:C6	2.55	0.41
22:a:417:C:H2'	22:a:418:C:C6	2.55	0.41
22:a:483:A:H5''	41:t:47:LYS:HD2	2.00	0.41
22:a:820:A:H4'	22:a:836:G:N2	2.36	0.41
22:a:1744:A:H3'	22:a:1745:A:H8	1.86	0.41
22:a:2098:U:H2'	22:a:2099:U:O4'	2.21	0.41
22:a:2627:G:N2	22:a:2777:G:OP2	2.53	0.41
41:t:14:LEU:HD11	41:t:71:ALA:HB2	2.01	0.41
54:Z:1:C:H2'	54:Z:2:G:H8	1.86	0.41
1:A:110:C:O2'	16:P:25:ARG:O	2.32	0.41
1:A:255:G:H2'	1:A:256:U:C6	2.55	0.41
7:G:27:VAL:HG11	7:G:40:GLU:HG3	2.03	0.41
9:I:25:ASN:OD1	9:I:25:ASN:N	2.54	0.41
11:K:97:ILE:HG22	21:U:12:PHE:HZ	1.86	0.41
12:L:106:GLY:O	12:L:108:LYS:NZ	2.54	0.41
13:M:48:LEU:HD23	13:M:48:LEU:HA	1.86	0.41
17:Q:58:VAL:HG12	17:Q:79:VAL:HB	2.03	0.41
22:a:553:G:H2'	22:a:554:U:H6	1.86	0.41
22:a:832:U:H2'	22:a:833:A:H8	1.86	0.41
22:a:1429:G:H2'	22:a:1430:G:H8	1.85	0.41
22:a:1637:A:H5'	22:a:1760:C:O2'	2.21	0.41
22:a:2100:G:N1	22:a:2189:U:N3	2.33	0.41
30:i:26:GLY:O	30:i:30:THR:HG23	2.20	0.41
41:t:98:SER:OG	41:t:98:SER:O	2.33	0.41
49:1:22:MET:HE3	49:1:22:MET:HB3	1.86	0.41
1:A:2:A:H4'	4:D:83:LYS:HZ2	1.85	0.41
1:A:1163:A:H2'	1:A:1164:G:C8	2.55	0.41
7:G:71:PRO:O	7:G:96:ARG:HG2	2.21	0.41
22:a:170:U:H2'	22:a:171:U:C6	2.56	0.41
22:a:194:G:H2'	22:a:195:A:O4'	2.20	0.41
22:a:438:G:H2'	22:a:439:A:C8	2.55	0.41
26:e:3:LEU:O	26:e:12:LEU:N	2.48	0.41
27:f:46:ASP:HB3	27:f:49:LEU:HG	2.02	0.41
29:h:2:GLN:HB3	29:h:39:ALA:HB3	2.03	0.41
29:h:12:LEU:HD12	29:h:13:GLY:N	2.36	0.41
32:k:19:LEU:HD13	32:k:31:GLY:HA3	2.02	0.41
1:A:219:U:H2'	1:A:220:G:C8	2.55	0.41
1:A:457:G:H3'	1:A:458:U:H6	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1412:C:H2'	1:A:1413:A:C8	2.55	0.41
3:C:72:ARG:HB3	3:C:75:ILE:HD12	2.02	0.41
6:F:10:VAL:HB	6:F:58:HIS:HB3	2.03	0.41
6:F:90:MET:HE1	18:R:23:TYR:OH	2.21	0.41
22:a:151:C:H2'	22:a:152:A:H8	1.85	0.41
22:a:273:G:H2'	22:a:274:C:H6	1.86	0.41
22:a:286:U:H2'	22:a:287:G:H8	1.85	0.41
22:a:835:C:C2	22:a:836:G:C8	3.08	0.41
22:a:852:U:H2'	22:a:853:C:C6	2.56	0.41
22:a:1361:G:H2'	22:a:1362:C:C6	2.56	0.41
22:a:1446:C:H2'	22:a:1447:C:C6	2.56	0.41
22:a:1614:A:C6	39:r:87:PRO:HB3	2.56	0.41
22:a:2700:A:H2'	22:a:2701:U:H6	1.86	0.41
24:c:240:PHE:O	24:c:242:LYS:HG3	2.21	0.41
25:d:152:PRO:HG3	25:d:156:PHE:CZ	2.56	0.41
33:l:56:ALA:HB2	33:l:119:LEU:HD12	2.03	0.41
47:z:43:ILE:HG22	47:z:49:TYR:HB2	2.02	0.41
1:A:31:G:O2'	1:A:48:C:N4	2.54	0.41
1:A:160:A:H2'	1:A:161:A:O4'	2.20	0.41
1:A:486:U:H2'	1:A:487:A:C8	2.56	0.41
1:A:707:U:H4'	11:K:22:HIS:CD2	2.56	0.41
1:A:1125:U:C2	1:A:1127:G:C8	3.09	0.41
1:A:1206:G:H2'	1:A:1207:2MG:O4'	2.20	0.41
1:A:1233:G:OP1	9:I:119:ARG:NH1	2.53	0.41
1:A:1266:G:N2	1:A:1269:A:OP2	2.43	0.41
2:B:167:ASP:HB2	2:B:191:SER:HB2	2.03	0.41
5:E:89:HIS:O	5:E:90:THR:C	2.64	0.41
9:I:23:PRO:HA	9:I:61:LEU:HD23	2.02	0.41
12:L:10:LYS:HB3	12:L:10:LYS:HE3	1.71	0.41
12:L:108:LYS:HA	12:L:108:LYS:HD3	1.90	0.41
13:M:69:LEU:O	13:M:73:ILE:HG12	2.21	0.41
22:a:176:A:O2'	22:a:177:G:H5'	2.21	0.41
22:a:184:C:H2'	22:a:185:G:C8	2.56	0.41
22:a:283:G:H2'	22:a:284:U:O4'	2.21	0.41
22:a:288:U:H2'	22:a:289:G:H8	1.85	0.41
22:a:839:U:H2'	22:a:840:C:C6	2.56	0.41
22:a:1028:A:N6	22:a:1125:G:H2'	2.36	0.41
22:a:1315:C:H2'	22:a:1316:U:C6	2.56	0.41
22:a:1354:A:H2'	22:a:1355:G:O4'	2.21	0.41
22:a:1473:G:C6	22:a:1519:G:C6	3.08	0.41
22:a:1710:G:H2'	22:a:1711:A:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2625:G:H2'	22:a:2626:C:O4'	2.20	0.41
22:a:2811:G:H5''	25:d:61:THR:HG23	2.03	0.41
22:a:2820:A:N3	22:a:2820:A:H2'	2.35	0.41
23:b:39:A:H2'	23:b:40:U:C6	2.56	0.41
37:p:58:ARG:HA	37:p:61:TRP:CE3	2.55	0.41
39:r:19:LEU:HD23	39:r:19:LEU:HA	1.89	0.41
52:4:16:CYS:SG	52:4:17:SER:N	2.94	0.41
54:Z:10:G:N2	54:Z:27:G:H1'	2.36	0.41
54:Z:44:A:H2'	54:Z:45:A:C8	2.56	0.41
1:A:3:A:N1	1:A:628:G:O2'	2.40	0.41
1:A:453:G:C4	1:A:454:G:C8	3.09	0.41
1:A:472:U:H2'	1:A:473:U:C6	2.56	0.41
1:A:696:A:H2'	1:A:697:U:C6	2.54	0.41
1:A:1060:U:H2'	1:A:1061:G:H8	1.85	0.41
1:A:1144:G:O6	1:A:1145:A:N6	2.54	0.41
1:A:1435:G:H2'	1:A:1436:U:C6	2.56	0.41
5:E:13:GLU:HG2	5:E:39:VAL:HG12	2.02	0.41
6:F:67:PRO:HB2	6:F:69:GLU:CD	2.46	0.41
22:a:2373:G:H2'	22:a:2374:C:C6	2.56	0.41
31:j:17:ARG:HB2	31:j:45:GLU:HG3	2.03	0.41
32:k:78:ARG:HG2	32:k:113:ALA:HB3	2.03	0.41
37:p:95:LEU:HD23	37:p:95:LEU:HA	1.93	0.41
47:z:38:HIS:ND1	47:z:39:LEU:O	2.53	0.41
50:2:55:LEU:HD23	50:2:55:LEU:HA	1.93	0.41
1:A:67:C:H2'	1:A:68:G:C8	2.56	0.40
1:A:184:G:H2'	1:A:185:U:H6	1.85	0.40
1:A:619:U:H2'	1:A:619:U:OP1	2.21	0.40
4:D:62:ARG:HE	4:D:62:ARG:HB3	1.76	0.40
16:P:52:LEU:HD12	16:P:78:VAL:HG11	2.03	0.40
20:T:4:ILE:O	20:T:8:LYS:HG3	2.21	0.40
22:a:40:U:H2'	22:a:41:C:C6	2.55	0.40
22:a:78:U:H2'	22:a:79:C:C6	2.57	0.40
22:a:765:C:H2'	22:a:766:U:C6	2.56	0.40
22:a:810:U:C4	32:k:29:LYS:O	2.74	0.40
22:a:1575:C:H2'	22:a:1576:U:O4'	2.22	0.40
22:a:1685:C:H2'	22:a:1686:C:H6	1.87	0.40
22:a:2301:C:H2'	22:a:2302:U:C6	2.56	0.40
22:a:2859:G:H2'	22:a:2860:A:C8	2.56	0.40
26:e:7:ASP:OD1	26:e:8:ALA:N	2.53	0.40
30:i:106:LYS:HG2	30:i:119:PHE:CD1	2.56	0.40
47:z:12:LYS:HB3	47:z:12:LYS:HE3	1.58	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:4:26:SER:OG	52:4:28:VAL:HG23	2.20	0.40
1:A:924:C:O2'	1:A:1502:A:N1	2.51	0.40
2:B:130:THR:O	2:B:132:LYS:N	2.54	0.40
3:C:134:MET:HE2	3:C:168:TYR:HD2	1.86	0.40
4:D:102:VAL:HG11	4:D:117:LEU:HD11	2.03	0.40
8:H:38:ASN:O	8:H:42:GLU:HG3	2.21	0.40
9:I:88:MET:HE1	9:I:95:ARG:HA	2.03	0.40
11:K:70:CYS:O	11:K:74:VAL:HG22	2.20	0.40
12:L:99:ARG:HB3	12:L:117:TYR:HA	2.02	0.40
13:M:71:ARG:NH2	27:f:113:ASP:OD2	2.54	0.40
14:N:83:LYS:HA	14:N:83:LYS:HD3	1.77	0.40
22:a:12:U:O2	22:a:2626:C:H4'	2.21	0.40
22:a:161:A:OP2	22:a:162:U:O2'	2.29	0.40
22:a:357:C:H2'	22:a:358:U:C6	2.57	0.40
22:a:1480:C:H2'	22:a:1481:U:O4'	2.22	0.40
22:a:1684:G:H2'	22:a:1685:C:H6	1.85	0.40
22:a:2364:C:H2'	22:a:2365:G:O4'	2.21	0.40
22:a:2818:U:H2'	22:a:2819:G:C8	2.56	0.40
33:l:53:MET:HE3	33:l:53:MET:HB2	1.97	0.40
54:Z:15:G:N2	54:Z:22:A:N3	2.70	0.40
1:A:244:U:O4	1:A:906:A:H1'	2.21	0.40
1:A:1158:C:C4	1:A:1160:G:C8	3.10	0.40
1:A:1263:C:H2'	1:A:1264:U:C6	2.56	0.40
5:E:81:LEU:HB2	5:E:98:PRO:HG3	2.02	0.40
13:M:22:ILE:HG23	13:M:66:GLU:OE2	2.21	0.40
22:a:896:A:N7	22:a:897:C:H1'	2.36	0.40
22:a:903:C:H2'	22:a:904:G:C8	2.54	0.40
22:a:1046:A:H5'	22:a:1047:G:H5''	2.04	0.40
22:a:1444:G:C4	22:a:1445:G:C8	3.09	0.40
22:a:1571:A:H2'	22:a:1572:A:C8	2.55	0.40
22:a:1874:C:H2'	22:a:1875:G:O4'	2.21	0.40
22:a:2292:U:H2'	22:a:2293:G:C8	2.56	0.40
22:a:2638:G:O2'	22:a:2775:G:N2	2.50	0.40
25:d:105:LYS:HA	25:d:105:LYS:HD3	1.70	0.40
39:r:13:SER:O	39:r:17:VAL:HG23	2.21	0.40
54:Z:20:G:H3'	54:Z:21:H2U:N3	2.37	0.40
1:A:41:G:H2'	1:A:42:G:H8	1.87	0.40
1:A:253:A:H2'	1:A:254:G:C8	2.57	0.40
1:A:490:C:H2'	1:A:491:G:H8	1.85	0.40
5:E:160:SER:O	5:E:164:ILE:HG12	2.21	0.40
7:G:113:ASP:HB2	7:G:119:ARG:CG	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:18:U:H2'	22:a:19:A:H8	1.86	0.40
22:a:157:C:H2'	22:a:158:U:O4'	2.22	0.40
22:a:340:A:O2'	26:e:162:ARG:NH1	2.54	0.40
22:a:493:G:H2'	22:a:494:G:O4'	2.21	0.40
22:a:729:G:OP1	24:c:10:SER:OG	2.35	0.40
22:a:1535:A:O2'	22:a:1537:G:N1	2.55	0.40
22:a:1683:U:H2'	22:a:1684:G:C8	2.56	0.40
22:a:1710:G:H4'	22:a:2858:C:O2	2.21	0.40
22:a:2728:U:HO2'	22:a:2729:G:H8	1.70	0.40
22:a:2728:U:O2'	22:a:2729:G:H8	2.05	0.40
23:b:48:U:H2'	23:b:49:C:C6	2.57	0.40
29:h:15:LEU:HD23	29:h:16:GLY:N	2.36	0.40
35:n:17:LYS:O	35:n:20:GLU:HG2	2.21	0.40
45:x:9:LYS:HB3	45:x:13:GLU:HB2	2.03	0.40
1:A:260:G:H2'	1:A:261:U:C6	2.56	0.40
1:A:538:G:H2'	1:A:539:A:C8	2.56	0.40
1:A:1037:C:H2'	1:A:1038:C:H6	1.86	0.40
2:B:136:MET:HE2	2:B:136:MET:HB3	2.00	0.40
4:D:109:ALA:H	4:D:113:GLU:HG2	1.85	0.40
6:F:4:TYR:CE2	6:F:71:ILE:HG13	2.56	0.40
12:L:36:ARG:HG2	12:L:38:TYR:HD1	1.87	0.40
22:a:287:G:H2'	22:a:288:U:C6	2.56	0.40
22:a:682:G:H5'	49:1:26:ASN:ND2	2.36	0.40
22:a:1495:A:H2'	22:a:1496:A:C8	2.57	0.40
22:a:1677:A:H2'	22:a:1678:A:C8	2.56	0.40
24:c:52:ARG:O	24:c:53:HIS:HB2	2.21	0.40
28:g:140:VAL:O	28:g:144:VAL:HG23	2.21	0.40
45:x:7:ARG:O	45:x:60:LYS:NZ	2.48	0.40
54:Z:17:C:H5'	54:Z:62:C:OP1	2.21	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	
2	B	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
3	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
5	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
6	F	101/135 (75%)	95 (94%)	6 (6%)	0	100	100
7	G	151/179 (84%)	139 (92%)	12 (8%)	0	100	100
8	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
9	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
10	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	28
11	K	113/129 (88%)	105 (93%)	8 (7%)	0	100	100
12	L	120/124 (97%)	111 (92%)	9 (8%)	0	100	100
13	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	77/84 (92%)	77 (100%)	0	0	100	100
18	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
19	S	82/92 (89%)	82 (100%)	0	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
24	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	d	206/209 (99%)	202 (98%)	3 (2%)	1 (0%)	24	46
26	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
27	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
28	g	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
29	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
30	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
31	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
32	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
33	l	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
34	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
35	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
39	r	108/110 (98%)	108 (100%)	0	0	100	100
40	s	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
41	t	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
42	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
43	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
44	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
45	x	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	54 (100%)	0	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	16
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5481/5913 (93%)	5281 (96%)	197 (4%)	3 (0%)	49	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	d	149	ASN
10	J	57	VAL
50	2	32	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	115 (99%)	1 (1%)	70	87
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	59/63 (94%)	59 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4573/4825 (95%)	4572 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	i	128	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	69	HIS
4	D	36	GLN
4	D	136	GLN
5	E	97	GLN
5	E	121	HIS
5	E	122	ASN
5	E	132	ASN
7	G	68	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	130	ASN
8	H	18	GLN
8	H	38	ASN
9	I	4	ASN
9	I	37	GLN
11	K	109	ASN
13	M	8	ASN
13	M	12	HIS
14	N	4	GLN
16	P	79	ASN
17	Q	9	GLN
20	T	48	GLN
24	c	90	ASN
24	c	115	GLN
24	c	134	ASN
25	d	173	GLN
26	e	9	GLN
26	e	62	GLN
26	e	115	GLN
28	g	22	GLN
28	g	73	ASN
28	g	88	GLN
29	h	11	ASN
31	j	93	GLN
33	l	13	HIS
33	l	97	GLN
35	n	98	GLN
36	o	66	ASN
40	s	48	GLN
40	s	70	HIS
40	s	72	GLN
41	t	74	ASN
43	v	12	ASN
44	w	36	HIS
45	x	15	ASN
45	x	45	GLN
49	1	26	ASN
52	4	30	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1542 (97%)	201 (13%)	6 (0%)
22	a	2757/2904 (94%)	301 (10%)	0
23	b	118/120 (98%)	13 (11%)	0
53	X	5/66 (7%)	0	0
54	Z	76/77 (98%)	10 (13%)	0
All	All	4464/4709 (94%)	525 (11%)	6 (0%)

All (525) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	A
1	A	4	U
1	A	7	A
1	A	9	G
1	A	22	G
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	71	A
1	A	73	C
1	A	74	A
1	A	78	A
1	A	91	U
1	A	94	G
1	A	95	C
1	A	116	A
1	A	121	U
1	A	122	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	143	A
1	A	144	G
1	A	149	A
1	A	164	G
1	A	166	U
1	A	177	G
1	A	182	A
1	A	183	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	189	A
1	A	197	A
1	A	199	A
1	A	200	G
1	A	204	G
1	A	215	C
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	392	C
1	A	397	A
1	A	406	G
1	A	411	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	416	G
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	453	G
1	A	457	G
1	A	458	U
1	A	467	U
1	A	468	A
1	A	474	G
1	A	478	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	479	U
1	A	481	G
1	A	482	A
1	A	484	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	497	G
1	A	499	A
1	A	505	G
1	A	509	A
1	A	511	C
1	A	513	C
1	A	517	G
1	A	518	C
1	A	521	G
1	A	527	G7M
1	A	530	G
1	A	532	A
1	A	533	A
1	A	545	C
1	A	546	A
1	A	547	A
1	A	559	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	596	A
1	A	619	U
1	A	620	C
1	A	633	G
1	A	637	C
1	A	639	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	687	A
1	A	721	G
1	A	723	U
1	A	724	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	734	G
1	A	747	A
1	A	748	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	802	A
1	A	815	A
1	A	817	C
1	A	819	A
1	A	832	G
1	A	890	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	965	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1009	U
1	A	1017	U
1	A	1024	G
1	A	1031	C
1	A	1032	G
1	A	1035	A
1	A	1036	A
1	A	1042	A
1	A	1044	A
1	A	1053	G
1	A	1065	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1137	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1139	G
1	A	1159	U
1	A	1171	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1227	A
1	A	1238	A
1	A	1260	G
1	A	1275	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1368	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1419	G
1	A	1432	G
1	A	1446	A
1	A	1451	U
1	A	1487	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1519	MA6
1	A	1529	G
1	A	1530	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	10	A
22	a	15	G
22	a	34	U
22	a	35	G
22	a	42	A
22	a	51	G
22	a	71	A
22	a	74	A
22	a	75	G
22	a	80	G
22	a	101	A
22	a	102	U
22	a	118	A
22	a	119	A
22	a	120	U
22	a	139	U
22	a	142	A
22	a	163	C
22	a	181	A
22	a	196	A
22	a	199	A
22	a	215	G
22	a	216	A
22	a	222	A
22	a	223	A
22	a	233	A
22	a	248	G
22	a	272	A
22	a	275	C
22	a	278	A
22	a	281	C
22	a	282	A
22	a	283	G
22	a	285	G
22	a	288	U
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	356	G
22	a	362	A
22	a	383	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	386	G
22	a	396	G
22	a	404	A
22	a	405	U
22	a	411	G
22	a	412	A
22	a	435	C
22	a	481	G
22	a	491	G
22	a	505	A
22	a	509	C
22	a	529	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	547	A
22	a	548	G
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	592	A
22	a	603	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C
22	a	647	G
22	a	654	A
22	a	686	U
22	a	717	C
22	a	730	A
22	a	738	G
22	a	747	5MU
22	a	764	A
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	789	A
22	a	792	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	805	G
22	a	811	U
22	a	812	C
22	a	827	U
22	a	828	U
22	a	845	A
22	a	846	U
22	a	847	U
22	a	859	G
22	a	883	G
22	a	884	U
22	a	888	C
22	a	890	C
22	a	891	G
22	a	893	C
22	a	895	U
22	a	896	A
22	a	897	C
22	a	910	A
22	a	931	U
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	996	A
22	a	1005	C
22	a	1012	U
22	a	1013	C
22	a	1033	U
22	a	1041	G
22	a	1045	C
22	a	1046	A
22	a	1047	G
22	a	1111	A
22	a	1112	G
22	a	1122	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1206	G
22	a	1212	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	1250	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1293	C
22	a	1300	G
22	a	1301	A
22	a	1329	U
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1411	U
22	a	1416	G
22	a	1427	A
22	a	1428	C
22	a	1452	G
22	a	1453	A
22	a	1475	G
22	a	1482	G
22	a	1493	C
22	a	1508	A
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1524	G
22	a	1529	G
22	a	1535	A
22	a	1537	G
22	a	1539	U
22	a	1554	U
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1608	A
22	a	1626	A
22	a	1646	C
22	a	1647	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1738	G
22	a	1764	C
22	a	1773	A
22	a	1786	A
22	a	1800	C
22	a	1801	A
22	a	1807	G
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1847	A
22	a	1848	A
22	a	1858	A
22	a	1862	G
22	a	1870	C
22	a	1871	A
22	a	1872	A
22	a	1905	C
22	a	1906	G
22	a	1913	A
22	a	1914	C
22	a	1915	3TD
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1955	U
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2020	A
22	a	2023	C
22	a	2027	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2093	G
22	a	2189	U
22	a	2190	G
22	a	2198	A
22	a	2204	G
22	a	2211	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2279	G
22	a	2283	C
22	a	2287	A
22	a	2288	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2336	A
22	a	2345	G
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2396	G
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2425	A
22	a	2429	G
22	a	2430	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	2435	A
22	a	2441	U
22	a	2445	2MG
22	a	2448	A
22	a	2469	A
22	a	2475	C
22	a	2476	A
22	a	2478	A
22	a	2491	U
22	a	2498	OMC
22	a	2502	G
22	a	2503	2MA
22	a	2505	G
22	a	2518	A
22	a	2529	G
22	a	2535	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2630	G
22	a	2661	G
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2716	C
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2757	A
22	a	2765	A
22	a	2778	A
22	a	2798	U
22	a	2799	A
22	a	2820	A
22	a	2821	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	2835	A
22	a	2849	U
22	a	2861	U
22	a	2873	A
22	a	2880	C
22	a	2884	U
22	a	2901	C
23	b	9	G
23	b	13	G
23	b	24	G
23	b	35	C
23	b	36	C
23	b	42	C
23	b	44	G
23	b	56	G
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	109	A
54	Z	8	4SU
54	Z	9	G
54	Z	18	U
54	Z	19	G
54	Z	20	G
54	Z	21	H2U
54	Z	22	A
54	Z	23	G
54	Z	48	U
54	Z	77	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	429	U
1	A	517	G
1	A	532	A
1	A	636	U
1	A	1030	U
1	A	1035	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	5MC	A	967	1	18,22,23	3.68	8 (44%)	26,32,35	1.02	1 (3%)
33	MS6	l	82	33	5,7,8	1.17	1 (20%)	2,7,9	2.05	1 (50%)
22	PSU	a	2580	22	18,21,22	1.11	3 (16%)	22,30,33	2.09	6 (27%)
22	OMU	a	2552	22	19,22,23	2.69	6 (31%)	26,31,34	1.82	5 (19%)
22	PSU	a	2457	22	18,21,22	1.08	2 (11%)	22,30,33	2.02	6 (27%)
22	2MA	a	2503	22,55	22,25,26	3.70	9 (40%)	33,37,40	2.81	8 (24%)
1	2MG	A	1207	1	23,26,27	2.57	8 (34%)	32,38,41	2.14	10 (31%)
22	OMC	a	2498	22,55	19,22,23	2.75	8 (42%)	26,31,34	0.86	0
22	6MZ	a	2030	22	22,25,26	2.67	4 (18%)	30,36,39	2.46	12 (40%)
22	PSU	a	2605	22	18,21,22	1.02	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A	516	1,55	18,21,22	1.03	1 (5%)	22,30,33	1.68	5 (22%)
1	4OC	A	1402	1,55	20,23,24	2.93	8 (40%)	26,32,35	1.01	2 (7%)
12	D2T	L	89	12	7,9,10	1.40	0	6,11,13	2.06	3 (50%)
1	5MC	A	1407	1	18,22,23	3.54	8 (44%)	26,32,35	1.02	2 (7%)
22	6MZ	a	1618	22	22,25,26	2.69	4 (18%)	30,36,39	2.40	11 (36%)
1	UR3	A	1498	1	19,22,23	2.60	7 (36%)	26,32,35	1.33	1 (3%)
11	IAS	K	119	11	6,7,8	1.02	0	6,8,10	1.26	1 (16%)
33	4D4	l	81	33	9,11,12	1.51	2 (22%)	8,13,15	2.04	3 (37%)
1	2MG	A	1516	1	23,26,27	2.52	7 (30%)	32,38,41	2.17	11 (34%)
1	MA6	A	1519	1	23,26,27	1.38	4 (17%)	34,38,41	2.32	12 (35%)
22	PSU	a	746	22,55	18,21,22	1.07	2 (11%)	22,30,33	1.71	3 (13%)
22	5MU	a	747	22	19,22,23	4.54	7 (36%)	28,32,35	3.79	10 (35%)
22	H2U	a	2449	22	18,21,22	1.29	3 (16%)	21,30,33	1.03	1 (4%)
22	2MG	a	2445	22	23,26,27	2.53	7 (30%)	32,38,41	2.24	10 (31%)
22	G7M	a	2069	22,55	23,26,27	2.72	8 (34%)	35,39,42	1.73	9 (25%)
22	5MC	a	1962	22	18,22,23	3.54	7 (38%)	26,32,35	1.09	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1518	1	23,26,27	1.41	5 (21%)	34,38,41	2.26	12 (35%)
54	5MU	Z	55	54	19,22,23	4.64	6 (31%)	28,32,35	3.67	9 (32%)
25	MEQ	d	150	25	8,9,10	1.10	0	5,10,12	1.50	2 (40%)
22	2MG	a	1835	22	23,26,27	2.54	7 (30%)	32,38,41	2.25	10 (31%)
22	PSU	a	2604	22	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
22	1MG	a	745	22	22,26,27	2.57	7 (31%)	33,39,42	1.78	8 (24%)
54	4SU	Z	8	54	18,21,22	4.10	8 (44%)	26,30,33	2.27	4 (15%)
54	H2U	Z	21	54	18,21,22	1.05	2 (11%)	21,30,33	0.74	0
54	OMC	Z	33	54	19,22,23	2.84	8 (42%)	26,31,34	0.75	0
1	2MG	A	966	1	23,26,27	2.61	7 (30%)	32,38,41	2.21	9 (28%)
1	G7M	A	527	1	23,26,27	2.76	8 (34%)	35,39,42	1.72	9 (25%)
22	PSU	a	1917	22	18,21,22	1.01	1 (5%)	22,30,33	1.86	5 (22%)
22	5MU	a	1939	22	19,22,23	4.51	7 (36%)	28,32,35	3.82	10 (35%)
22	PSU	a	1911	22	18,21,22	1.02	1 (5%)	22,30,33	1.84	3 (13%)
22	OMG	a	2251	54,22	23,26,27	2.53	10 (43%)	33,38,41	1.93	9 (27%)
22	PSU	a	2504	22	18,21,22	1.04	1 (5%)	22,30,33	1.82	4 (18%)
22	PSU	a	955	22	18,21,22	1.08	2 (11%)	22,30,33	1.92	5 (22%)
22	3TD	a	1915	22	18,22,23	4.06	6 (33%)	22,32,35	1.74	3 (13%)
54	PSU	Z	56	54	18,21,22	1.06	1 (5%)	22,30,33	1.86	5 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
33	MS6	l	82	33	-	1/4/6/8	-
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	1/9/27/28	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	2MA	a	2503	22,55	-	1/7/25/26	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
22	OMC	a	2498	22,55	-	0/9/27/28	0/2/2/2
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,55	-	2/7/25/26	0/2/2/2
1	4OC	A	1402	1,55	-	1/9/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	D2T	L	89	12	-	3/7/12/14	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
33	4D4	l	81	33	-	3/11/12/14	-
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
22	PSU	a	746	22,55	-	1/7/25/26	0/2/2/2
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	2MG	a	2445	22	-	2/9/27/28	0/3/3/3
22	G7M	a	2069	22,55	-	1/7/25/26	0/3/3/3
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
54	5MU	Z	55	54	-	2/7/25/26	0/2/2/2
25	MEQ	d	150	25	-	2/8/9/11	-
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
54	H2U	Z	21	54	-	7/7/38/39	0/2/2/2
54	OMC	Z	33	54	-	0/9/27/28	0/2/2/2
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
1	G7M	A	527	1	-	3/7/25/26	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	54,22	-	1/9/27/28	0/3/3/3
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	2/7/25/26	0/2/2/2
54	PSU	Z	56	54	-	0/7/25/26	0/2/2/2

All (214) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	12.17	1.49	1.35
22	a	2503	2MA	C4-N3	11.28	1.48	1.34
22	a	1618	6MZ	C6-N6	11.19	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2030	6MZ	C6-N6	10.98	1.46	1.34
54	Z	55	5MU	C6-N1	10.58	1.56	1.38
54	Z	55	5MU	C2-N1	10.35	1.55	1.38
22	a	747	5MU	C6-N1	10.25	1.55	1.38
22	a	1939	5MU	C6-N1	10.04	1.55	1.38
22	a	747	5MU	C2-N1	10.02	1.54	1.38
22	a	1939	5MU	C2-N1	9.79	1.54	1.38
54	Z	8	4SU	C4-N3	9.33	1.47	1.37
1	A	967	5MC	C6-C5	9.27	1.49	1.34
54	Z	55	5MU	C4-C5	9.15	1.60	1.44
1	A	1407	5MC	C6-C5	9.06	1.49	1.34
22	a	1962	5MC	C6-C5	8.83	1.49	1.34
22	a	747	5MU	C4-C5	8.73	1.59	1.44
22	a	1939	5MU	C4-C5	8.71	1.59	1.44
22	a	1915	3TD	C2-N1	8.57	1.48	1.37
22	a	1939	5MU	C4-N3	-7.85	1.24	1.38
22	a	747	5MU	C4-N3	-7.67	1.24	1.38
54	Z	8	4SU	C2-N1	7.62	1.50	1.38
1	A	966	2MG	C2-N3	7.61	1.46	1.31
54	Z	55	5MU	C4-N3	-7.40	1.25	1.38
1	A	1207	2MG	C2-N3	7.31	1.45	1.31
22	a	1835	2MG	C2-N3	7.21	1.45	1.31
22	a	2445	2MG	C2-N3	7.18	1.45	1.31
1	A	1516	2MG	C2-N3	7.11	1.45	1.31
1	A	967	5MC	C4-N3	7.08	1.46	1.34
22	a	2503	2MA	C2-N3	6.96	1.46	1.34
22	a	2251	OMG	C4-N3	6.94	1.50	1.34
22	a	1962	5MC	C4-N3	6.91	1.45	1.34
1	A	1407	5MC	C4-N3	6.61	1.45	1.34
54	Z	8	4SU	C2-N3	6.47	1.49	1.38
1	A	1498	UR3	C2-N1	6.46	1.47	1.38
54	Z	55	5MU	C6-C5	6.42	1.45	1.34
1	A	966	2MG	C4-N3	6.39	1.49	1.34
1	A	1402	4OC	C4-N3	6.36	1.43	1.32
1	A	527	G7M	C2-N2	6.35	1.49	1.34
1	A	967	5MC	C2-N3	6.33	1.49	1.36
1	A	1207	2MG	C4-N3	6.31	1.49	1.34
22	a	1835	2MG	C4-N3	6.26	1.49	1.34
22	a	2069	G7M	C2-N2	6.21	1.48	1.34
1	A	527	G7M	C4-N3	6.19	1.49	1.34
22	a	747	5MU	C6-C5	6.17	1.44	1.34
1	A	1516	2MG	C4-N3	6.15	1.48	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1962	5MC	C2-N3	6.13	1.48	1.36
22	a	1939	5MU	C6-C5	6.10	1.44	1.34
22	a	2445	2MG	C4-N3	6.10	1.48	1.34
22	a	2069	G7M	C4-N3	6.05	1.48	1.34
22	a	745	1MG	C2-N3	6.04	1.45	1.34
54	Z	33	OMC	C2-N3	6.00	1.48	1.36
22	a	2552	OMU	C2-N1	6.00	1.48	1.38
1	A	1402	4OC	C6-C5	6.00	1.49	1.35
22	a	2552	OMU	C2-N3	5.97	1.48	1.38
1	A	1407	5MC	C2-N3	5.95	1.48	1.36
22	a	2503	2MA	C2-N1	5.93	1.44	1.34
22	a	745	1MG	C4-N3	5.92	1.48	1.34
54	Z	8	4SU	C6-C5	5.91	1.48	1.35
1	A	1498	UR3	C6-C5	5.87	1.48	1.35
22	a	745	1MG	C2-N2	5.78	1.44	1.34
22	a	1915	3TD	C6-N1	5.76	1.45	1.36
22	a	2498	OMC	C2-N3	5.74	1.48	1.36
54	Z	33	OMC	C6-C5	5.72	1.48	1.35
22	a	2498	OMC	C6-C5	5.57	1.48	1.35
22	a	2552	OMU	C6-C5	5.56	1.48	1.35
54	Z	8	4SU	C4-S4	-5.47	1.58	1.68
1	A	1402	4OC	C2-N3	5.47	1.47	1.36
1	A	527	G7M	C2-N3	5.42	1.46	1.33
54	Z	8	4SU	C5-C4	5.38	1.49	1.42
22	a	2069	G7M	C2-N3	5.16	1.45	1.33
22	a	2503	2MA	C6-N6	-5.07	1.21	1.34
22	a	2251	OMG	C2-N3	5.04	1.45	1.33
22	a	2503	2MA	C5-C6	5.00	1.54	1.41
1	A	967	5MC	C6-N1	4.92	1.46	1.38
22	a	2069	G7M	C5-N7	-4.91	1.33	1.39
1	A	966	2MG	C2-N1	4.84	1.44	1.36
22	a	2251	OMG	C2-N2	4.83	1.45	1.34
1	A	1207	2MG	C2-N1	4.80	1.44	1.36
54	Z	33	OMC	C4-N3	4.77	1.44	1.34
54	Z	33	OMC	C4-N4	4.72	1.45	1.33
1	A	527	G7M	C5-N7	-4.71	1.33	1.39
1	A	1407	5MC	C6-N1	4.70	1.46	1.38
1	A	1498	UR3	C2-N3	4.68	1.48	1.39
22	a	1962	5MC	C6-N1	4.58	1.45	1.38
22	a	2498	OMC	C4-N4	4.57	1.44	1.33
1	A	1516	2MG	C2-N1	4.46	1.43	1.36
22	a	1835	2MG	C2-N1	4.46	1.43	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2498	OMC	C4-N3	4.45	1.43	1.34
22	a	1915	3TD	C2-N3	4.35	1.48	1.38
22	a	2445	2MG	C2-N1	4.35	1.43	1.36
1	A	1402	4OC	C4-N4	4.20	1.44	1.35
54	Z	33	OMC	C2-N1	4.06	1.48	1.40
1	A	967	5MC	C4-N4	4.01	1.44	1.34
22	a	2498	OMC	C2-N1	3.94	1.48	1.40
1	A	967	5MC	C2-N1	3.92	1.48	1.40
1	A	1407	5MC	C4-N4	3.91	1.44	1.34
22	a	1962	5MC	C4-N4	3.89	1.44	1.34
1	A	1402	4OC	C2-N1	3.73	1.48	1.40
22	a	1962	5MC	C2-N1	3.69	1.48	1.40
1	A	1402	4OC	C5-C4	3.61	1.48	1.40
1	A	1407	5MC	C2-N1	3.59	1.47	1.40
1	A	527	G7M	C5-C6	3.54	1.53	1.43
22	a	2069	G7M	C5-C6	3.50	1.53	1.43
22	a	745	1MG	C5-N7	-3.44	1.32	1.39
22	a	2503	2MA	C5-N7	-3.43	1.32	1.39
22	a	2251	OMG	C5-N7	-3.39	1.32	1.39
22	a	2445	2MG	C5-N7	-3.39	1.32	1.39
22	a	1835	2MG	C5-N7	-3.37	1.32	1.39
1	A	1519	MA6	C5-C4	-3.29	1.32	1.39
1	A	1402	4OC	O2-C2	-3.25	1.17	1.23
1	A	1518	MA6	C5-C4	-3.25	1.32	1.39
22	a	2030	6MZ	C5-C4	-3.23	1.33	1.39
22	a	2552	OMU	O2-C2	-3.21	1.17	1.23
54	Z	56	PSU	C6-C5	3.20	1.39	1.35
22	a	2449	H2U	C2-N3	-3.20	1.32	1.38
54	Z	8	4SU	O2-C2	-3.20	1.17	1.23
1	A	966	2MG	C5-N7	-3.16	1.33	1.39
22	a	2498	OMC	O2-C2	-3.14	1.17	1.23
22	a	2503	2MA	C6-N1	3.13	1.39	1.35
22	a	2449	H2U	C4-N3	-3.13	1.32	1.37
22	a	2251	OMG	O6-C6	-3.10	1.17	1.23
54	Z	8	4SU	C6-N1	3.08	1.45	1.38
1	A	1207	2MG	C5-N7	-3.06	1.33	1.39
22	a	2552	OMU	O4-C4	-3.04	1.18	1.24
22	a	1618	6MZ	C5-C4	-3.03	1.33	1.39
1	A	1516	2MG	C5-N7	-2.99	1.33	1.39
54	Z	33	OMC	O2-C2	-2.93	1.18	1.23
22	a	2069	G7M	O6-C6	-2.90	1.18	1.23
1	A	1518	MA6	C6-N6	2.84	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1518	MA6	C5-N7	-2.84	1.33	1.39
1	A	516	PSU	C6-C5	2.83	1.38	1.35
33	l	81	4D4	OB-CB	-2.83	1.37	1.43
54	Z	33	OMC	C6-N1	2.81	1.44	1.38
1	A	1402	4OC	C6-N1	2.80	1.44	1.38
22	a	745	1MG	C5-C6	2.79	1.52	1.45
1	A	1519	MA6	C6-N6	2.78	1.45	1.36
22	a	2552	OMU	C4-N3	2.77	1.43	1.38
1	A	527	G7M	O6-C6	-2.76	1.18	1.23
1	A	1519	MA6	C5-N7	-2.76	1.33	1.39
1	A	527	G7M	C2-N1	2.75	1.44	1.37
1	A	1498	UR3	C6-N1	2.75	1.44	1.38
1	A	1407	5MC	O2-C2	-2.74	1.18	1.23
54	Z	21	H2U	C2-N3	-2.73	1.33	1.38
22	a	2504	PSU	C6-C5	2.71	1.38	1.35
22	a	1911	PSU	C6-C5	2.71	1.38	1.35
1	A	1519	MA6	C8-N9	-2.68	1.32	1.37
22	a	746	PSU	C6-C5	2.68	1.38	1.35
1	A	1518	MA6	C8-N9	-2.68	1.32	1.37
22	a	2457	PSU	C6-C5	2.67	1.38	1.35
22	a	2604	PSU	C6-C5	2.67	1.38	1.35
22	a	1917	PSU	C6-C5	2.66	1.38	1.35
22	a	2445	2MG	O6-C6	-2.64	1.18	1.23
22	a	1835	2MG	O6-C6	-2.64	1.18	1.23
22	a	2069	G7M	C2-N1	2.63	1.44	1.37
1	A	527	G7M	C6-N1	2.62	1.43	1.38
22	a	2251	OMG	C5-C6	2.60	1.54	1.44
22	a	2498	OMC	C6-N1	2.59	1.44	1.38
54	Z	21	H2U	C4-N3	-2.58	1.33	1.37
1	A	1516	2MG	O6-C6	-2.58	1.18	1.23
22	a	955	PSU	C6-C5	2.57	1.38	1.35
22	a	1962	5MC	O2-C2	-2.55	1.19	1.23
22	a	1939	5MU	O2-C2	-2.54	1.18	1.23
22	a	2069	G7M	C6-N1	2.52	1.43	1.38
22	a	1915	3TD	C4-N3	2.50	1.45	1.40
22	a	2605	PSU	C6-C5	2.49	1.38	1.35
33	l	81	4D4	CZ-NE	2.48	1.38	1.33
22	a	2030	6MZ	C5-N7	-2.46	1.34	1.39
1	A	1207	2MG	C5-C6	2.46	1.53	1.44
1	A	967	5MC	O2-C2	-2.46	1.19	1.23
1	A	1498	UR3	O2-C2	-2.46	1.18	1.22
33	l	82	MS6	CB-CA	2.45	1.56	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O4-C4	-2.45	1.18	1.23
22	a	2580	PSU	C6-C5	2.44	1.38	1.35
22	a	2030	6MZ	C8-N9	-2.43	1.33	1.37
1	A	1207	2MG	O6-C6	-2.42	1.19	1.23
22	a	745	1MG	O6-C6	-2.42	1.18	1.23
22	a	747	5MU	O2-C2	-2.42	1.18	1.23
1	A	1516	2MG	C5-C6	2.41	1.53	1.44
22	a	745	1MG	C4-N9	-2.40	1.31	1.38
22	a	1618	6MZ	C8-N9	-2.38	1.33	1.37
1	A	966	2MG	C5-C6	2.38	1.53	1.44
22	a	1618	6MZ	C5-N7	-2.38	1.34	1.39
22	a	2445	2MG	C5-C6	2.38	1.53	1.44
1	A	966	2MG	O6-C6	-2.38	1.19	1.23
1	A	1516	2MG	C4-N9	-2.36	1.31	1.38
22	a	2449	H2U	C2-N1	-2.33	1.32	1.35
22	a	2580	PSU	O4'-C1'	-2.31	1.40	1.43
22	a	1915	3TD	O4-C4	-2.31	1.18	1.23
22	a	2445	2MG	C4-N9	-2.28	1.32	1.38
22	a	1835	2MG	C5-C6	2.26	1.52	1.44
22	a	2251	OMG	C8-N9	-2.19	1.32	1.37
22	a	1939	5MU	O4-C4	-2.19	1.19	1.23
22	a	2580	PSU	C4-C5	-2.18	1.37	1.44
1	A	967	5MC	CM5-C5	2.15	1.56	1.50
54	Z	33	OMC	C5-C4	2.13	1.47	1.42
1	A	1207	2MG	C6-N1	2.13	1.42	1.38
1	A	966	2MG	C6-N1	2.13	1.42	1.38
22	a	2503	2MA	CM2-C2	2.13	1.55	1.49
22	a	2251	OMG	C6-N1	2.13	1.42	1.38
22	a	746	PSU	C4-C5	-2.12	1.38	1.44
1	A	1207	2MG	C4-N9	-2.12	1.32	1.38
22	a	955	PSU	C4-C5	-2.11	1.38	1.44
22	a	2251	OMG	C4-N9	-2.11	1.32	1.38
22	a	2251	OMG	C2-N1	2.11	1.42	1.37
22	a	1835	2MG	C4-N9	-2.09	1.32	1.38
22	a	2503	2MA	C8-N9	-2.08	1.33	1.37
22	a	2605	PSU	C4-C5	-2.07	1.38	1.44
1	A	1498	UR3	C5-C4	2.06	1.49	1.43
54	Z	55	5MU	O2-C2	-2.06	1.19	1.23
1	A	1518	MA6	C4-N9	-2.05	1.33	1.37
22	a	747	5MU	O4-C4	-2.04	1.19	1.23
22	a	2457	PSU	C4-C5	-2.03	1.38	1.44
1	A	1407	5MC	CM5-C5	2.02	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2498	OMC	C5-C4	2.01	1.47	1.42

All (249) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	747	5MU	C5-C4-N3	12.47	125.95	115.31
22	a	1939	5MU	C5-C4-N3	12.46	125.95	115.31
54	Z	55	5MU	C5-C4-N3	12.28	125.79	115.31
22	a	1939	5MU	C5-C6-N1	-10.87	112.16	123.34
22	a	747	5MU	C5-C6-N1	-10.71	112.33	123.34
54	Z	55	5MU	C5-C6-N1	-10.21	112.83	123.34
22	a	2503	2MA	C5-C4-N3	-8.49	117.64	127.19
54	Z	8	4SU	C4-N3-C2	-7.92	119.64	127.34
22	a	2503	2MA	C4-N9-C1'	-6.63	110.80	126.59
22	a	1835	2MG	C2-N3-C4	6.60	120.22	112.04
22	a	2503	2MA	C1'-N9-C8	6.57	141.96	127.14
22	a	2445	2MG	C2-N3-C4	6.54	120.14	112.04
1	A	966	2MG	C2-N3-C4	6.50	120.10	112.04
1	A	1207	2MG	C2-N3-C4	6.17	119.69	112.04
1	A	1516	2MG	C2-N3-C4	6.08	119.58	112.04
22	a	2030	6MZ	C9-N6-C6	-5.95	117.75	122.87
1	A	1518	MA6	N1-C2-N3	-5.84	119.47	128.60
1	A	1519	MA6	N1-C2-N3	-5.78	119.56	128.60
22	a	2552	OMU	C4-N3-C2	-5.70	119.07	126.58
54	Z	8	4SU	C5-C4-N3	5.65	119.93	114.69
22	a	2503	2MA	N3-C4-N9	5.63	134.79	126.99
22	a	1915	3TD	N1-C2-N3	5.62	120.57	116.14
22	a	2030	6MZ	N1-C2-N3	-5.54	119.93	128.60
22	a	1618	6MZ	N1-C2-N3	-5.47	120.05	128.60
22	a	1835	2MG	C5-C4-N3	-5.47	119.59	128.46
1	A	966	2MG	C5-C4-N3	-5.45	119.62	128.46
22	a	2251	OMG	C5-C4-N3	-5.41	119.68	128.46
22	a	1618	6MZ	C5-C4-N3	-5.39	119.72	126.75
22	a	1939	5MU	C4-N3-C2	-5.33	120.45	127.35
22	a	2457	PSU	N1-C2-N3	5.28	121.11	115.13
22	a	2580	PSU	N1-C2-N3	5.25	121.07	115.13
22	a	2445	2MG	C5-C4-N3	-5.24	119.96	128.46
22	a	747	5MU	C4-N3-C2	-5.24	120.57	127.35
22	a	747	5MU	O4-C4-C5	-5.15	118.93	124.90
1	A	1498	UR3	C4-N3-C2	-5.14	119.72	124.56
22	a	2605	PSU	C4-N3-C2	-5.02	119.10	126.34
22	a	1939	5MU	O4-C4-C5	-5.00	119.11	124.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2457	PSU	C4-N3-C2	-4.98	119.16	126.34
22	a	955	PSU	N1-C2-N3	4.96	120.75	115.13
22	a	955	PSU	C4-N3-C2	-4.96	119.20	126.34
22	a	745	1MG	C5-C4-N3	-4.95	120.43	128.46
22	a	2580	PSU	C4-N3-C2	-4.94	119.22	126.34
22	a	1911	PSU	C4-N3-C2	-4.92	119.25	126.34
54	Z	55	5MU	O4-C4-C5	-4.90	119.22	124.90
1	A	1519	MA6	C5-C4-N3	-4.90	120.35	126.75
22	a	2445	2MG	C2-N1-C6	-4.89	118.86	124.48
22	a	2604	PSU	C4-N3-C2	-4.88	119.30	126.34
54	Z	55	5MU	C4-N3-C2	-4.88	121.03	127.35
22	a	1917	PSU	C4-N3-C2	-4.87	119.32	126.34
22	a	2030	6MZ	N9-C8-N7	-4.83	107.30	113.91
22	a	2030	6MZ	C5-C4-N3	-4.83	120.44	126.75
22	a	746	PSU	C4-N3-C2	-4.83	119.38	126.34
22	a	2605	PSU	N1-C2-N3	4.80	120.57	115.13
1	A	1207	2MG	C5-C4-N3	-4.78	120.71	128.46
22	a	2504	PSU	N1-C2-N3	4.78	120.54	115.13
22	a	1618	6MZ	C9-N6-C6	-4.77	118.76	122.87
22	a	2504	PSU	C4-N3-C2	-4.74	119.51	126.34
22	a	1835	2MG	C2-N1-C6	-4.73	119.03	124.48
54	Z	56	PSU	C4-N3-C2	-4.70	119.56	126.34
22	a	1939	5MU	N3-C2-N1	4.67	121.09	114.89
22	a	2604	PSU	N1-C2-N3	4.66	120.41	115.13
22	a	1917	PSU	N1-C2-N3	4.66	120.41	115.13
54	Z	56	PSU	N1-C2-N3	4.66	120.41	115.13
1	A	966	2MG	C2-N1-C6	-4.64	119.14	124.48
1	A	1516	2MG	C5-C4-N3	-4.62	120.96	128.46
1	A	1518	MA6	C5-C4-N3	-4.60	120.75	126.75
1	A	1519	MA6	N9-C8-N7	-4.59	107.64	113.91
22	a	747	5MU	N3-C2-N1	4.57	120.95	114.89
22	a	1911	PSU	N1-C2-N3	4.56	120.30	115.13
1	A	1518	MA6	C2-N1-C6	4.55	122.49	111.75
1	A	1207	2MG	C2-N1-C6	-4.45	119.36	124.48
22	a	1618	6MZ	N9-C8-N7	-4.43	107.86	113.91
22	a	2552	OMU	N3-C2-N1	4.41	120.75	114.89
1	A	1518	MA6	N9-C8-N7	-4.40	107.89	113.91
1	A	1516	2MG	C2-N1-C6	-4.40	119.42	124.48
1	A	516	PSU	C4-N3-C2	-4.37	120.04	126.34
54	Z	55	5MU	N3-C2-N1	4.35	120.67	114.89
22	a	746	PSU	N1-C2-N3	4.32	120.02	115.13
22	a	2251	OMG	C2-N3-C4	4.31	119.98	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	C2-N1-C6	4.31	121.92	111.75
22	a	1939	5MU	C5M-C5-C6	-4.30	117.11	122.85
1	A	1518	MA6	C4-C5-C6	4.30	120.69	115.88
22	a	2069	G7M	C2-N3-C4	4.25	119.87	112.30
22	a	747	5MU	C5M-C5-C6	-4.22	117.21	122.85
1	A	1519	MA6	C4-C5-C6	4.21	120.59	115.88
1	A	527	G7M	C2-N3-C4	4.13	119.65	112.30
1	A	516	PSU	N1-C2-N3	4.12	119.79	115.13
22	a	1915	3TD	C4-N3-C2	-4.11	120.14	124.61
54	Z	55	5MU	C5M-C5-C6	-4.10	117.38	122.85
54	Z	55	5MU	C5M-C5-C4	4.07	123.24	118.77
1	A	527	G7M	C5-C6-N1	4.00	120.14	111.79
22	a	2069	G7M	C5-C6-N1	3.99	120.12	111.79
22	a	1939	5MU	C5M-C5-C4	3.93	123.09	118.77
22	a	747	5MU	C5M-C5-C4	3.89	123.05	118.77
1	A	966	2MG	N9-C4-N3	3.88	133.73	125.94
22	a	1618	6MZ	C4-C5-C6	3.86	119.80	116.81
22	a	1835	2MG	N9-C4-N3	3.82	133.60	125.94
1	A	1519	MA6	C5-N7-C8	3.69	108.76	103.51
54	Z	8	4SU	N3-C2-N1	3.69	119.79	114.89
54	Z	8	4SU	C5-C4-S4	-3.68	119.72	124.47
22	a	2069	G7M	C5-C4-N3	-3.67	121.12	128.15
1	A	527	G7M	C5-C4-N3	-3.64	121.16	128.15
33	l	81	4D4	NE-CZ-NH2	3.64	127.09	120.70
22	a	1618	6MZ	C2-N3-C4	3.63	120.32	111.75
1	A	1516	2MG	N9-C8-N7	-3.59	106.62	113.39
22	a	2503	2MA	N9-C8-N7	-3.54	109.07	113.91
22	a	2030	6MZ	C2-N3-C4	3.54	120.11	111.75
22	a	1962	5MC	C5-C6-N1	-3.54	119.70	123.34
22	a	745	1MG	C2-N3-C4	3.52	119.89	111.98
22	a	2251	OMG	N9-C4-N3	3.51	132.99	125.94
1	A	1407	5MC	C5-C6-N1	-3.50	119.74	123.34
1	A	527	G7M	O6-C6-C5	-3.50	120.17	128.06
1	A	1518	MA6	C5-N7-C8	3.46	108.43	103.51
1	A	1519	MA6	C2-N3-C4	3.43	119.85	111.75
1	A	1207	2MG	N9-C8-N7	-3.43	106.93	113.39
22	a	2069	G7M	O6-C6-C5	-3.42	120.35	128.06
22	a	2552	OMU	C5-C4-N3	3.41	119.94	114.84
22	a	2445	2MG	N9-C8-N7	-3.38	107.02	113.39
22	a	2445	2MG	N9-C4-N3	3.38	132.72	125.94
22	a	745	1MG	C1'-N9-C8	-3.36	117.14	126.70
22	a	2251	OMG	C2-N1-C6	-3.29	119.09	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2580	PSU	O2-C2-N1	-3.28	119.18	122.79
22	a	2030	6MZ	C5-N7-C8	3.27	108.16	103.51
22	a	1835	2MG	N9-C8-N7	-3.26	107.24	113.39
1	A	1518	MA6	C2-N3-C4	3.23	119.39	111.75
22	a	1618	6MZ	N3-C4-N9	3.22	132.39	127.08
12	L	89	D2T	OD2-CG-CB	3.21	120.09	113.15
22	a	745	1MG	N9-C8-N7	-3.20	107.37	113.39
22	a	2251	OMG	N9-C8-N7	-3.18	107.40	113.39
1	A	1207	2MG	N9-C4-N3	3.14	132.24	125.94
22	a	2503	2MA	C6-C5-C4	3.14	121.40	117.18
1	A	966	2MG	N9-C8-N7	-3.11	107.53	113.39
1	A	1519	MA6	C4-C5-N7	-3.07	106.88	110.62
22	a	1618	6MZ	C5-N7-C8	3.07	107.87	103.51
1	A	967	5MC	C5-C6-N1	-3.04	120.21	123.34
22	a	745	1MG	N9-C4-N3	3.03	132.03	125.94
1	A	527	G7M	C2-N1-C6	-3.03	119.57	125.10
22	a	2503	2MA	N3-C2-N1	-3.03	120.14	125.72
22	a	2069	G7M	C2-N1-C6	-3.03	119.57	125.10
22	a	2030	6MZ	C4-C5-C6	2.93	119.08	116.81
12	L	89	D2T	OD1-CG-CB	-2.93	116.31	122.44
22	a	2445	2MG	C5-C6-N1	2.90	120.54	113.19
54	Z	56	PSU	O2-C2-N1	-2.89	119.61	122.79
22	a	1835	2MG	C5-C6-N1	2.88	120.49	113.19
22	a	2457	PSU	O2-C2-N1	-2.87	119.64	122.79
33	l	82	MS6	CE-SD-CG	2.86	110.23	100.40
22	a	2503	2MA	C5-N7-C8	2.83	107.53	103.51
1	A	527	G7M	N9-C4-N3	2.83	131.61	125.94
22	a	2449	H2U	C4-N3-C2	-2.81	123.46	125.79
1	A	1518	MA6	C4-C5-N7	-2.80	107.20	110.62
1	A	1516	2MG	C5-C6-N1	2.80	120.31	113.19
1	A	1207	2MG	C5-C6-N1	2.80	120.30	113.19
1	A	966	2MG	C5-C6-N1	2.79	120.28	113.19
22	a	745	1MG	C5-C6-N1	2.78	120.28	114.91
33	l	81	4D4	CB-CA-C	-2.77	107.34	111.77
22	a	2251	OMG	C5-C6-N1	2.76	120.21	113.19
1	A	1516	2MG	N9-C4-N3	2.76	131.48	125.94
22	a	2580	PSU	C6-N1-C2	-2.75	119.88	122.68
1	A	966	2MG	O6-C6-C5	-2.73	119.35	126.60
22	a	1939	5MU	O2-C2-N1	-2.72	119.17	122.79
22	a	1939	5MU	O4-C4-N3	-2.70	114.94	120.12
22	a	2580	PSU	C6-C5-C4	2.70	120.08	118.20
22	a	1835	2MG	O6-C6-C5	-2.70	119.45	126.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Z	55	5MU	O4-C4-N3	-2.67	114.99	120.12
22	a	2069	G7M	N9-C4-N3	2.67	131.31	125.94
22	a	2069	G7M	CN7-N7-C5	2.67	130.09	126.77
22	a	2457	PSU	C6-C5-C4	2.66	120.06	118.20
1	A	527	G7M	CN7-N7-C5	2.66	130.07	126.77
1	A	1207	2MG	O6-C6-C5	-2.61	119.68	126.60
22	a	747	5MU	O4-C4-N3	-2.61	115.12	120.12
22	a	1911	PSU	O2-C2-N1	-2.60	119.93	122.79
22	a	2552	OMU	O4-C4-C5	-2.59	120.61	125.16
25	d	150	MEQ	OE1-CD-CG	2.58	126.74	122.02
22	a	2580	PSU	O4'-C1'-C2'	2.58	108.78	105.14
22	a	2457	PSU	C6-N1-C2	-2.58	120.05	122.68
22	a	2445	2MG	CM2-N2-C2	-2.58	118.17	123.86
22	a	2030	6MZ	N3-C4-N9	2.57	131.32	127.08
22	a	2030	6MZ	C4-N9-C8	2.57	108.51	105.73
1	A	1519	MA6	N1-C6-N6	-2.53	114.31	117.08
22	a	2445	2MG	O6-C6-C5	-2.53	119.88	126.60
1	A	1519	MA6	C5-C4-N9	2.53	108.72	105.78
22	a	955	PSU	O2-C2-N1	-2.52	120.02	122.79
1	A	516	PSU	O2-C2-N1	-2.51	120.02	122.79
22	a	2552	OMU	O2-C2-N1	-2.51	119.45	122.79
22	a	2604	PSU	O2-C2-N1	-2.50	120.04	122.79
22	a	747	5MU	O2-C2-N1	-2.49	119.47	122.79
22	a	2251	OMG	O6-C6-C5	-2.49	119.99	126.60
22	a	745	1MG	C1'-N9-C4	2.48	133.87	126.50
22	a	2504	PSU	O2-C2-N1	-2.48	120.06	122.79
22	a	1917	PSU	O2-C2-N1	-2.44	120.10	122.79
12	L	89	D2T	O-C-CA	-2.44	118.38	124.78
1	A	1518	MA6	N1-C6-N6	-2.44	114.42	117.08
1	A	1402	4OC	C6-C5-C4	2.43	119.94	116.96
1	A	1516	2MG	O6-C6-C5	-2.42	120.17	126.60
33	l	81	4D4	O-C-CA	-2.41	118.47	124.78
22	a	2251	OMG	C1'-N9-C4	-2.37	119.48	126.50
54	Z	55	5MU	O2-C2-N1	-2.36	119.65	122.79
1	A	1516	2MG	C8-N7-C5	2.35	108.50	104.24
1	A	1518	MA6	C5-C4-N9	2.35	108.52	105.78
1	A	1516	2MG	C1'-N9-C4	-2.34	119.55	126.50
22	a	1618	6MZ	C4-N9-C8	2.34	108.27	105.73
1	A	1207	2MG	N1-C2-N3	-2.33	120.35	123.95
1	A	1519	MA6	N3-C4-N9	2.33	130.92	127.08
22	a	1835	2MG	N1-C2-N3	-2.33	120.36	123.95
22	a	2030	6MZ	C4-C5-N7	-2.33	107.79	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	1835	2MG	CM2-N2-C2	-2.32	118.74	123.86
22	a	955	PSU	C6-N1-C2	-2.32	120.31	122.68
1	A	1516	2MG	N1-C2-N3	-2.32	120.37	123.95
22	a	2504	PSU	C6-N1-C2	-2.31	120.32	122.68
1	A	966	2MG	N1-C2-N3	-2.31	120.39	123.95
22	a	2445	2MG	C8-N7-C5	2.26	108.33	104.24
54	Z	56	PSU	C6-N1-C2	-2.26	120.37	122.68
22	a	2605	PSU	O2-C2-N1	-2.26	120.30	122.79
22	a	1915	3TD	C6-C5-C4	2.26	119.78	118.22
22	a	2445	2MG	N1-C2-N3	-2.24	120.50	123.95
54	Z	56	PSU	C6-C5-C4	2.22	119.75	118.20
1	A	1207	2MG	C8-N7-C5	2.22	108.26	104.24
1	A	1518	MA6	N3-C4-N9	2.21	130.73	127.08
1	A	527	G7M	N9-C8-N7	-2.20	106.76	112.21
22	a	1917	PSU	C6-C5-C4	2.20	119.74	118.20
22	a	1618	6MZ	C5-C6-N1	2.17	120.52	118.20
1	A	1407	5MC	CM5-C5-C6	-2.17	119.95	122.85
22	a	2251	OMG	C8-N7-C5	2.17	108.17	104.24
1	A	1207	2MG	CM2-N2-C2	-2.15	119.12	123.86
22	a	2030	6MZ	C5-C6-N1	2.14	120.48	118.20
22	a	746	PSU	O2-C2-N1	-2.13	120.44	122.79
1	A	516	PSU	C6-N1-C2	-2.13	120.50	122.68
22	a	1835	2MG	C8-N7-C5	2.13	108.10	104.24
22	a	745	1MG	C8-N7-C5	2.13	108.09	104.24
1	A	516	PSU	O4'-C1'-C2'	2.13	108.14	105.14
22	a	955	PSU	C6-C5-C4	2.12	119.68	118.20
1	A	527	G7M	CN7-N7-C8	-2.12	121.57	124.84
1	A	1516	2MG	CM2-N2-C2	-2.12	119.18	123.86
22	a	1939	5MU	C6-C5-C4	2.12	119.80	118.03
22	a	2030	6MZ	C5-C4-N9	2.11	108.24	105.78
1	A	1519	MA6	C4-N9-C8	2.10	108.00	105.73
1	A	966	2MG	C8-N7-C5	2.07	107.98	104.24
25	d	150	MEQ	CG-CD-NE2	-2.06	113.42	116.29
1	A	1518	MA6	C4-N9-C8	2.06	107.96	105.73
22	a	1618	6MZ	C4-C5-N7	-2.06	108.11	110.62
22	a	747	5MU	C6-C5-C4	2.05	119.74	118.03
22	a	1962	5MC	CM5-C5-C6	-2.05	120.11	122.85
22	a	2069	G7M	N9-C8-N7	-2.03	107.18	112.21
22	a	2457	PSU	O4'-C1'-C2'	2.03	108.00	105.14
11	K	119	IAS	OXT-C-CA	2.03	120.29	113.38
22	a	1917	PSU	C6-N1-C2	-2.02	120.62	122.68
22	a	2604	PSU	C6-N1-C2	-2.02	120.62	122.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2069	G7M	CN7-N7-C8	-2.01	121.73	124.84
1	A	1402	4OC	O2-C2-N3	-2.01	119.06	122.33

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	966	2MG	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C4'-C5'-O5'
54	Z	21	H2U	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C1'-N1-C6
54	Z	21	H2U	C2'-C1'-N1-C6
22	a	1915	3TD	C3'-C4'-C5'-O5'
22	a	1915	3TD	O4'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2251	OMG	C1'-C2'-O2'-CM2
22	a	2445	2MG	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C1'-N1-C2
54	Z	21	H2U	C2'-C1'-N1-C2
1	A	516	PSU	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	516	PSU	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
22	a	2504	PSU	O4'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
54	Z	55	5MU	O4'-C4'-C5'-O5'
22	a	2445	2MG	O4'-C4'-C5'-O5'
54	Z	55	5MU	C3'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
12	L	89	D2T	SB-CB-CG-OD1
22	a	2552	OMU	C3'-C2'-O2'-CM2
33	l	82	MS6	CB-CG-SD-CE
33	l	81	4D4	NE-CD-CG-CB
54	Z	21	H2U	C4'-C5'-O5'-P
22	a	2504	PSU	C3'-C4'-C5'-O5'
1	A	527	G7M	C4'-C5'-O5'-P
33	l	81	4D4	CG-CD-NE-CZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	a	2069	G7M	O4'-C4'-C5'-O5'
12	L	89	D2T	SB-CB-CG-OD2
1	A	1402	4OC	O4'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C6
22	a	2503	2MA	O4'-C4'-C5'-O5'
33	l	81	4D4	O-C-CA-CB

There are no ring outliers.

10 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	1	0
22	a	2030	6MZ	2	0
1	A	1516	2MG	1	0
1	A	1519	MA6	1	0
54	Z	55	5MU	1	0
54	Z	21	H2U	1	0
1	A	966	2MG	1	0
22	a	1939	5MU	1	0
22	a	1915	3TD	1	0
54	Z	56	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 457 ligands modelled in this entry, 457 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

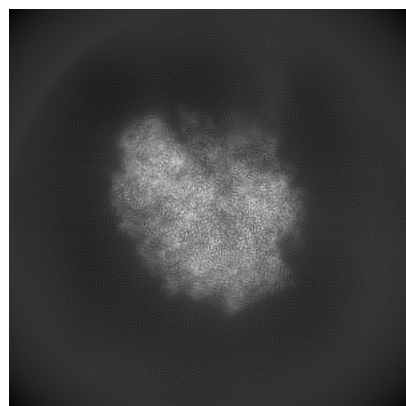
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60059. These allow visual inspection of the internal detail of the map and identification of artifacts.

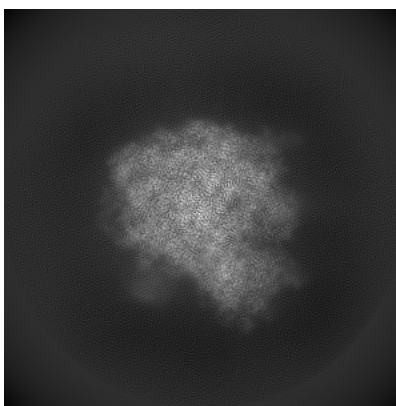
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

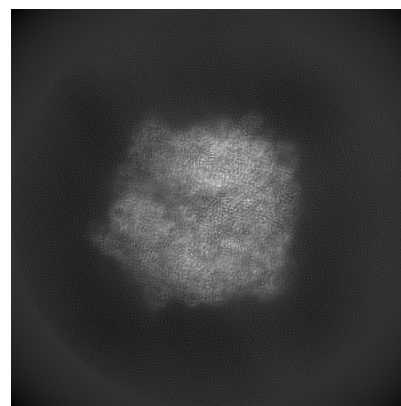
6.1.1 Primary map



X

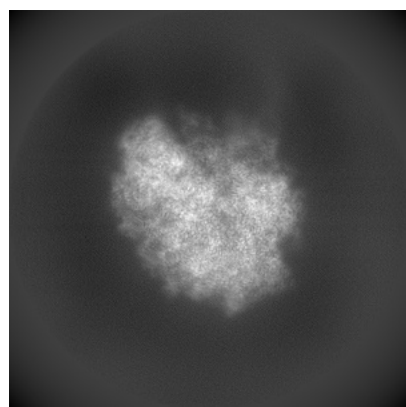


Y

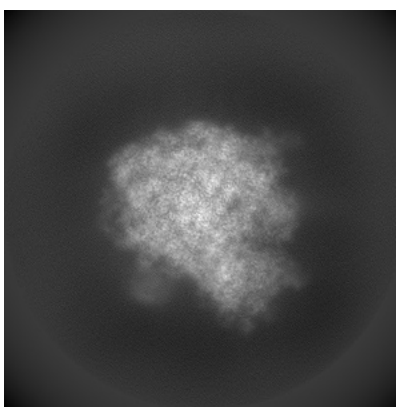


Z

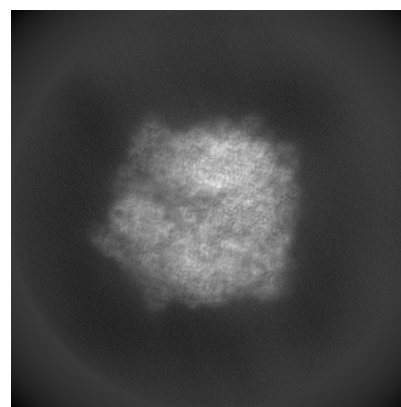
6.1.2 Raw map



X



Y

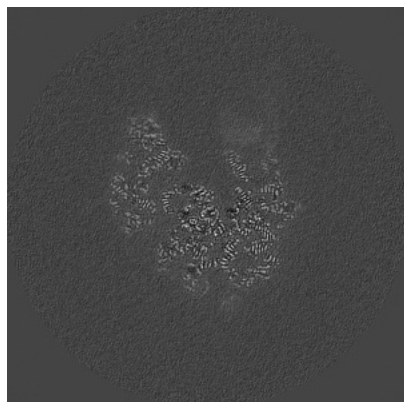


Z

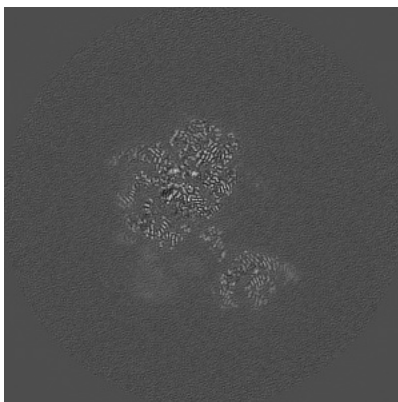
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

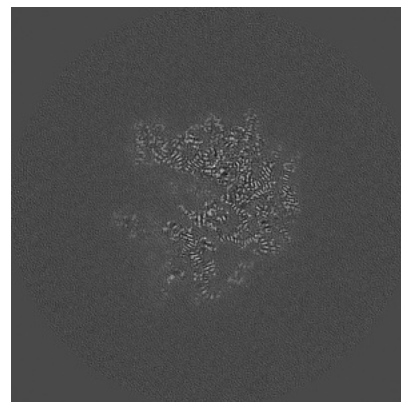
6.2.1 Primary map



X Index: 265

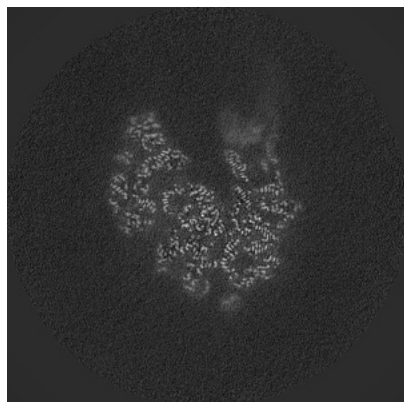


Y Index: 265

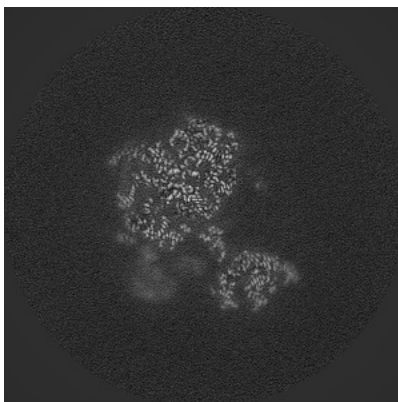


Z Index: 265

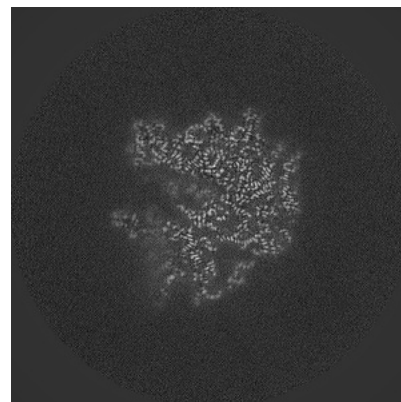
6.2.2 Raw map



X Index: 265



Y Index: 265

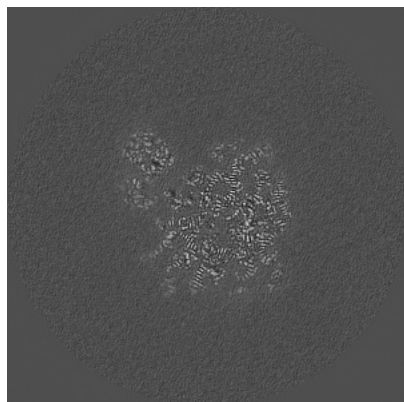


Z Index: 265

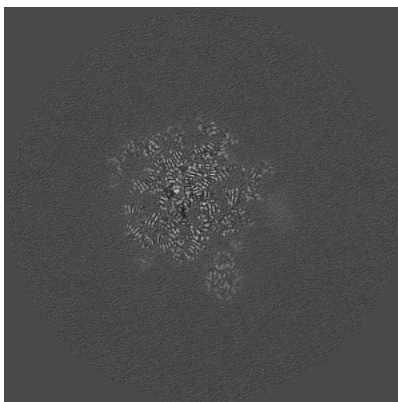
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

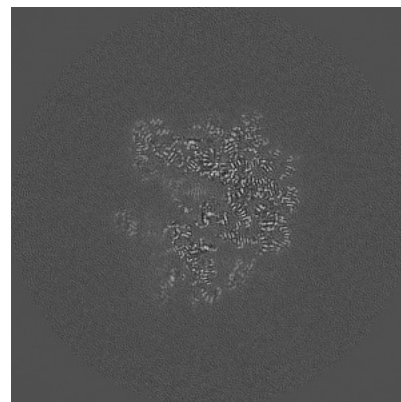
6.3.1 Primary map



X Index: 298

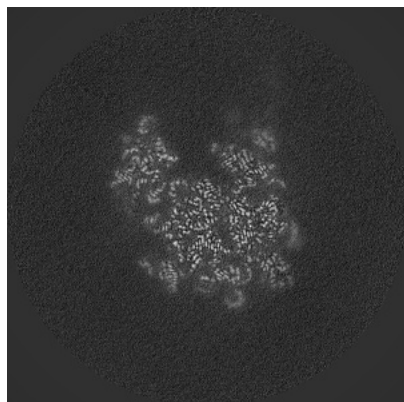


Y Index: 319

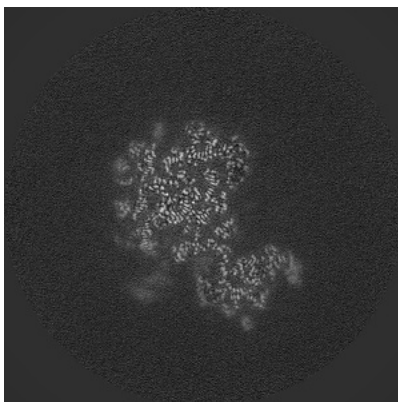


Z Index: 269

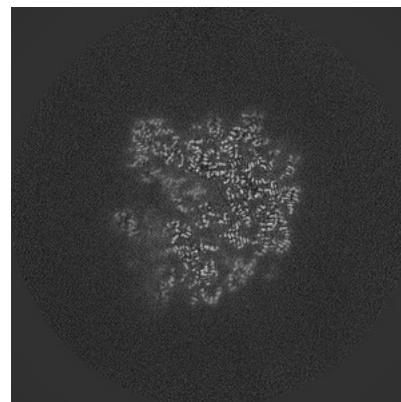
6.3.2 Raw map



X Index: 285



Y Index: 244

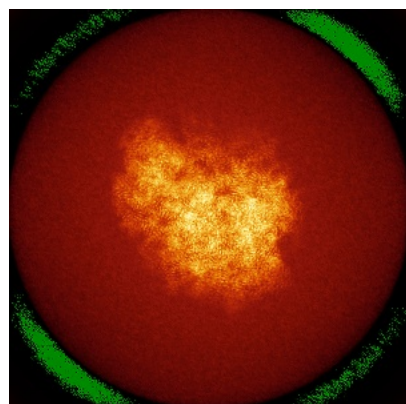


Z Index: 270

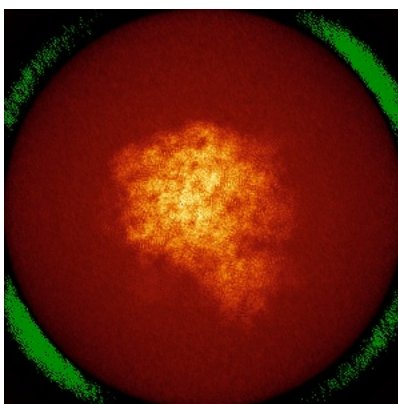
The images above show the largest variance slices of the map in three orthogonal directions.

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

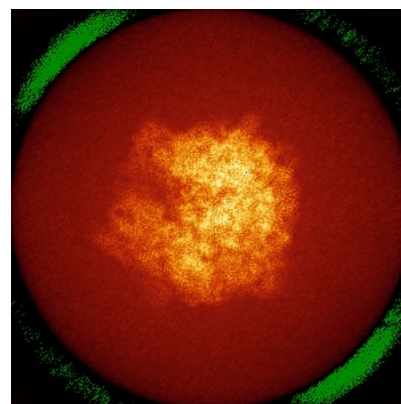
6.4.1 Primary map



X

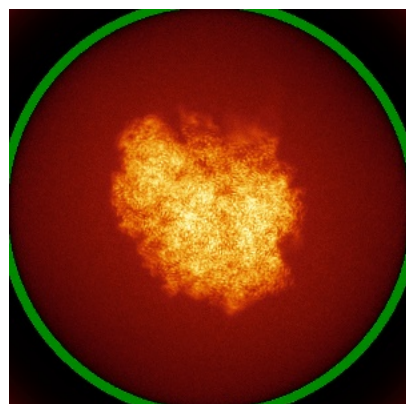


Y

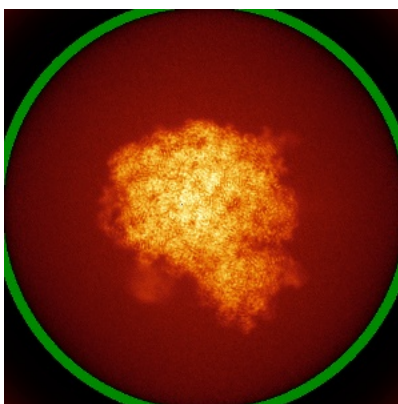


Z

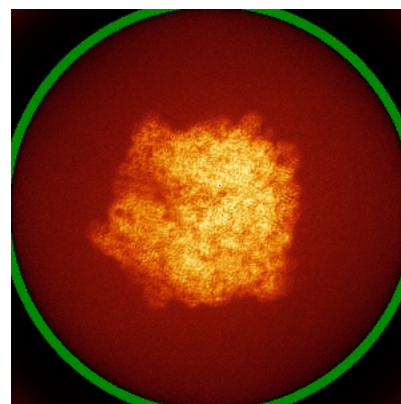
6.4.2 Raw map



X



Y

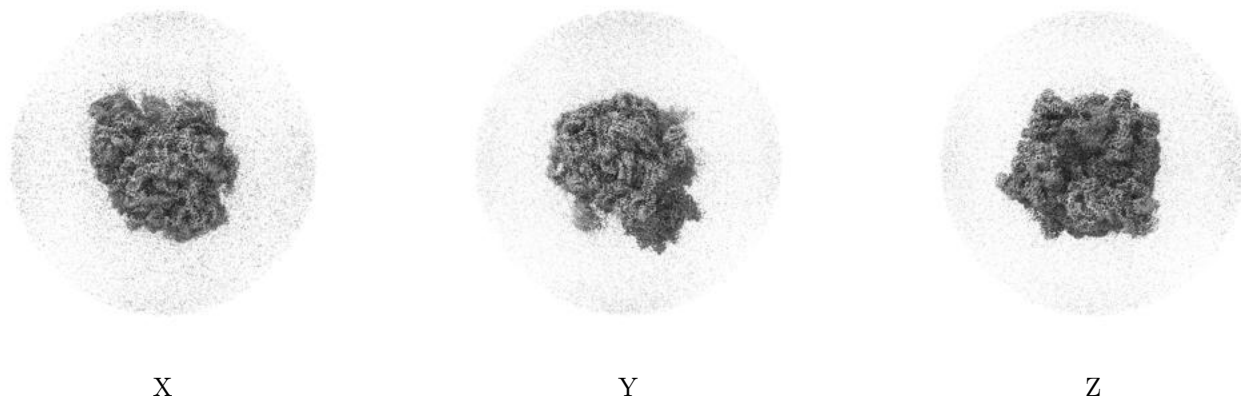


Z

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.

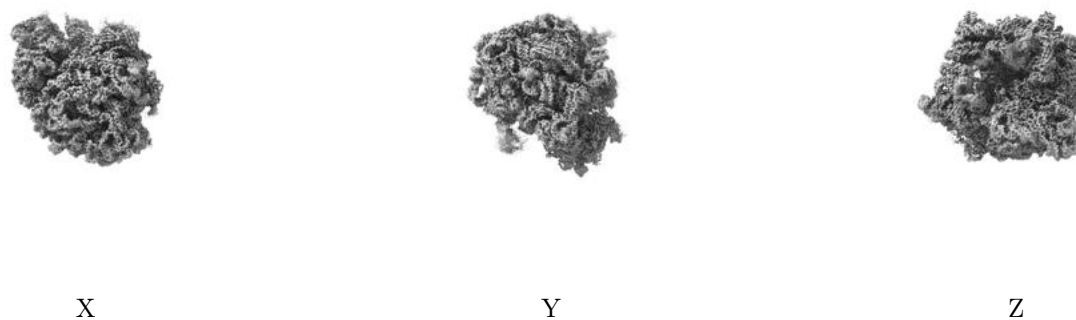
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. 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.

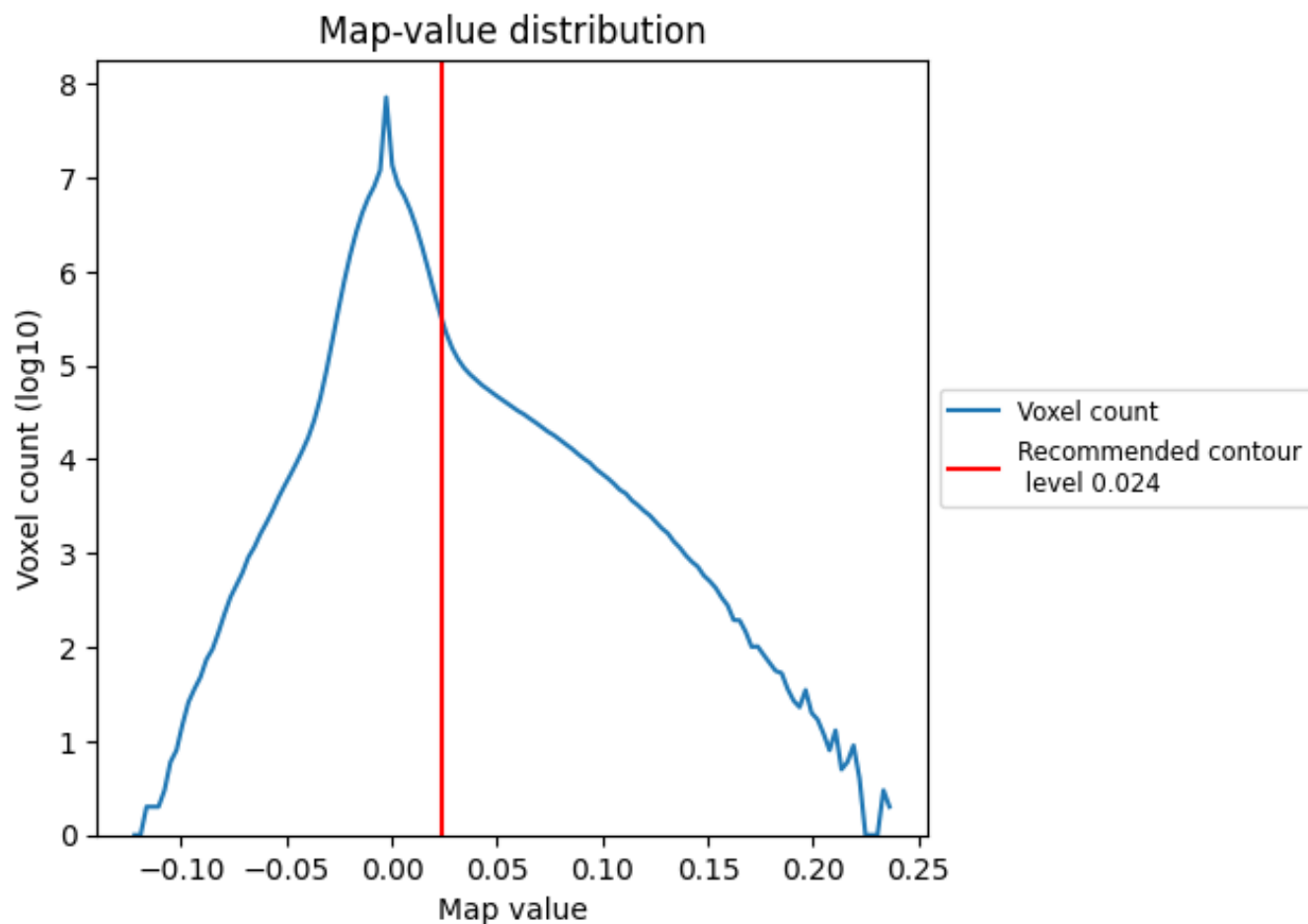
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

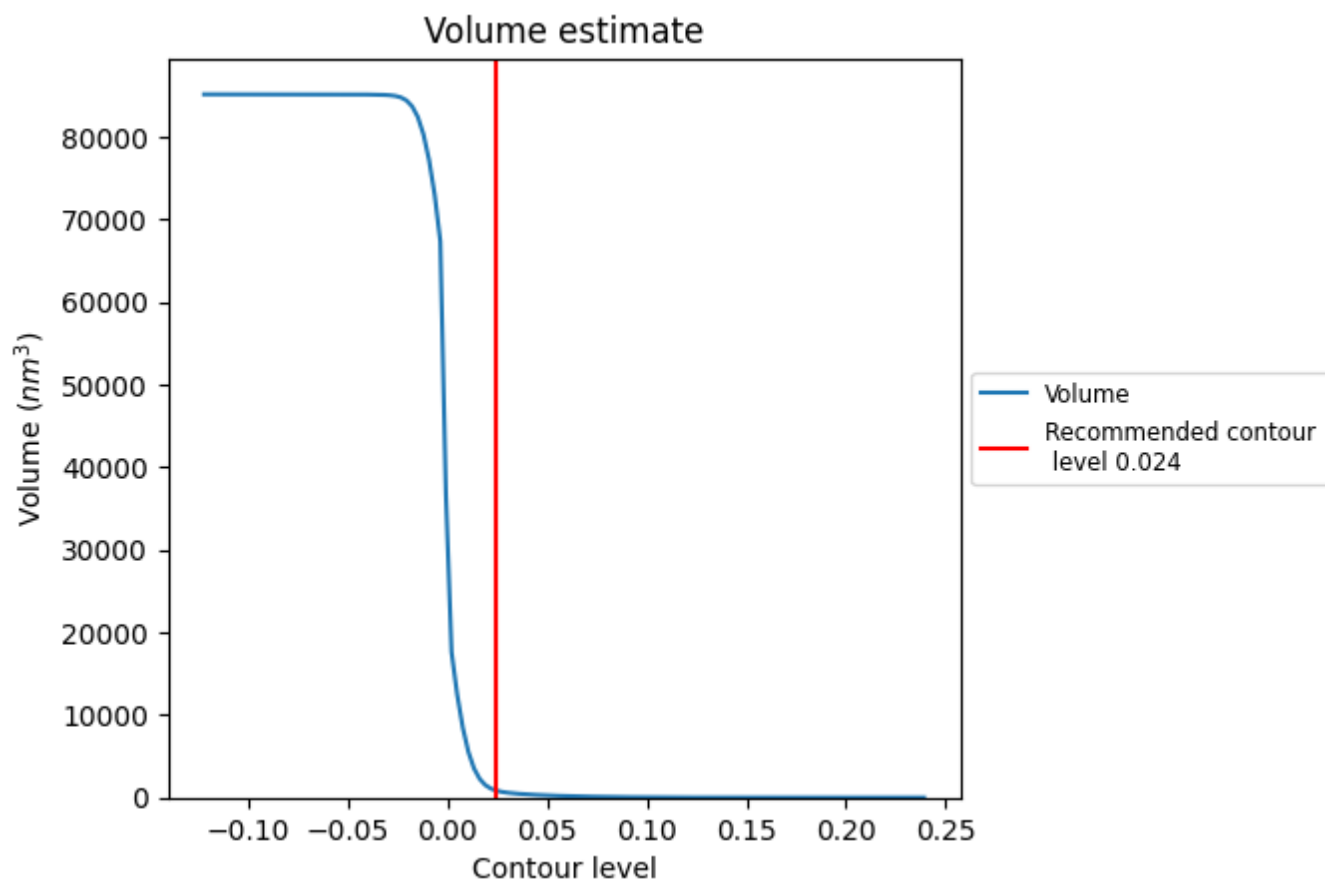
This section contains the results of statistical analysis of the map.

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.

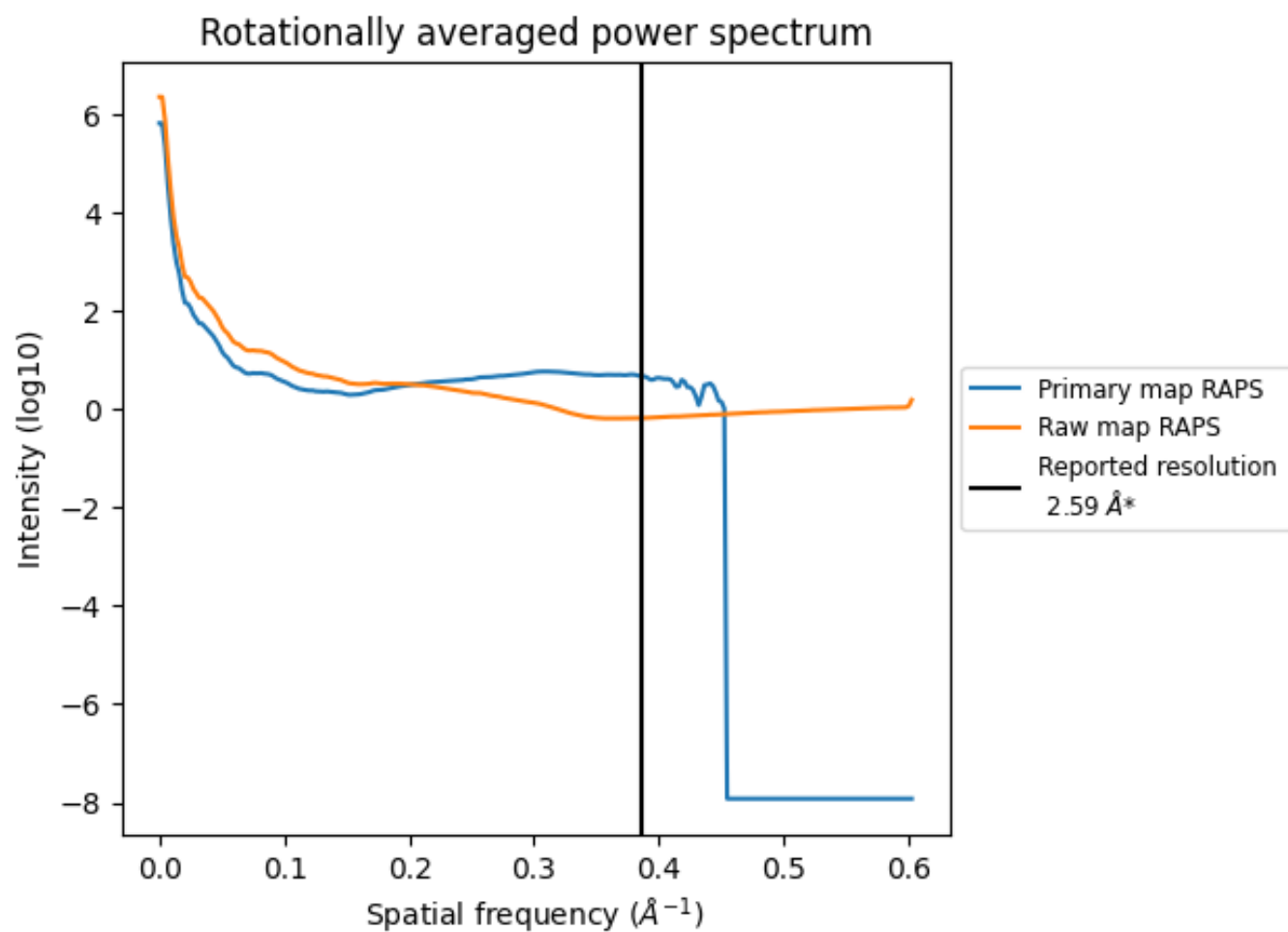
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 892 nm^3 ; this corresponds to an approximate mass of 806 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 ⓘ

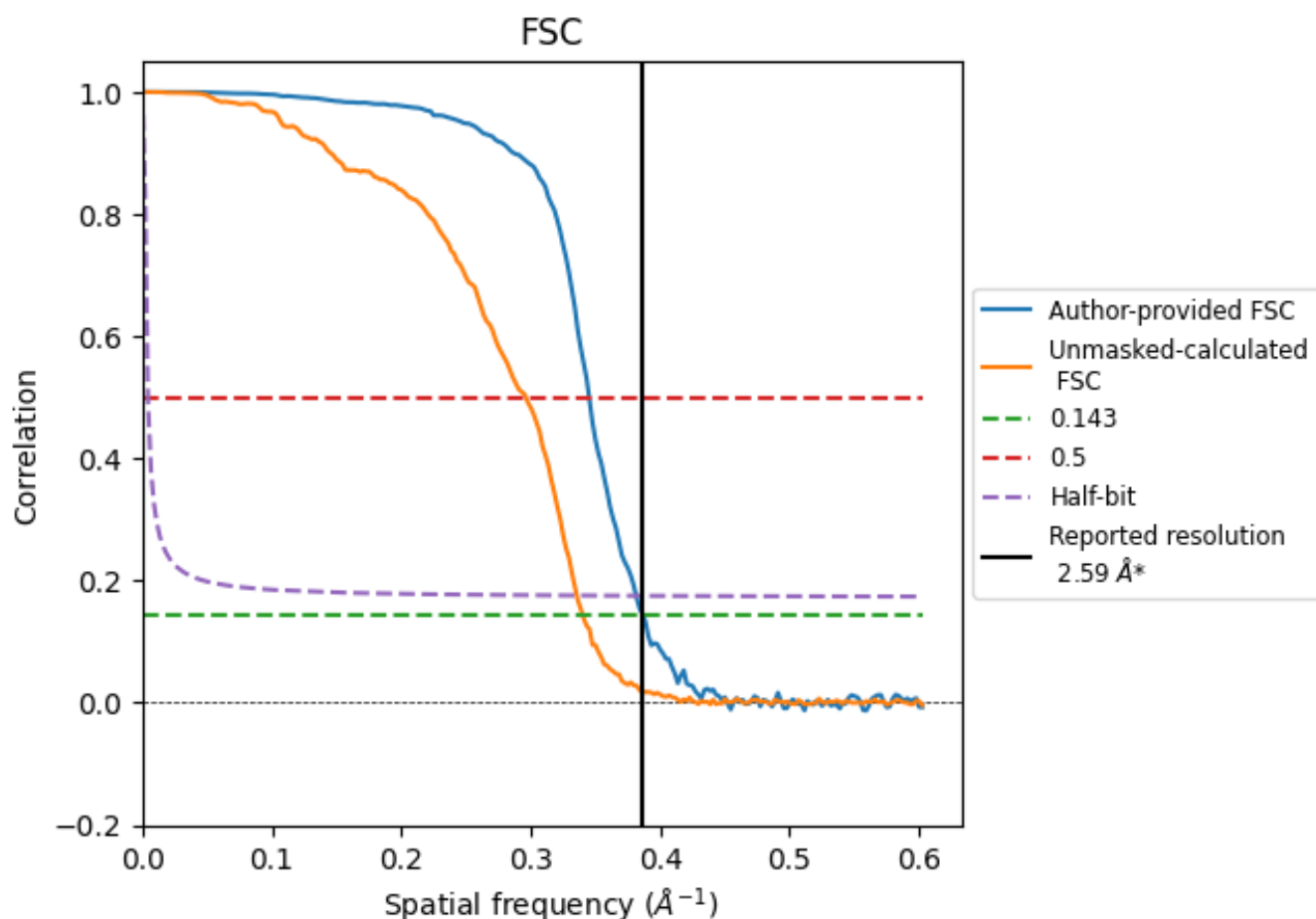


*Reported resolution corresponds to spatial frequency of $0.386 \text{ \AA}^{-1}$

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 0.386 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

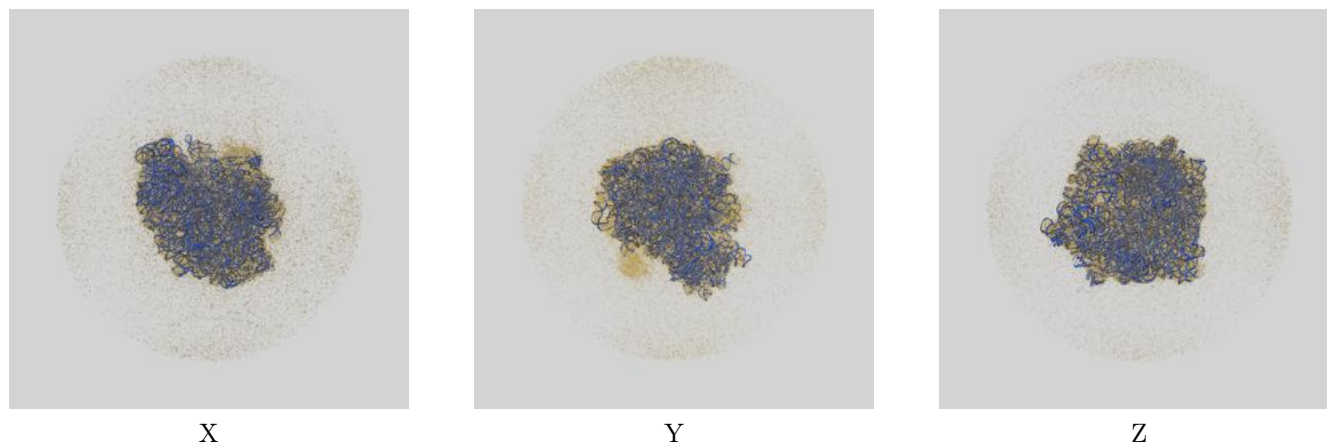
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.90	2.62
Unmasked-calculated*	2.94	3.37	2.98

*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 2.94 differs from the reported value 2.59 by more than 10 %

9 Map-model fit [i](#)

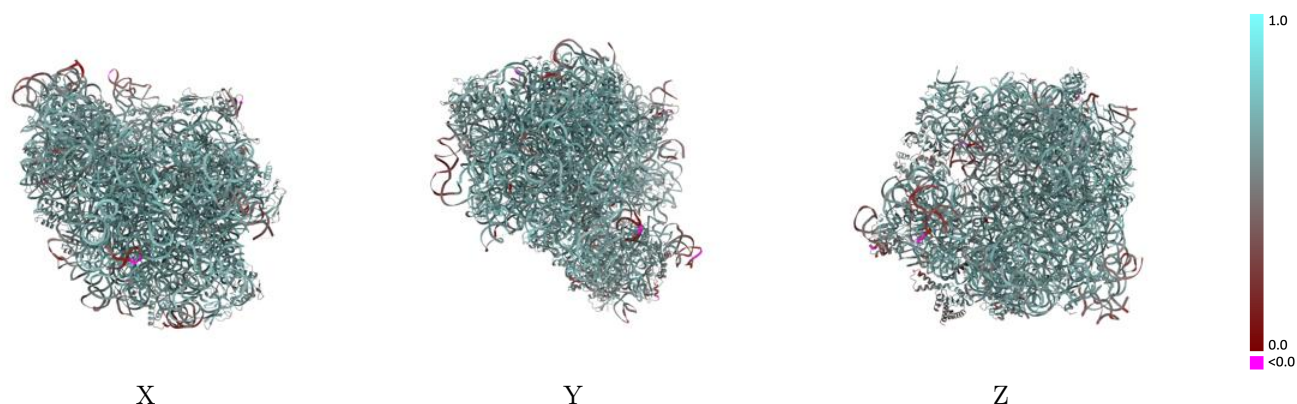
This section contains information regarding the fit between EMDB map EMD-60059 and PDB model 8ZFF. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



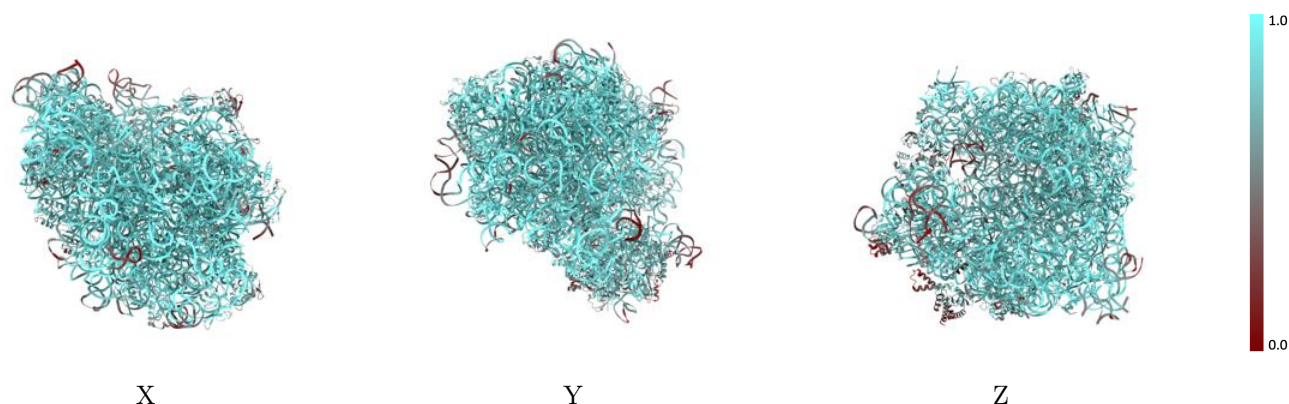
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



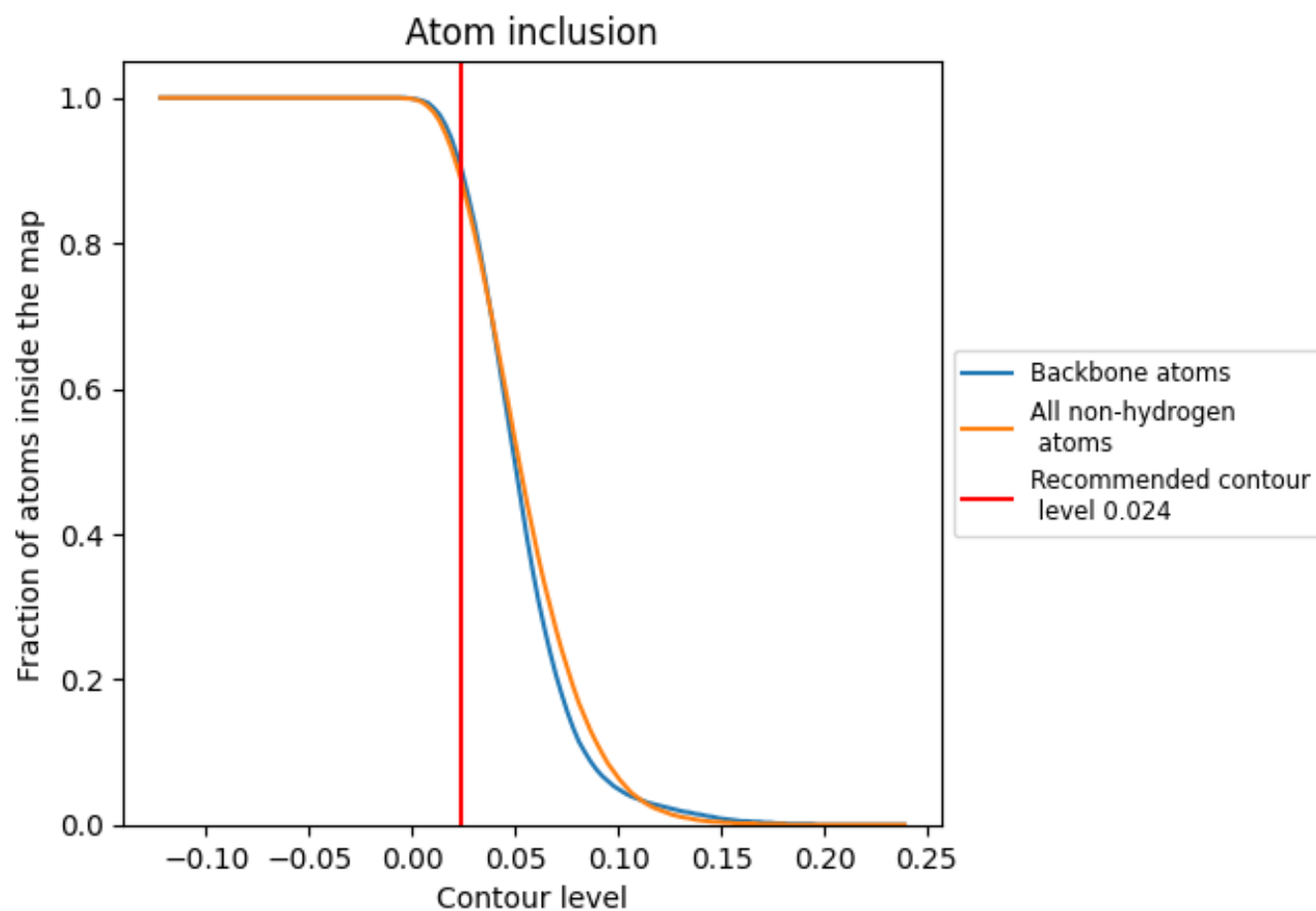
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.6220
0	 0.8510	 0.6340
1	 0.9610	 0.6730
2	 0.9550	 0.6740
3	 0.9250	 0.6440
4	 0.5500	 0.5030
A	 0.9030	 0.6210
B	 0.4960	 0.4960
C	 0.7730	 0.6030
D	 0.7530	 0.5780
E	 0.8720	 0.6420
F	 0.7160	 0.5480
G	 0.6400	 0.5330
H	 0.8810	 0.6420
I	 0.7500	 0.5660
J	 0.5810	 0.4960
K	 0.8070	 0.5880
L	 0.8750	 0.6240
M	 0.7440	 0.5640
N	 0.8140	 0.6060
O	 0.8360	 0.6150
P	 0.8650	 0.6070
Q	 0.8030	 0.5880
R	 0.7670	 0.5740
S	 0.7270	 0.5600
T	 0.8570	 0.6080
U	 0.5190	 0.4790
X	 0.7390	 0.5210
Z	 0.7720	 0.5410
a	 0.9330	 0.6390
b	 0.9080	 0.6140
c	 0.9640	 0.6810
d	 0.9170	 0.6600
e	 0.8070	 0.6060
f	 0.7360	 0.5660



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.6550	 0.5210
h	 0.6830	 0.4990
i	 0.9260	 0.6570
j	 0.9160	 0.6570
k	 0.8950	 0.6410
l	 0.9220	 0.6580
m	 0.9640	 0.6730
n	 0.8600	 0.6170
o	 0.9020	 0.6570
p	 0.9540	 0.6700
q	 0.8410	 0.6110
r	 0.8930	 0.6340
s	 0.8260	 0.5920
t	 0.7450	 0.5630
u	 0.7980	 0.6070
v	 0.9220	 0.6640
w	 0.8980	 0.6440
x	 0.7180	 0.5310
y	 0.8900	 0.6250
z	 0.8810	 0.6400