



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 10:12 AM EDT

PDB ID : 9Q43 / pdb_00009q43
EMDB ID : EMD-72219
Title : Pseudomonas aeruginosa 50S ribosome bound to RsfS (L1 stalk in 'out' conformation)
Authors : Findlay, J.L.; Kanik, M.; Gauvin, C.C.; Franklin, M.J.; Lawrence, C.M.
Deposited on : 2025-08-19
Resolution : 2.29 Å (reported)
Based on initial models : 7UNW, .

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:

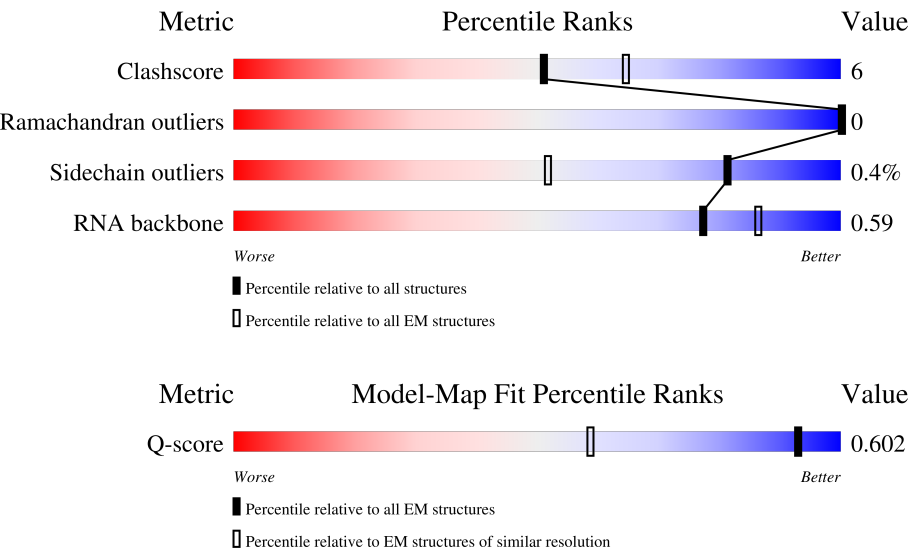
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.29 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	3699 (1.79 - 2.79)

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	2892	
2	B	121	
3	C	231	

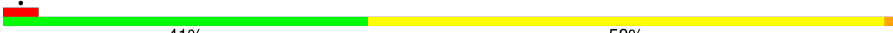
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	273	
5	E	211	
6	F	200	
7	G	179	
8	H	177	
9	I	148	
10	L	142	
11	M	122	
12	N	144	
13	O	137	
14	P	129	
15	Q	116	
16	R	116	
17	S	118	
18	T	103	
19	U	110	
20	V	99	
21	W	104	
22	X	204	
23	Y	85	
24	Z	78	
25	1	63	
26	2	58	
27	4	60	
28	5	51	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	6	44	 73%25%•
30	7	64	 84%14%•
31	8	38	 84%16%
32	9	118	 72%16%12%
33	v	76	 41%58%•
34	J	166	 6%57%10%33%
35	K	143	 5%85%15%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2837	Total	C	N	O	P	0	0
			60895	27173	11178	19708	2836		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	P	0	0
			2535	1132	452	832	119		

- Molecule 3 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	0	0
			918	582	163	172	1		

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	272	Total	C	N	O	S	0	0
			2072	1276	426	364	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	208	Total	C	N	O	S	0	0
			1564	968	298	293	5		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	200	Total	C	N	O	S	0	0
			1521	955	283	280	3		

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	179	Total	C	N	O	S	0	0
			1435	914	256	260	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	174	Total	C	N	O	S	0	0
			1314	828	242	242	2		

- Molecule 9 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	115	Total	C	N	O	S	0	0
			858	539	152	166	1		

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	142	Total	C	N	O	S	0	0
			1130	718	206	202	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	144	Total	C	N	O	S	0	0
			1066	654	215	194	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	137	Total	C	N	O	S	0	0
			1085	689	211	181	4		

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	119	Total	C	N	O	S	0	0
			952	595	191	161	5		

- Molecule 15 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 16 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	114	Total	C	N	O	S	0	0
			901	567	171	162	1		

- Molecule 17 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	117	Total	C	N	O	S	0	0
			936	592	196	148			

- Molecule 18 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	103	Total	C	N	O	S	0	0
			822	521	156	143	2		

- Molecule 19 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	110	Total	C	N	O	S	0	0
			833	515	161	153	4		

- Molecule 20 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	94	Total	C	N	O	S	0	0
			739	472	134	132	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	95	Total	C	N	O	S	0	0
			738	466	142	129	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	190	Total	C	N	O	S	0	0
			1445	915	262	265	3		

- Molecule 23 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	77	Total	C	N	O	S	0	0
			581	367	112	102			

- Molecule 24 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	77	Total	C	N	O	S	0	0
			630	391	134	103	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	61	Total	C	N	O	S	0	0
			490	301	96	91	2		

- Molecule 26 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	56	Total	C	N	O	S	0	0
			440	275	86	77	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	54	Total	C	N	O	S	0	0
			431	258	91	81	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	51	Total	C	N	O	S	0	0
			426	272	78	75	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	44	Total	C	N	O	S	0	0
			365	222	87	54	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

- Molecule 31 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	8	38	Total	C	N	O	S	0	0
			307	186	69	48	4		

- Molecule 32 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	104	Total	C	N	O	S	0	0
			804	504	135	162	3		

- Molecule 33 is a RNA chain called tRNA-Ala.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	v	76	Total	C	N	O	P	0	0
			1623	723	289	535	76		

- Molecule 34 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	J	111	Total	C	N	O	S	0	0
			840	533	151	155	1		

- Molecule 35 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	143	Total	C	N	O	S	0	0
			1046	655	186	201	4		

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	195	Total	Mg	0
			195	195	
36	B	3	Total	Mg	0
			3	3	
36	D	1	Total	Mg	0
			1	1	
36	E	1	Total	Mg	0
			1	1	
36	S	1	Total	Mg	0
			1	1	
36	4	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	8	1	Total	Zn	0
			1	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	4039	Total	O	0
			4039	4039	
38	B	76	Total	O	0
			76	76	
38	D	91	Total	O	0
			91	91	
38	E	81	Total	O	0
			81	81	
38	F	49	Total	O	0
			49	49	
38	G	10	Total	O	0
			10	10	
38	H	4	Total	O	0
			4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
38	I	1	Total 1	O 1	0
38	L	31	Total 31	O 31	0
38	M	20	Total 20	O 20	0
38	N	64	Total 64	O 64	0
38	O	36	Total 36	O 36	0
38	P	32	Total 32	O 32	0
38	Q	7	Total 7	O 7	0
38	R	26	Total 26	O 26	0
38	S	46	Total 46	O 46	0
38	T	35	Total 35	O 35	0
38	U	39	Total 39	O 39	0
38	V	30	Total 30	O 30	0
38	W	9	Total 9	O 9	0
38	X	22	Total 22	O 22	0
38	Y	25	Total 25	O 25	0
38	Z	21	Total 21	O 21	0
38	1	4	Total 4	O 4	0
38	2	18	Total 18	O 18	0
38	4	32	Total 32	O 32	0
38	5	3	Total 3	O 3	0
38	6	19	Total 19	O 19	0

Continued on next page...

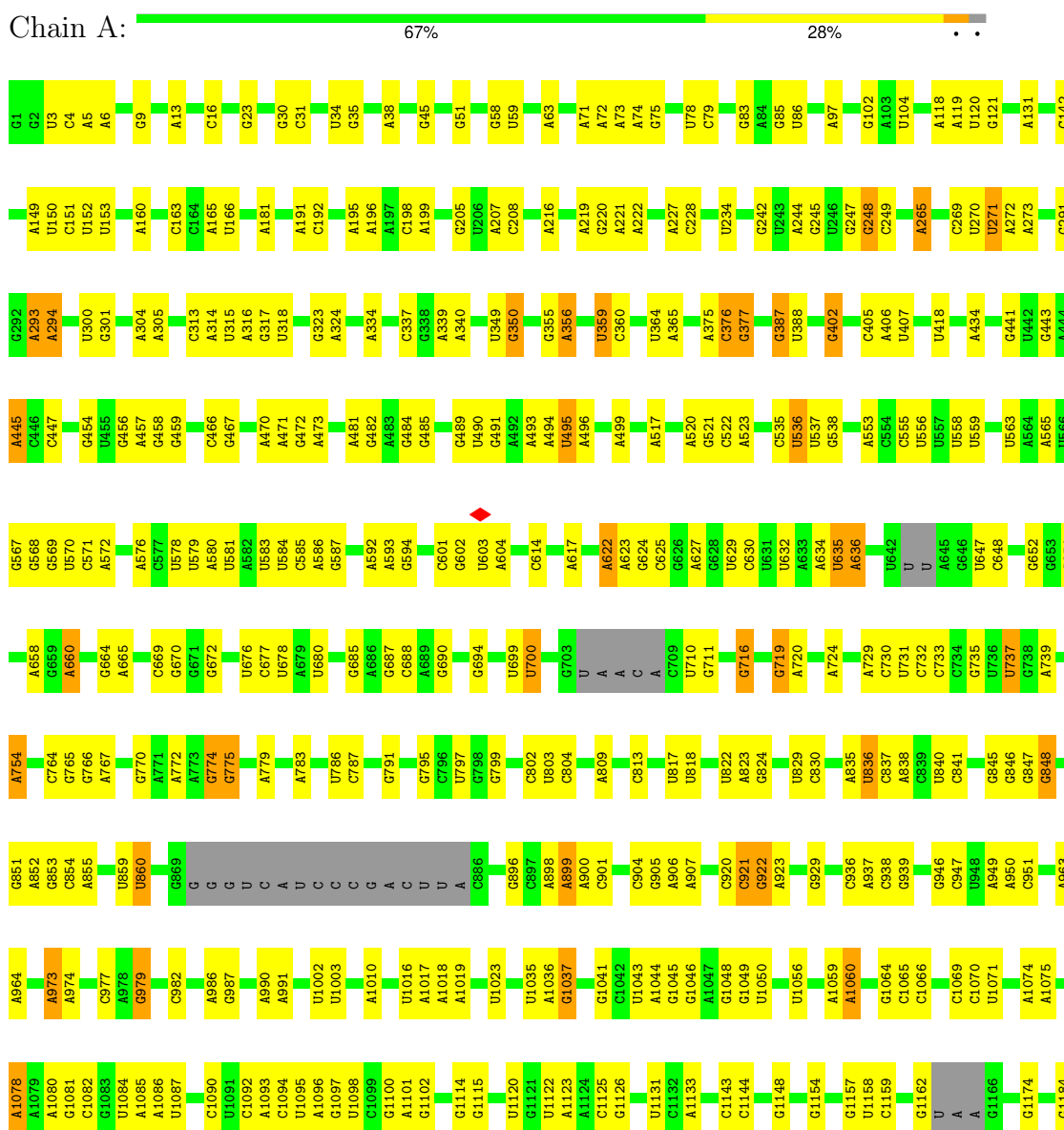
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
38	7	24	Total 24	O 24	0
38	8	9	Total 9	O 9	0

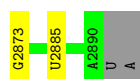
3 Residue-property plots

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: 23S rRNA

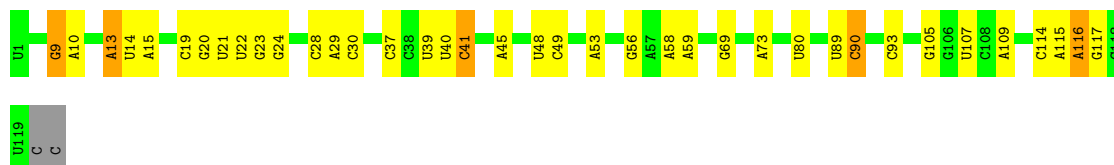


A2740	U2600	G2481	G2376	U2292	U2176	G2102	U2013	A	G1761	A1627	G1461	A1352	U1185
U2743	U2601	C2488	U2377	C2293	G2179	G2103	A2017	C	C1782	G1635	G1469	G1357	U1186
A2744	U2602	G2378	G2378	G2294	G2180	A2104	G2019	G	U1783	C1636	G1469	C1358	C1187
G2750	C2603	G2489	A2379	G2295	G2181	G2108	U2019	G1909	C1784	U1637	A1496	A1365	A1192
A2753	U2604	A2490	U2388	U2298	C2183	G2110	A2020	U1911	C1787	U1638	A1496	U1366	G1193
A2752	G2605	U2491	U	A2299	U2184	G2111	G2025	C1912	A1788	G1649	G1511	G1199	G1199
U2760	G2614	U2493	C2390	C2300	U2185	G2112	U2026	U1913	A1789	G1656	A1515	A1372	G1223
U2765	U2616	U2498	U2393	C2304	C2186	A2113	U2030	A1915	A1790	G1657	A1515	A1374	G1223
A2766	G2619	C2499	A2394	G2305	C2187	G2114	U2030	U1916	A1796	A1658	G1519	G1237	G1237
G2767	G2620	A2500	G2397	A2307	C2187	G2115	U2038	U1917	A1796	G1684	U	A1240	A1240
A2768	U2624	C2502	A2398	A2308	G2191	G2120	U2043	U1918	A1797	U1684	C	A1241	U1241
U2771	G2625	A2505	C2405	A2309	G2195	A2121	C2042	A1923	C1803	G1672	U	U1242	U1242
A2775	A2626	U2509	U2406	A2312	A2198	A2122	G2043	A1925	C1673	A1674	U	G1243	G1243
C2776	G2627	U2535	U2406	A2316	C2201	G2125	A2047	U1926	G1811	G1689	U	U1250	U1250
C2783	C2633	G2516	A2412	A2318	A2212	G2131	G2048	U1933	A1816	G1692	G1530	G1403	G1403
U	U2634	A2517	A2413	A2316	U2220	U2136	A2057	U1942	U1821	G1693	A1531	C1404	C1404
G2785	G2635	G2522	G2415	G2318	G2221	U2137	C2051	U1950	G1833	U1708	A1532	G1405	C1257
G2786	C2636	A2534	G2416	A2323	G2225	G2138	A2057	G1951	A1834	G1709	G1533	A1406	G1258
A2787	U2637	U2535	A2417	G2327	G2226	G2140	C2059	C1952	A1835	A1710	A1534	A1259	A1259
G2795	U2643	U2539	U2419	G2332	G2228	U2142	C2060	C1954	A1840	G1711	G1536	G1265	G1265
A2796	C2645	U2544	A2422	G2333	U2230	G2144	U2061	C1957	U1842	G1712	A1556	A1414	A1414
C2805	G2648	G2545	U2428	G2332	U2231	G2145	U2062	U1958	U1843	U1717	A1556	C1276	C1276
A2807	A2652	U2553	C2429	G2333	U2232	G2146	U2066	G1959	G1844	C1722	A1559	G1416	A1277
A2808	G2665	A2553	C2430	G2335	G2233	C2147	U2066	G1971	U1846	G1723	U1568	A1418	C1284
G2809	A2666	U2555	G2432	G2336	A2234	G2148	U2066	C1986	A1845	U1724	A1569	A1420	A1287
A2810	C2667	U2559	A2435	G2337	G2238	U2149	U2073	G1989	U1871	G1732	C1572	A1421	A1288
G2821	U2674	G2565	C2439	A2341	C2245	C2151	U2074	C1993	A1872	G1736	U1573	G1422	A1289
A2822	G2675	U2566	A2440	C2346	A2255	U2153	G2080	G1997	C1892	G1743	C1575	G1423	G1296
U2823	U2676	G2569	G2441	C2347	A2255	U2154	A2082	U1998	G1893	G1740	A1576	U1425	U1425
G2826	U2677	U2572	G2442	C2348	U2259	A2156	C2083	G1999	G1894	G1743	G1577	A1426	U1303
U2834	U2685	C2578	C2443	C2351	A2260	A2158	U2085	A2001	C	G1743	A1587	C1433	G1304
G2835	C2686	G2579	C2448	G2352	A2261	U2159	U2086	A2002	C	C1747	A1588	U1434	A1308
U2836	G2701	U2582	C2449	G2358	G2266	A2160	G2087	G2006	U	G1751	C1594	U1435	U1316
A2846	C2710	G2582	C2454	U2359	G2266	C2161	G2088	G2007	C1892	G1751	C1594	G1439	U1359
A2847	U2711	U2585	A2455	A2360	U2270	C2162	G2090	A2008	G1893	G1751	C1594	U1447	A1340
G2854	A2712	U2585	A2456	C2361	A2271	A2163	C2091	A2009	C	G1757	A1598	A1451	C1344
A2859	U2713	U2585	U2460	G2362	C2272	C2165	G2093	A2002	G	A1760	A1599	G1452	A1345
A2860	G2719	G2590	U2461	A2365	G2273	G2169	U2096	A2006	U	U1766	A1608	A1451	C1344
A2866	A2720	U2591	C2462	G2366	A2274	C2170	G2097	A2007	A	U1769	A1608	A1451	A1346
C2867	G2731	U2592	G2471	U2367	U2278	A2171	U2098	A2008	C	A1770	G1621	A1451	G1347
U2871	A2735	G2593	G2472	G2370	G2279	U2172	G2100	U2009	U	A1622	G1621	A1451	G1348
U2872	U2872	G2594	G2475	U2371	U2279	G2173	G2109	G2011	A	A1772	G1623	A1451	C1349
		U2596		C2372	U2283	U2175	A2101	C2012	A	A1773	A1624	U1460	G1351



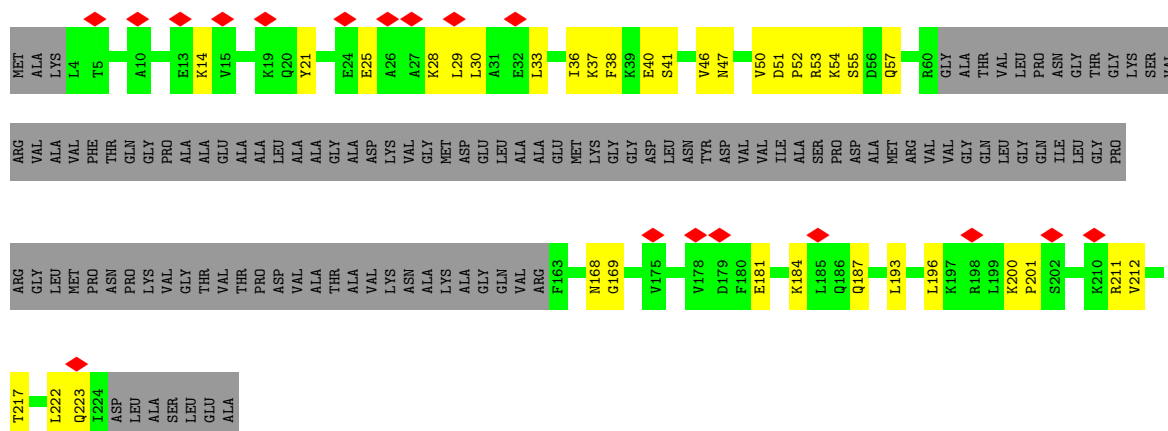
- Molecule 2: 5S rRNA

Chain B: 67% 27%



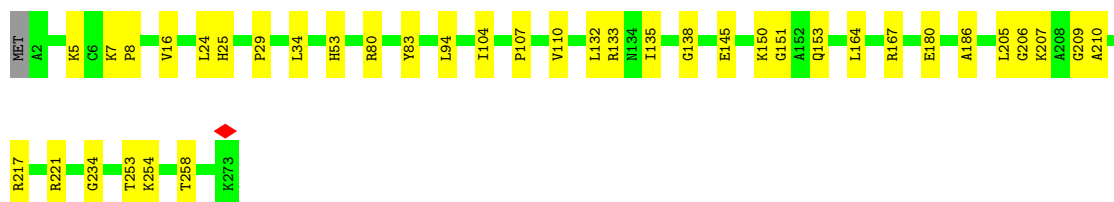
- Molecule 3: Large ribosomal subunit protein uL1

Chain C: 8% 36% 15% 48%



- Molecule 4: Large ribosomal subunit protein uL2

Chain D: 86% 14%



- Molecule 5: Large ribosomal subunit protein uL3

Chain E: 85% 14%



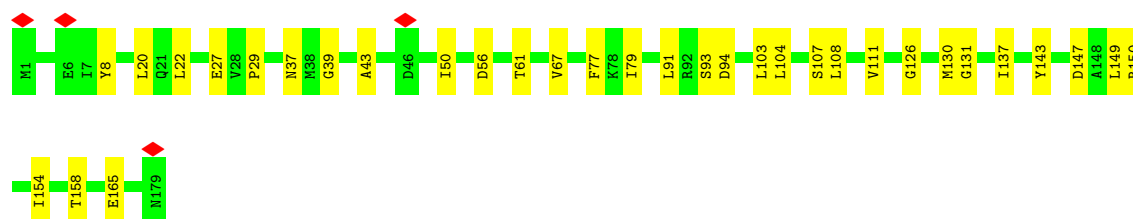
- Molecule 6: Large ribosomal subunit protein uL4

Chain F:  82% 18%



- Molecule 7: Large ribosomal subunit protein uL5

Chain G:  82% 18%



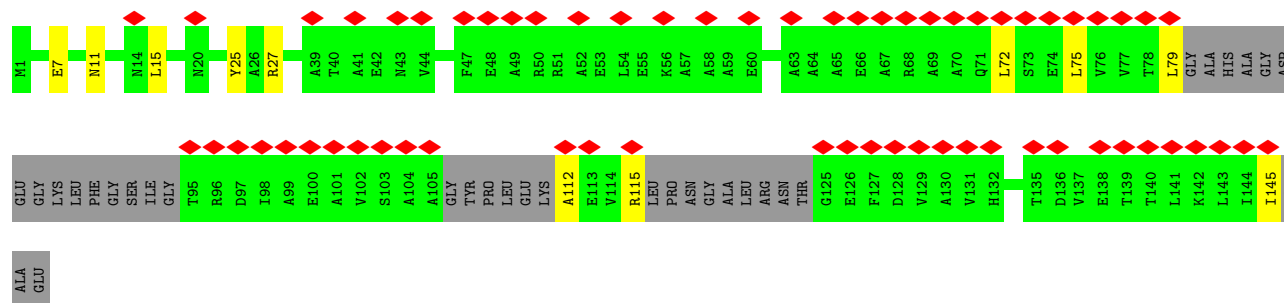
- Molecule 8: Large ribosomal subunit protein uL6

Chain H:  84% 15%



- Molecule 9: Large ribosomal subunit protein bL9

Chain I:  43% 70% 7% 22%



- Molecule 10: Large ribosomal subunit protein uL13

Chain L:  89% 11%

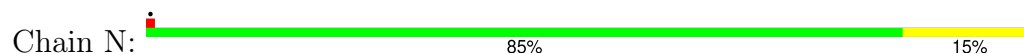


- Molecule 11: Large ribosomal subunit protein uL14

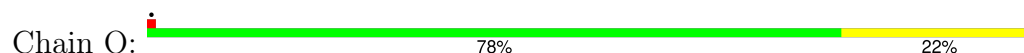
Chain M:  83% 17%



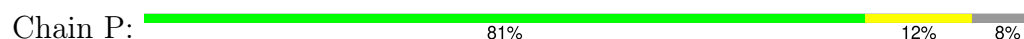
- Molecule 12: Large ribosomal subunit protein uL15



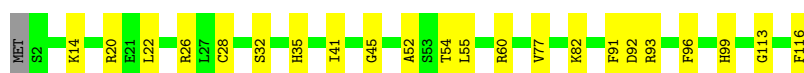
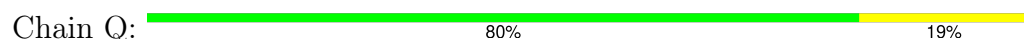
- Molecule 13: Large ribosomal subunit protein uL16



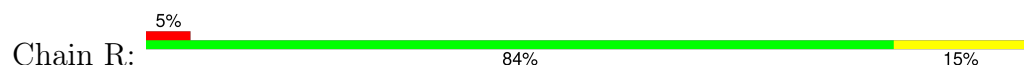
- Molecule 14: Large ribosomal subunit protein bL17



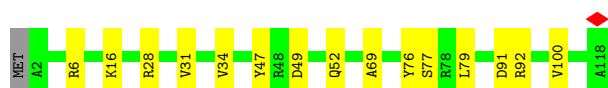
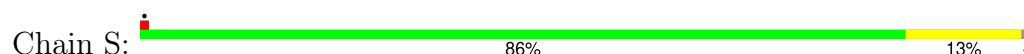
- Molecule 15: Large ribosomal subunit protein uL18



- Molecule 16: Large ribosomal subunit protein bL19



- Molecule 17: Large ribosomal subunit protein bL20



- Molecule 18: Large ribosomal subunit protein bL21

Chain T:  85% 15%



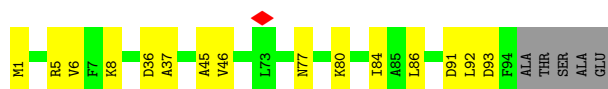
- Molecule 19: Large ribosomal subunit protein uL22

Chain U:  88% 12%



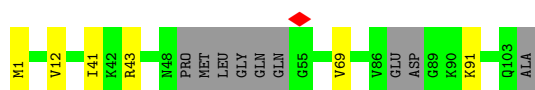
- Molecule 20: Large ribosomal subunit protein uL23

Chain V:  80% 15% 5%



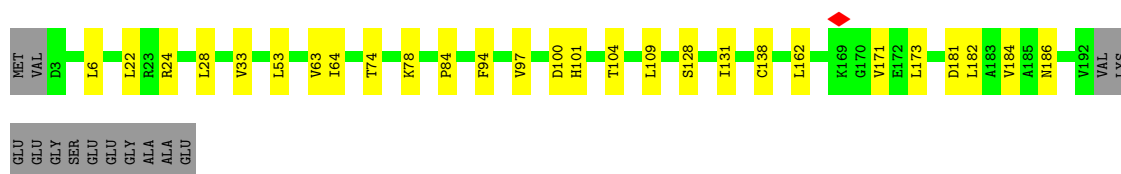
- Molecule 21: Large ribosomal subunit protein uL24

Chain W:  86% 6% 9%



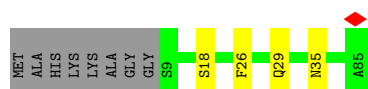
- Molecule 22: Large ribosomal subunit protein bL25

Chain X:  80% 13% 7%



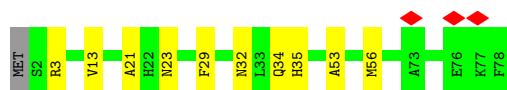
- Molecule 23: Large ribosomal subunit protein bL27

Chain Y:  86% 5% 9%

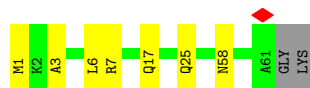
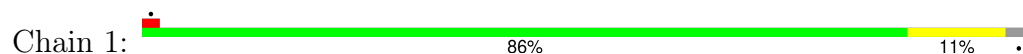


- Molecule 24: Large ribosomal subunit protein bL28

Chain Z:  86% 13%



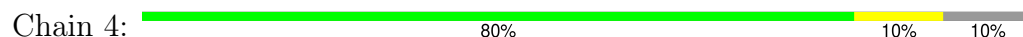
- Molecule 25: Large ribosomal subunit protein uL29



- Molecule 26: Large ribosomal subunit protein uL30



- Molecule 27: Large ribosomal subunit protein bL32



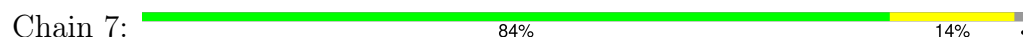
- Molecule 28: Large ribosomal subunit protein bL33



- Molecule 29: Large ribosomal subunit protein bL34



- Molecule 30: Large ribosomal subunit protein bL35



- Molecule 31: Large ribosomal subunit protein bL36A

Chain 8:  84% 16%



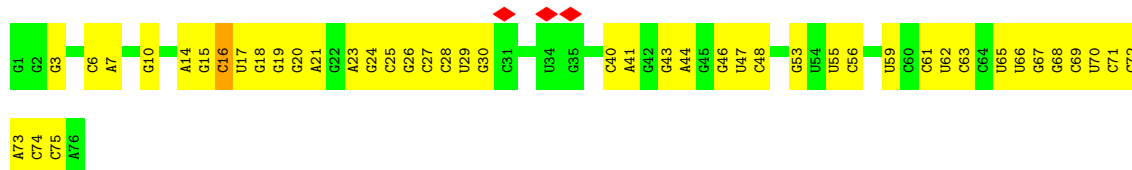
- Molecule 32: Ribosomal silencing factor RsfS

Chain 9:  72% 16% 12%



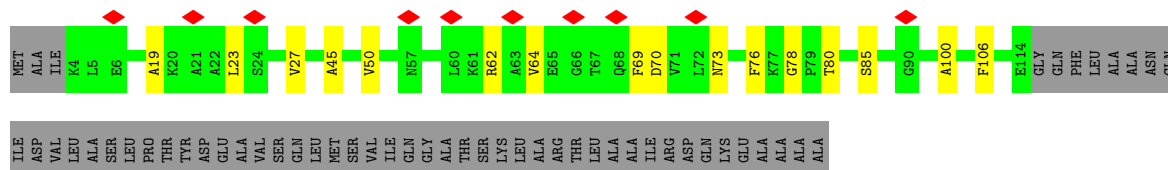
- Molecule 33: tRNA-Ala

Chain v:  41% 58%



- Molecule 34: Large ribosomal subunit protein uL10

Chain J:  6% 57% 10% 33%



- Molecule 35: Large ribosomal subunit protein uL10

Chain K:  5% 85% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	452165	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	67.584	Depositor
Minimum map value	-42.340	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.110	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	468.408, 468.408, 468.408	wwPDB
Map dimensions	696, 696, 696	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.673, 0.673, 0.673	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 5MU, OMU, 7MG, 6MZ, OMC, 2MA, OMG, PSU, 2MG, 1MG, 5MC

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	0.23	0/67882	0.26	0/105870
2	B	0.12	0/2833	0.21	0/4413
3	C	0.12	0/927	0.32	0/1243
4	D	0.16	0/2108	0.29	0/2831
5	E	0.17	0/1587	0.31	0/2138
6	F	0.09	0/1541	0.23	0/2075
7	G	0.13	0/1456	0.26	0/1953
8	H	0.10	0/1332	0.22	0/1794
9	I	0.14	0/861	0.30	0/1159
10	L	0.12	0/1156	0.28	0/1559
11	M	0.10	0/947	0.26	0/1268
12	N	0.08	0/1078	0.23	0/1436
13	O	0.08	0/1105	0.21	0/1476
14	P	0.17	0/968	0.36	0/1294
15	Q	0.18	0/888	0.23	0/1183
16	R	0.20	0/910	0.32	0/1218
17	S	0.16	0/946	0.31	0/1257
18	T	0.09	0/835	0.21	0/1117
19	U	0.10	0/837	0.22	0/1114
20	V	0.08	0/749	0.23	0/1002
21	W	0.09	0/743	0.27	0/988
22	X	0.13	0/1468	0.26	0/1987
23	Y	0.13	0/589	0.37	0/782
24	Z	0.15	0/641	0.25	0/854
25	1	0.14	0/491	0.23	0/654
26	2	0.19	0/444	0.27	0/597
27	4	0.09	0/437	0.23	0/583
28	5	0.12	0/433	0.27	0/576
29	6	0.18	0/368	0.36	0/482
30	7	0.15	0/511	0.34	0/668
31	8	0.09	0/308	0.19	0/404
32	9	0.17	0/813	0.35	0/1103

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	v	0.25	0/1767	0.31	0/2752
34	J	0.08	0/850	0.22	0/1142
35	K	0.08	0/1061	0.23	0/1435
All	All	0.21	0/101870	0.26	0/152407

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	60895	0	30645	522	0
2	B	2535	0	1283	20	0
3	C	918	0	977	26	0
4	D	2072	0	2152	26	0
5	E	1564	0	1575	21	0
6	F	1521	0	1581	27	0
7	G	1435	0	1504	21	0
8	H	1314	0	1373	15	0
9	I	858	0	890	9	0
10	L	1130	0	1160	11	0
11	M	938	0	1012	16	0
12	N	1066	0	1112	15	0
13	O	1085	0	1157	21	0
14	P	952	0	996	11	0
15	Q	881	0	920	14	0
16	R	901	0	958	14	0
17	S	936	0	1025	13	0
18	T	822	0	858	11	0
19	U	833	0	897	8	0
20	V	739	0	788	10	0
21	W	738	0	806	4	0
22	X	1445	0	1486	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Y	581	0	603	3	0
24	Z	630	0	653	8	0
25	1	490	0	520	4	0
26	2	440	0	469	2	0
27	4	431	0	424	6	0
28	5	426	0	457	10	0
29	6	365	0	409	10	0
30	7	506	0	569	11	0
31	8	307	0	342	4	0
32	9	804	0	809	13	0
33	v	1623	0	824	44	0
34	J	840	0	867	10	0
35	K	1046	0	1089	14	0
36	4	1	0	0	0	0
36	A	195	0	0	0	0
36	B	3	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	S	1	0	0	0	0
37	8	1	0	0	0	0
38	1	4	0	0	0	0
38	2	18	0	0	0	0
38	4	32	0	0	1	0
38	5	3	0	0	1	0
38	6	19	0	0	1	0
38	7	24	0	0	1	0
38	8	9	0	0	0	0
38	A	4039	0	0	16	0
38	B	76	0	0	1	0
38	D	91	0	0	1	0
38	E	81	0	0	0	0
38	F	49	0	0	1	0
38	G	10	0	0	0	0
38	H	4	0	0	0	0
38	I	1	0	0	0	0
38	L	31	0	0	0	0
38	M	20	0	0	0	0
38	N	64	0	0	0	0
38	O	36	0	0	0	0
38	P	32	0	0	0	0
38	Q	7	0	0	0	0
38	R	26	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	S	46	0	0	2	0
38	T	35	0	0	0	0
38	U	39	0	0	1	0
38	V	30	0	0	0	0
38	W	9	0	0	1	0
38	X	22	0	0	0	0
38	Y	25	0	0	0	0
38	Z	21	0	0	1	0
All	All	99173	0	63190	849	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 (849) 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:2419:A:H1'	33:v:75:C:O4'	1.76	0.84
1:A:79:C:HO2'	1:A:340:A:H8	1.25	0.81
3:C:54:LYS:HB2	3:C:57:GLN:HE22	1.52	0.73
8:H:16:GLU:HB2	8:H:27:LYS:HB3	1.71	0.72
1:A:1692:G:N7	38:A:3104:HOH:O	2.22	0.72
1:A:558:U:H1'	1:A:2017:6MZ:H9C1	1.73	0.70
1:A:1046:G:O2'	1:A:1093:A:N6	2.25	0.69
8:H:164:TYR:HB2	8:H:167:GLU:HB2	1.73	0.69
1:A:339:A:N1	38:A:3123:HOH:O	2.25	0.68
2:B:41:C:N4	7:G:67:VAL:O	2.26	0.68
33:v:3:G:H1	33:v:70:U:H3	1.41	0.68
35:K:100:THR:HG22	35:K:139:ASN:HB2	1.74	0.68
1:A:291:G:N7	38:A:3138:HOH:O	2.27	0.67
29:6:1:MET:SD	29:6:3:ARG:NH2	2.68	0.67
3:C:54:LYS:HB2	3:C:57:GLN:NE2	2.09	0.67
1:A:920:C:OP2	26:2:29:ARG:NH1	2.25	0.66
1:A:2315:A:H2'	1:A:2316:A:C8	2.31	0.66
35:K:9:ILE:HB	35:K:59:ILE:HB	1.78	0.66
34:J:27:VAL:HG13	34:J:80:THR:HG23	1.77	0.65
1:A:2162:C:H2'	1:A:2163:A:H8	1.63	0.64
1:A:694:G:O2'	1:A:716:G:N2	2.25	0.64
3:C:51:ASP:O	3:C:57:GLN:NE2	2.31	0.63
8:H:87:LEU:HB2	8:H:131:ILE:HB	1.81	0.63
1:A:1997:G:N7	38:A:3193:HOH:O	2.31	0.63
1:A:2010:C:H5'	1:A:2604:U:H4'	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2292:U:H5''	7:G:131:GLY:HA3	1.80	0.63
1:A:1085:A:H61	35:K:30:GLN:HE22	1.47	0.63
1:A:896:G:H5'	13:O:23:ARG:HB3	1.80	0.62
16:R:95:LYS:NZ	38:R:202:HOH:O	2.31	0.62
1:A:1084:U:H1'	1:A:1087:U:H5	1.64	0.62
1:A:1095:U:H2'	1:A:1096:A:H8	1.63	0.62
1:A:2156:A:C4	33:v:56:C:C5	2.88	0.62
1:A:963:A:H5''	18:T:81:LYS:HD2	1.82	0.62
22:X:162:LEU:HD12	22:X:182:LEU:H	1.63	0.62
13:O:67:ARG:NH1	13:O:105:GLU:OE2	2.32	0.62
16:R:101:LEU:HD11	16:R:111:ILE:HD11	1.82	0.61
5:E:41:GLU:HG3	5:E:47:ARG:HG3	1.82	0.61
13:O:78:PRO:HG2	13:O:81:VAL:HG21	1.82	0.61
6:F:147:ILE:HG23	6:F:186:LEU:HD23	1.82	0.61
27:4:2:ALA:N	38:4:203:HOH:O	2.34	0.61
1:A:2645:C:OP1	8:H:160:LYS:NZ	2.33	0.61
25:1:1:MET:SD	25:1:17:GLN:NE2	2.74	0.61
1:A:2278:U:H2'	1:A:2279:G:C8	2.36	0.60
1:A:896:G:OP1	13:O:24:GLY:N	2.33	0.60
1:A:2158:A:H4'	1:A:2159:U:H5'	1.83	0.60
1:A:1788:A:OP2	4:D:150:LYS:NZ	2.34	0.60
1:A:160:A:N3	1:A:2195:C:O2'	2.33	0.60
1:A:459:G:N7	29:6:39:ARG:NH2	2.40	0.60
1:A:1071:U:H4'	35:K:124:ALA:HB1	1.84	0.60
1:A:1834:A:O2'	1:A:1835:A:N7	2.35	0.60
1:A:2835:G:O2'	1:A:2854:G:N2	2.26	0.60
1:A:2293:C:H42	7:G:39:GLY:HA3	1.65	0.59
1:A:688:C:O2'	1:A:724:A:N6	2.35	0.59
35:K:28:LEU:HD12	35:K:35:ILE:HG23	1.84	0.59
1:A:1766:U:OP2	1:A:1771:A:N6	2.31	0.59
1:A:2114:G:H5'	3:C:37:LYS:HD3	1.83	0.59
1:A:2156:A:C4	33:v:56:C:C6	2.90	0.59
4:D:53:HIS:HA	4:D:217:ARG:HB2	1.84	0.59
33:v:43:G:H2'	33:v:44:A:H8	1.68	0.59
22:X:128:SER:OG	22:X:186:ASN:OD1	2.20	0.59
1:A:1689:G:N3	38:A:3227:HOH:O	2.32	0.58
1:A:2124:C:H2'	1:A:2125:G:C8	2.38	0.58
1:A:2156:A:N3	33:v:56:C:C5	2.70	0.58
1:A:2775:A:H2'	1:A:2776:C:C6	2.38	0.58
1:A:2170:C:H2'	1:A:2171:A:C8	2.39	0.58
1:A:1049:G:H21	35:K:128:THR:HG23	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1710:A:N7	1:A:1724:U:O2'	2.33	0.58
1:A:359:U:H5''	1:A:360:C:H5'	1.86	0.58
3:C:181:GLU:HG2	3:C:184:LYS:H	1.69	0.58
18:T:14:VAL:HG13	18:T:98:ILE:HG13	1.85	0.58
1:A:1420:A:H2'	1:A:1421:A:C8	2.39	0.57
1:A:1766:U:H5	1:A:1771:A:N7	2.03	0.57
1:A:1587:A:H5''	1:A:1588:A:H5'	1.87	0.57
3:C:211:ARG:HE	3:C:223:GLN:HB2	1.68	0.57
1:A:2260:A:H2'	1:A:2261:A:C8	2.40	0.57
1:A:5:A:H2'	1:A:6:A:C8	2.40	0.57
32:9:2:GLN:HB3	32:9:5:GLN:HG2	1.87	0.57
1:A:921:C:H4'	1:A:922:G:H5'	1.85	0.57
1:A:1404:C:HO2'	1:A:1577:G:HO2'	1.52	0.57
11:M:25:LEU:HD12	11:M:38:ILE:HG22	1.86	0.57
13:O:122:ALA:HA	13:O:125:LEU:HD12	1.87	0.57
28:5:6:ARG:NH2	28:5:50:ILE:O	2.37	0.57
14:P:79:LEU:HA	14:P:83:LEU:HB2	1.87	0.56
1:A:1237:G:O6	12:N:18:ARG:NH2	2.37	0.56
13:O:76:LYS:HB2	13:O:91:GLU:HG3	1.87	0.56
1:A:2156:A:C2	33:v:56:C:C5	2.92	0.56
11:M:64:ARG:HB2	11:M:83:ALA:HB3	1.87	0.56
1:A:797:U:OP2	12:N:41:ARG:NH2	2.38	0.56
1:A:1060:A:N7	1:A:1086:A:O2'	2.36	0.56
6:F:3:LEU:HD12	6:F:13:VAL:HG11	1.87	0.56
1:A:2080:G:O2'	9:I:25:TYR:CD1	2.59	0.56
1:A:1018:A:H2'	1:A:1019:A:C8	2.41	0.56
1:A:1056:U:N3	1:A:1059:A:OP2	2.34	0.56
1:A:1284:C:O2'	1:A:1289:A:N1	2.34	0.56
15:Q:20:ARG:HH21	15:Q:45:GLY:HA3	1.71	0.56
1:A:853:G:H2'	1:A:854:C:C6	2.41	0.55
22:X:78:LYS:NZ	22:X:104:THR:O	2.39	0.55
33:v:66:U:H2'	33:v:67:G:C8	2.42	0.55
35:K:56:PRO:HD3	35:K:75:PRO:HD3	1.87	0.55
1:A:2162:C:H2'	1:A:2163:A:C8	2.42	0.55
1:A:2775:A:O2'	1:A:2796:A:N3	2.39	0.55
2:B:13:A:N1	2:B:69:G:O2'	2.35	0.55
2:B:15:A:OP2	2:B:69:G:N2	2.33	0.55
33:v:43:G:H2'	33:v:44:A:C8	2.40	0.55
8:H:9:VAL:HG13	8:H:73:ASN:HD22	1.71	0.55
19:U:92:ARG:NH1	38:U:205:HOH:O	2.38	0.55
1:A:1821:U:H5''	1:A:1822:2MG:H5'	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2406:U:H4'	28:5:18:THR:HG21	1.89	0.55
1:A:59:U:OP2	20:V:77:ASN:ND2	2.40	0.55
1:A:72:A:H61	25:1:58:ASN:HD22	1.52	0.55
4:D:138:GLY:H	4:D:164:LEU:HB3	1.72	0.55
28:5:2:ARG:HB3	28:5:20:ASP:HB2	1.89	0.55
1:A:1373:C:H2'	1:A:1374:A:C8	2.42	0.55
1:A:1419:G:H2'	1:A:1420:A:C8	2.41	0.55
20:V:5:ARG:NH2	20:V:36:ASP:OD2	2.39	0.55
22:X:53:LEU:HD21	22:X:64:ILE:HD13	1.88	0.55
1:A:219:A:N3	1:A:234:U:O2'	2.37	0.55
1:A:1926:5MU:OP1	1:A:2591:U:O2'	2.23	0.55
1:A:2805:C:OP2	14:P:42:LYS:HE2	2.06	0.55
1:A:1074:A:N3	1:A:1095:U:O2'	2.32	0.55
1:A:1788:A:OP2	4:D:153:GLN:NE2	2.29	0.55
11:M:120:GLU:OE1	16:R:66:SER:OG	2.25	0.54
1:A:567:G:O2'	1:A:1241:A:OP1	2.26	0.54
1:A:1456:A:H2'	1:A:1457:A:C8	2.42	0.54
1:A:907:A:N3	2:B:80:U:O2'	2.39	0.54
1:A:2084:U:H3	1:A:2179:G:H1	1.55	0.54
1:A:571:C:H2'	1:A:572:A:C8	2.42	0.54
1:A:2498:U:H5''	5:E:128:ARG:HG3	1.90	0.54
33:v:26:G:H1	33:v:44:A:H61	1.56	0.54
1:A:1406:A:O2'	1:A:1408:G:N7	2.40	0.54
1:A:2534:A:H2'	1:A:2535:U:C6	2.43	0.54
4:D:132:LEU:HA	4:D:135:ILE:HD12	1.90	0.54
1:A:592:A:O2'	1:A:594:G:O2'	2.21	0.54
1:A:2300:C:O4'	7:G:37:ASN:ND2	2.40	0.54
21:W:43:ARG:NH2	38:W:201:HOH:O	2.41	0.54
1:A:2165:C:O2'	3:C:168:ASN:ND2	2.41	0.54
1:A:2230:U:H2'	1:A:2231:U:C6	2.42	0.54
11:M:98:ILE:HD13	11:M:114:ILE:HG23	1.90	0.54
1:A:570:U:H2'	1:A:571:C:C6	2.43	0.54
1:A:733:C:O2'	1:A:1649:G:OP1	2.24	0.54
1:A:2245:C:O2'	1:A:2414:C:OP2	2.25	0.53
13:O:34:LEU:HD13	13:O:118:PHE:HB3	1.90	0.53
1:A:78:U:H2'	1:A:79:C:C6	2.44	0.53
1:A:2102:G:O2'	1:A:2154:U:O2	2.24	0.53
1:A:2170:C:H2'	1:A:2171:A:H8	1.71	0.53
14:P:54:LEU:HD21	14:P:65:LEU:HB3	1.90	0.53
1:A:848:G:O2'	1:A:905:G:O6	2.24	0.53
1:A:1783:U:H2'	1:A:1784:C:C6	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2061:U:H2'	1:A:2062:U:C6	2.44	0.53
1:A:2087:G:H2'	1:A:2088:A:H8	1.72	0.53
9:I:79:LEU:HD21	9:I:145:ILE:HG12	1.90	0.53
1:A:786:U:H2'	1:A:787:C:C6	2.44	0.53
1:A:632:U:O2'	1:A:634:A:N7	2.40	0.53
1:A:1453:U:O3'	1:A:1536:G:O2'	2.27	0.53
3:C:47:ASN:ND2	3:C:211:ARG:HB3	2.24	0.53
1:A:677:C:H5''	29:6:2:LYS:HE2	1.90	0.53
1:A:244:A:H5''	12:N:67:VAL:HG11	1.91	0.53
1:A:680:U:O2'	1:A:770:G:OP1	2.25	0.53
1:A:764:C:O2'	1:A:767:A:N3	2.41	0.53
3:C:36:ILE:HD11	3:C:40:GLU:HB3	1.90	0.53
1:A:2019:G:O2'	5:E:150:GLN:NE2	2.42	0.52
1:A:2052:C:H2'	1:A:2053:C:H6	1.74	0.52
33:v:29:U:H2'	33:v:30:G:H8	1.74	0.52
22:X:74:THR:HG22	22:X:97:VAL:HB	1.90	0.52
1:A:823:A:H2'	1:A:824:G:C8	2.44	0.52
10:L:18:VAL:HG11	10:L:28:LEU:HD11	1.92	0.52
1:A:937:A:H2'	1:A:938:C:C6	2.45	0.52
1:A:1352:A:OP1	24:Z:3:ARG:NH1	2.38	0.52
1:A:2082:A:H4'	9:I:11:ASN:ND2	2.25	0.52
1:A:754:A:H5'	4:D:209:GLY:HA2	1.91	0.52
1:A:2125:G:N1	1:A:2141:G:O6	2.42	0.52
1:A:2605:G:H21	5:E:155:VAL:HG21	1.74	0.52
7:G:93:SER:OG	7:G:94:ASP:N	2.42	0.52
8:H:28:GLY:HA3	8:H:79:VAL:HB	1.91	0.52
11:M:77:ILE:HG12	16:R:73:ARG:HD2	1.92	0.52
13:O:54:LEU:HD12	13:O:117:ALA:HB1	1.91	0.52
28:5:41:GLN:NE2	38:5:101:HOH:O	2.42	0.52
29:6:25:LYS:NZ	38:6:101:HOH:O	2.43	0.52
32:9:34:THR:HG21	32:9:86:VAL:HG23	1.91	0.52
1:A:899:A:H2'	1:A:900:A:C8	2.45	0.52
7:G:103:LEU:HD12	7:G:107:SER:HB2	1.92	0.52
15:Q:82:LYS:HD2	15:Q:113:GLY:HA3	1.92	0.52
1:A:2161:C:H2'	1:A:2162:C:H6	1.75	0.52
22:X:131:ILE:HD11	22:X:184:VAL:HG22	1.92	0.52
38:B:305:HOH:O	22:X:24:ARG:NH2	2.42	0.52
17:S:16:LYS:NZ	38:S:303:HOH:O	2.43	0.52
8:H:42:GLU:HG2	8:H:55:ARG:HD3	1.91	0.51
10:L:31:GLU:OE2	10:L:35:ARG:NE	2.42	0.51
1:A:1046:G:N1	1:A:1092:C:OP2	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:156:PHE:HB3	10:L:81:PRO:HG3	1.92	0.51
19:U:82:LEU:HB2	19:U:98:LYS:HB2	1.91	0.51
1:A:441:G:N1	1:A:445:A:OP2	2.37	0.51
1:A:2585:A:H5''	4:D:234:GLY:HA3	1.93	0.51
1:A:5:A:H2'	1:A:6:A:H8	1.76	0.51
18:T:6:VAL:HG22	18:T:11:GLN:HG2	1.91	0.51
30:7:53:ASP:OD1	30:7:56:ARG:NH2	2.43	0.51
1:A:247:G:H4'	1:A:377:G:C5	2.45	0.51
1:A:1085:A:N6	35:K:30:GLN:HE22	2.09	0.51
1:A:2179:G:H2'	1:A:2180:G:H8	1.76	0.51
1:A:2633:C:OP2	1:A:2719:G:O2'	2.29	0.51
7:G:20:LEU:HD13	7:G:165:GLU:HG2	1.92	0.51
24:Z:13:VAL:HG23	24:Z:29:PHE:HB2	1.91	0.51
1:A:265:A:N1	1:A:418:U:O2'	2.44	0.51
1:A:2220:U:H2'	1:A:2221:G:C8	2.45	0.51
22:X:181:ASP:OD1	22:X:181:ASP:N	2.43	0.51
1:A:300:U:H2'	1:A:301:G:O4'	2.10	0.51
1:A:629:U:H2'	1:A:630:C:C6	2.46	0.51
1:A:1043:U:O4	1:A:1044:A:N6	2.44	0.51
1:A:1044:A:H2'	1:A:1045:G:C8	2.46	0.51
1:A:1434:U:O2'	1:A:1534:A:N3	2.38	0.51
1:A:1783:U:H2'	1:A:1784:C:H6	1.76	0.51
1:A:2432:2MG:OP1	6:F:68:ARG:NH1	2.42	0.51
12:N:78:ARG:HB2	12:N:81:GLU:HG3	1.93	0.51
1:A:1348:G:H2'	1:A:1349:C:C6	2.45	0.51
1:A:1373:C:H2'	1:A:1374:A:H8	1.76	0.51
1:A:2087:G:H2'	1:A:2088:A:C8	2.46	0.51
3:C:193:LEU:HD13	3:C:196:LEU:HD21	1.92	0.51
6:F:17:THR:OG1	6:F:200:GLY:O	2.29	0.51
1:A:1185:U:H2'	1:A:1186:U:C6	2.45	0.51
1:A:2058:A:H2'	1:A:2059:C:C6	2.46	0.51
1:A:2711:U:OP1	5:E:123:LYS:NZ	2.44	0.51
1:A:2821:G:H2'	1:A:2866:A:H61	1.75	0.51
11:M:122:LEU:HD13	16:R:71:VAL:HG11	1.93	0.51
21:W:1:MET:HE3	21:W:91:LYS:HE3	1.93	0.51
1:A:2086:U:H2'	1:A:2087:G:H8	1.76	0.50
1:A:2114:G:H2'	1:A:2115:G:H8	1.77	0.50
19:U:4:ALA:HB2	19:U:106:LYS:HG2	1.93	0.50
20:V:1:MET:HB3	20:V:5:ARG:HB3	1.93	0.50
33:v:23:A:H2'	33:v:24:G:H8	1.76	0.50
1:A:191:A:H2'	1:A:192:C:C6	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:G:H2'	1:A:1065:C:C6	2.46	0.50
1:A:2330:U:O2'	1:A:2360:A:O2'	2.26	0.50
30:7:41:ARG:NH1	38:7:105:HOH:O	2.44	0.50
1:A:836:U:H5	1:A:923:A:N7	2.09	0.50
3:C:200:LYS:HD2	3:C:201:PRO:HD2	1.93	0.50
1:A:456:G:OP1	29:6:12:ARG:NH2	2.44	0.50
1:A:1095:U:H2'	1:A:1096:A:C8	2.45	0.50
1:A:1781:A:H2'	1:A:1782:C:C6	2.46	0.50
38:A:6877:HOH:O	15:Q:14:LYS:CD	2.59	0.50
1:A:2554:G:H2'	1:A:2555:U:C6	2.46	0.50
1:A:2602:U:H1'	27:4:4:GLN:HB3	1.94	0.50
5:E:36:THR:HG22	5:E:74:VAL:HG21	1.94	0.50
16:R:89:ARG:NH2	16:R:111:ILE:O	2.35	0.50
32:9:33:VAL:HG12	32:9:34:THR:HG23	1.93	0.50
1:A:405:C:H2'	1:A:406:A:C8	2.46	0.50
7:G:61:THR:HB	7:G:91:LEU:HD21	1.93	0.50
33:v:68:G:H2'	33:v:69:C:H6	1.76	0.50
1:A:2080:G:O2'	9:I:25:TYR:HB2	2.12	0.50
1:A:2283:U:O2'	1:A:2307:A:N6	2.44	0.50
9:I:7:GLU:HA	9:I:15:LEU:HD12	1.94	0.50
9:I:72:LEU:HA	9:I:75:LEU:HD23	1.94	0.50
1:A:293:A:N3	1:A:313:C:O2'	2.41	0.50
13:O:35:LYS:NZ	22:X:84:PRO:O	2.34	0.50
31:8:2:LYS:HG2	31:8:4:ARG:HD2	1.94	0.50
33:v:68:G:H2'	33:v:69:C:C6	2.47	0.50
1:A:700:U:H3	1:A:711:G:H1	1.60	0.50
1:A:1392:U:H2'	1:A:1393:U:C6	2.47	0.50
1:A:1434:U:H2'	1:A:1435:U:C6	2.46	0.50
1:A:2182:U:H2'	1:A:2183:C:H6	1.77	0.50
8:H:121:ILE:HD11	8:H:140:LEU:HG	1.94	0.50
20:V:6:VAL:HG23	20:V:45:ALA:HA	1.94	0.50
33:v:14:A:C2	33:v:15:G:H1'	2.47	0.50
1:A:672:G:H5'	29:6:26:ASN:CG	2.37	0.49
1:A:2578:C:H2'	1:A:2579:G:C8	2.46	0.49
1:A:625:C:O2'	1:A:629:U:OP1	2.30	0.49
1:A:2582:G:N2	1:A:2585:A:OP2	2.34	0.49
1:A:2846:G:H2'	1:A:2847:A:C8	2.47	0.49
13:O:63:LYS:HD3	13:O:65:TRP:CZ2	2.47	0.49
1:A:729:A:H1'	1:A:730:C:H5	1.77	0.49
1:A:2517:A:N6	8:H:156:PRO:HG3	2.26	0.49
6:F:97:LYS:NZ	38:F:311:HOH:O	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:C:H2'	1:A:1066:C:C6	2.47	0.49
9:I:112:ALA:O	9:I:115:ARG:NH1	2.44	0.49
33:v:6:C:H2'	33:v:7:A:C8	2.47	0.49
1:A:658:A:H2'	1:A:660:A:H62	1.77	0.49
1:A:803:U:H2'	1:A:804:C:C6	2.47	0.49
1:A:2001:A:H2'	1:A:2002:A:C8	2.47	0.49
1:A:2179:G:H2'	1:A:2180:G:C8	2.47	0.49
2:B:28:C:OP1	15:Q:32:SER:OG	2.28	0.49
32:9:19:ALA:HB3	32:9:22:ILE:HD11	1.93	0.49
1:A:491:G:N1	1:A:494:A:OP2	2.41	0.49
1:A:1186:U:H2'	1:A:1187:C:C6	2.46	0.49
28:5:36:ASP:HB3	28:5:39:VAL:HG22	1.95	0.49
10:L:49:ASP:OD1	10:L:121:LYS:NZ	2.45	0.49
33:v:23:A:H2'	33:v:24:G:C8	2.47	0.49
1:A:2098:U:O4	1:A:2131:G:O2'	2.31	0.49
1:A:2114:G:N1	1:A:2149:A:H1'	2.27	0.49
7:G:77:PHE:HB2	7:G:79:ILE:HG13	1.93	0.49
1:A:1404:C:O2'	1:A:1577:G:O2'	2.26	0.49
1:A:2379:A:H5'	30:7:27:PHE:CD2	2.47	0.49
38:A:6877:HOH:O	15:Q:14:LYS:HD3	2.13	0.49
7:G:111:VAL:HG22	7:G:137:ILE:HG21	1.94	0.49
1:A:1010:A:N1	1:A:1131:U:O2'	2.44	0.49
1:A:1018:A:N6	1:A:1115:G:H2'	2.28	0.49
1:A:2834:U:H2'	1:A:2835:G:O4'	2.13	0.49
1:A:1097:G:H4'	34:J:78:GLY:C	2.38	0.48
34:J:45:ALA:HB1	34:J:50:VAL:HB	1.94	0.48
34:J:70:ASP:OD1	34:J:73:ASN:ND2	2.46	0.48
1:A:837:C:H2'	1:A:838:A:C8	2.49	0.48
1:A:1036:A:OP2	34:J:62:ARG:NH2	2.46	0.48
1:A:1350:U:O2'	1:A:1796:A:N3	2.42	0.48
6:F:142:LEU:HD13	6:F:145:VAL:HG21	1.95	0.48
6:F:169:ARG:NH1	6:F:175:ASP:OD1	2.44	0.48
29:6:41:ARG:HD3	29:6:44:VAL:HG23	1.95	0.48
1:A:16:C:H5''	27:4:14:ASP:HB2	1.95	0.48
1:A:1303:U:H2'	1:A:1304:G:C8	2.49	0.48
1:A:1303:U:H2'	1:A:1304:G:H8	1.78	0.48
1:A:1656:G:HO2'	11:M:6:SER:HG	1.61	0.48
1:A:1781:A:H2'	1:A:1782:C:H6	1.78	0.48
1:A:2012:C:H2'	1:A:2013:U:C6	2.48	0.48
1:A:2278:U:OP1	1:A:2367:U:O2'	2.30	0.48
1:A:2685:U:H2'	1:A:2686:C:C6	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:49:ASP:HA	17:S:52:GLN:HB2	1.95	0.48
1:A:2278:U:H2'	1:A:2279:G:H8	1.78	0.48
1:A:2471:G:OP1	13:O:45:ARG:NH1	2.37	0.48
1:A:938:C:H2'	1:A:939:G:H8	1.78	0.48
14:P:99:LYS:HB3	27:4:41:HIS:CE1	2.48	0.48
2:B:115:A:H2'	2:B:116:A:C8	2.49	0.48
4:D:145:GLU:HG2	4:D:151:GLY:C	2.39	0.48
10:L:4:TYR:CG	17:S:100:VAL:HG11	2.48	0.48
29:6:12:ARG:HE	29:6:44:VAL:HG12	1.77	0.48
19:U:73:THR:HB	19:U:106:LYS:HD2	1.96	0.48
31:8:16:ILE:HD13	31:8:25:VAL:HG22	1.95	0.48
1:A:293:A:H2'	1:A:294:A:C8	2.48	0.48
1:A:2771:U:H4'	5:E:44:ASP:OD1	2.14	0.48
1:A:150:U:H2'	1:A:151:C:C6	2.49	0.47
1:A:334:A:O2'	6:F:161:ARG:NH2	2.47	0.47
1:A:576:A:N1	1:A:799:G:O2'	2.40	0.47
1:A:1989:G:OP1	14:P:17:ARG:NH2	2.47	0.47
1:A:2152:C:N4	1:A:2159:U:O4	2.47	0.47
1:A:2181:U:H2'	1:A:2182:U:O4'	2.14	0.47
1:A:2404:C:OP1	30:7:24:LYS:NZ	2.47	0.47
22:X:162:LEU:HD22	22:X:173:LEU:HD13	1.95	0.47
33:v:70:U:H2'	33:v:71:C:H6	1.79	0.47
1:A:121:G:H4'	1:A:149:A:H5'	1.95	0.47
1:A:269:C:H5''	1:A:271:U:H5'	1.96	0.47
1:A:580:A:H2'	1:A:581:U:C6	2.49	0.47
1:A:733:C:OP1	5:E:135:GLY:HA2	2.14	0.47
1:A:2740:A:N7	38:A:3318:HOH:O	2.36	0.47
1:A:840:U:H2'	1:A:841:C:C6	2.48	0.47
1:A:1143:C:H4'	17:S:77:SER:HA	1.96	0.47
1:A:2052:C:H2'	1:A:2053:C:C6	2.49	0.47
33:v:67:G:H2'	33:v:68:G:H8	1.78	0.47
33:v:72:C:H2'	33:v:73:A:C8	2.49	0.47
34:J:19:ALA:HB1	34:J:69:PHE:HD2	1.79	0.47
34:J:100:ALA:HB2	34:J:106:PHE:HD2	1.79	0.47
1:A:719:G:C6	4:D:207:LYS:HB2	2.49	0.47
12:N:19:PRO:HA	12:N:27:LEU:HB3	1.97	0.47
28:5:25:THR:HG22	28:5:26:LYS:HE3	1.96	0.47
1:A:690:G:O2'	1:A:1622:A:N3	2.44	0.47
1:A:791:G:C8	6:F:49:SER:HB3	2.49	0.47
1:A:1980:U:H4'	5:E:133:THR:OG1	2.15	0.47
1:A:2140:C:H2'	1:A:2141:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2341:A:H4'	23:Y:35:ASN:ND2	2.30	0.47
1:A:2602:U:C2	27:4:4:GLN:HA	2.49	0.47
2:B:39:U:H2'	2:B:40:U:C6	2.49	0.47
22:X:63:VAL:HG13	22:X:74:THR:HG23	1.96	0.47
1:A:1276:C:H2'	1:A:1277:A:C8	2.50	0.47
1:A:1340:A:H2'	1:A:1341:A:C8	2.50	0.47
1:A:1757:G:N7	38:A:3313:HOH:O	2.35	0.47
1:A:2378:G:C6	1:A:2414:C:H1'	2.49	0.47
1:A:739:A:H4'	1:A:1258:G:N3	2.30	0.47
1:A:1424:C:H2'	1:A:1425:U:C6	2.50	0.47
1:A:1672:G:H2'	1:A:1673:C:C6	2.50	0.47
1:A:1840:A:H2'	1:A:1841:A:C8	2.49	0.47
1:A:2088:A:H2'	1:A:2089:G:C8	2.50	0.47
1:A:2619:A:H2'	1:A:2620:G:C8	2.50	0.47
6:F:170:ASP:OD1	6:F:171:VAL:N	2.45	0.47
6:F:171:VAL:O	6:F:174:SER:OG	2.31	0.47
11:M:24:VAL:HG13	11:M:33:ALA:HB2	1.97	0.47
11:M:97:ARG:NH2	32:9:98:TYR:O	2.48	0.47
11:M:98:ILE:HD12	11:M:117:LEU:HB2	1.96	0.47
28:5:9:SER:HB3	28:5:45:TYR:CZ	2.49	0.47
1:A:1740:G:H5''	16:R:94:ARG:HD2	1.97	0.47
1:A:1892:C:H4'	1:A:1916:G:H8	1.79	0.47
1:A:2057:A:H2'	1:A:2058:A:C8	2.50	0.47
22:X:33:VAL:HG22	22:X:94:PHE:HB2	1.97	0.47
1:A:402:G:OP2	1:A:2393:U:O2'	2.32	0.47
1:A:837:C:H2'	1:A:838:A:H8	1.80	0.47
1:A:859:U:H2'	1:A:860:U:H5''	1.95	0.47
1:A:1045:G:H21	1:A:1075:A:H2	1.63	0.47
1:A:2051:C:H2'	1:A:2052:C:C6	2.50	0.47
1:A:2307:A:H8	1:A:2309:A:C5	2.33	0.47
1:A:2667:C:H5'	5:E:194:PRO:HA	1.97	0.47
7:G:8:TYR:OH	7:G:29:PRO:O	2.28	0.47
1:A:467:G:H4'	1:A:493:A:N1	2.29	0.47
1:A:979:G:OP2	26:2:11:SER:OG	2.23	0.47
1:A:2090:C:H2'	1:A:2091:C:C6	2.50	0.47
1:A:2337:C:OP2	30:7:44:ARG:NH1	2.48	0.47
1:A:2454:C:O2	13:O:124:LYS:NZ	2.36	0.47
1:A:797:U:O2'	1:A:2047:A:N1	2.45	0.46
4:D:221:ARG:NH2	38:D:414:HOH:O	2.47	0.46
20:V:46:VAL:HG21	20:V:84:ILE:HD13	1.97	0.46
1:A:559:U:O2'	1:A:973:A:N1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1789:A:H2'	1:A:1790:A:C8	2.51	0.46
1:A:2220:U:H2'	1:A:2221:G:H8	1.80	0.46
1:A:2316:A:H2'	1:A:2317:G:C8	2.50	0.46
1:A:2636:C:H2'	1:A:2637:U:C6	2.51	0.46
1:A:2137:U:H2'	1:A:2138:C:C6	2.49	0.46
4:D:29:PRO:HG2	4:D:34:LEU:HD11	1.98	0.46
8:H:115:TYR:OH	8:H:147:GLU:OE1	2.28	0.46
20:V:37:ALA:O	20:V:80:LYS:NZ	2.47	0.46
1:A:1708:U:H2'	1:A:1709:G:O4'	2.15	0.46
33:v:27:C:H2'	33:v:28:C:C6	2.50	0.46
1:A:1184:G:H2'	1:A:1185:U:H6	1.81	0.46
1:A:1851:U:OP1	1:A:2397:G:O2'	2.25	0.46
33:v:66:U:H2'	33:v:67:G:H8	1.80	0.46
1:A:2509:U:O2'	1:A:2634:U:OP1	2.25	0.46
14:P:56:LYS:HE2	14:P:87:TYR:O	2.15	0.46
33:v:26:G:H1	33:v:44:A:N6	2.14	0.46
1:A:38:A:N3	6:F:42:SER:HB3	2.30	0.46
1:A:647:U:H2'	1:A:648:C:C6	2.50	0.46
1:A:977:C:O2'	1:A:990:A:N3	2.43	0.46
1:A:1041:G:H1	1:A:1098:U:H3	1.61	0.46
1:A:1344:C:H2'	1:A:1345:G:O4'	2.15	0.46
1:A:2278:U:O2'	1:A:2361:C:O2	2.34	0.46
1:A:2636:C:H2'	1:A:2637:U:H6	1.81	0.46
19:U:97:VAL:HG12	19:U:99:ARG:HG2	1.98	0.46
23:Y:26:PHE:H	23:Y:29:GLN:HE21	1.64	0.46
33:v:62:U:H2'	33:v:63:C:H6	1.81	0.46
1:A:13:A:O4'	1:A:517:A:N6	2.48	0.46
1:A:195:A:H61	1:A:198:C:H3'	1.81	0.46
1:A:1415:C:C5	1:A:1559:A:H5''	2.50	0.46
1:A:1425:U:H2'	1:A:1426:A:C8	2.50	0.46
3:C:30:LEU:HD23	3:C:33:LEU:HD21	1.98	0.46
3:C:53:ARG:NH2	33:v:62:U:H5'	2.31	0.46
1:A:207:A:H2'	1:A:208:C:O4'	2.16	0.46
4:D:135:ILE:O	4:D:167:ARG:NH2	2.49	0.46
34:J:27:VAL:HG21	34:J:76:PHE:HE1	1.81	0.46
1:A:571:C:H2'	1:A:572:A:H8	1.80	0.45
1:A:783:A:OP2	1:A:2058:A:O2'	2.32	0.45
1:A:1393:U:H2'	1:A:1394:C:H6	1.82	0.45
1:A:1784:C:O2'	4:D:258:THR:OG1	2.30	0.45
2:B:90:C:H5'	13:O:18:ARG:HG2	1.97	0.45
13:O:29:PHE:HB3	13:O:65:TRP:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:U:O2'	1:A:636:A:OP1	2.30	0.45
1:A:652:G:H5'	12:N:16:LYS:HB3	1.99	0.45
1:A:665:A:N3	1:A:2430:C:O2'	2.43	0.45
1:A:2025:G:H2'	1:A:2026:U:O4'	2.16	0.45
3:C:184:LYS:O	3:C:187:GLN:HG3	2.16	0.45
5:E:39:LYS:NZ	5:E:82:GLU:OE2	2.38	0.45
8:H:40:SER:HB2	8:H:61:THR:HG23	1.98	0.45
1:A:2085:U:H2'	1:A:2086:U:C6	2.52	0.45
1:A:2626:A:H2'	1:A:2627:G:O4'	2.16	0.45
10:L:121:LYS:HE2	10:L:121:LYS:HB2	1.79	0.45
11:M:112:MET:HE1	32:9:33:VAL:HG11	1.98	0.45
33:v:69:C:H2'	33:v:70:U:H6	1.81	0.45
1:A:454:G:N2	1:A:457:A:OP2	2.40	0.45
1:A:569:G:O2'	1:A:2006:A:OP1	2.34	0.45
1:A:822:U:H2'	1:A:823:A:C8	2.51	0.45
1:A:929:G:OP1	30:7:64:ARG:NH2	2.50	0.45
1:A:2233:G:H2'	1:A:2234:A:C8	2.51	0.45
3:C:46:VAL:HG13	3:C:212:VAL:HG12	1.98	0.45
6:F:96:ASN:HB2	6:F:99:MET:HG3	1.98	0.45
1:A:774:G:H5'	1:A:775:G:OP1	2.16	0.45
1:A:1048:G:N1	1:A:1071:U:C2	2.84	0.45
1:A:1673:C:H2'	1:A:1674:A:C8	2.52	0.45
1:A:2298:A:N3	7:G:79:ILE:HD11	2.31	0.45
4:D:94:LEU:HD11	4:D:104:ILE:HD13	1.96	0.45
8:H:118:PRO:HD2	8:H:121:ILE:HD13	1.98	0.45
15:Q:28:CYS:HA	15:Q:92:ASP:HB3	1.99	0.45
20:V:86:LEU:HD11	20:V:92:LEU:HG	1.98	0.45
32:9:58:LYS:HA	32:9:58:LYS:HD2	1.75	0.45
1:A:835:A:O2'	1:A:836:U:O2	2.27	0.45
1:A:990:A:H2'	1:A:991:A:C8	2.52	0.45
27:4:37:HIS:ND1	27:4:38:LEU:O	2.49	0.45
1:A:2735:A:H5'	8:H:4:VAL:HG21	1.98	0.45
2:B:114:C:H2'	2:B:115:A:H8	1.81	0.45
13:O:43:THR:HG22	13:O:94:VAL:HG12	1.98	0.45
1:A:1069:C:H2'	1:A:1070:C:C6	2.52	0.45
1:A:1833:G:H2'	1:A:1834:A:O4'	2.17	0.45
11:M:38:ILE:HD11	11:M:111:PHE:HZ	1.82	0.45
31:8:1:MET:HE3	31:8:1:MET:HB2	1.86	0.45
33:v:27:C:H2'	33:v:28:C:H6	1.80	0.45
33:v:71:C:H2'	33:v:72:C:C6	2.52	0.45
1:A:58:G:O2'	1:A:73:A:N1	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:SER:O	3:C:217:THR:OG1	2.32	0.45
3:C:50:VAL:O	3:C:52:PRO:HD3	2.17	0.45
7:G:108:LEU:HD21	7:G:130:MET:HE1	1.98	0.45
33:v:40:C:H2'	33:v:41:A:C8	2.52	0.45
1:A:388:U:H5''	24:Z:32:ASN:HB2	1.99	0.45
1:A:829:U:H2'	1:A:830:C:C6	2.52	0.45
1:A:2337:C:H5''	30:7:41:ARG:HD2	1.99	0.45
1:A:2439:C:H2'	1:A:2440:A:C8	2.52	0.45
2:B:29:A:H2'	2:B:30:C:C6	2.53	0.45
1:A:570:U:O3'	17:S:31:VAL:HG13	2.18	0.44
1:A:1796:A:H2'	1:A:1797:A:C8	2.53	0.44
1:A:2092:U:H2'	1:A:2093:G:C8	2.51	0.44
1:A:2096:U:H2'	1:A:2097:G:C8	2.52	0.44
1:A:2114:G:H2'	1:A:2115:G:C8	2.52	0.44
1:A:2534:A:H4'	11:M:29:HIS:NE2	2.31	0.44
12:N:55:GLN:O	12:N:60:ARG:NH1	2.40	0.44
1:A:568:G:OP1	1:A:1242:U:O2'	2.30	0.44
1:A:617:A:N7	12:N:113:SER:HB2	2.31	0.44
1:A:982:C:OP1	17:S:47:TYR:OH	2.32	0.44
1:A:1843:U:H2'	1:A:1844:G:O4'	2.17	0.44
1:A:2114:G:H4'	3:C:38:PHE:CD1	2.52	0.44
7:G:130:MET:HG3	7:G:154:ILE:HB	1.99	0.44
8:H:133:ILE:HG22	8:H:141:VAL:HG13	1.98	0.44
18:T:41:VAL:HG11	18:T:103:ALA:HA	1.99	0.44
24:Z:53:ALA:HA	24:Z:56:MET:HE3	1.98	0.44
33:v:70:U:H2'	33:v:71:C:C6	2.53	0.44
1:A:1425:U:H2'	1:A:1426:A:H8	1.83	0.44
7:G:126:GLY:O	7:G:158:THR:OG1	2.29	0.44
8:H:149:ARG:HA	8:H:162:VAL:HB	2.00	0.44
1:A:405:C:H2'	1:A:406:A:H8	1.82	0.44
1:A:1421:A:H2'	1:A:1422:G:O4'	2.17	0.44
1:A:1782:C:O2	4:D:254:LYS:NZ	2.46	0.44
1:A:2146:G:H2'	1:A:2147:C:C6	2.53	0.44
33:v:71:C:H2'	33:v:72:C:H6	1.81	0.44
35:K:133:ALA:HB1	35:K:138:LEU:HB2	1.99	0.44
1:A:938:C:H2'	1:A:939:G:C8	2.53	0.44
1:A:2272:C:OP2	28:5:2:ARG:NH1	2.50	0.44
38:A:4313:HOH:O	16:R:54:ARG:HD2	2.16	0.44
2:B:115:A:H2'	2:B:116:A:H8	1.81	0.44
12:N:51:GLU:OE2	30:7:56:ARG:NH1	2.51	0.44
1:A:86:U:H4'	1:A:104:U:H1'	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:C:H1'	38:A:3967:HOH:O	2.17	0.44
1:A:737:U:O2	1:A:2001:A:H1'	2.17	0.44
1:A:845:G:H2'	1:A:846:G:C8	2.52	0.44
1:A:1097:G:H2'	1:A:1098:U:C6	2.53	0.44
1:A:2088:A:H2'	1:A:2089:G:H8	1.83	0.44
1:A:2136:U:H2'	1:A:2137:U:C6	2.52	0.44
1:A:2269:G:H4'	1:A:2376:G:O2'	2.17	0.44
32:9:5:GLN:O	32:9:9:VAL:HG23	2.16	0.44
1:A:791:G:OP1	6:F:49:SER:HB2	2.18	0.44
1:A:1374:A:H5'	1:A:1456:A:H1'	1.99	0.44
1:A:1394:C:H2'	1:A:1395:U:H6	1.82	0.44
1:A:1627:A:H5'	1:A:1747:C:O2'	2.18	0.44
1:A:2346:C:H5''	30:7:50:ASN:ND2	2.33	0.44
1:A:2826:G:O2'	14:P:49:GLU:OE1	2.21	0.44
17:S:69:ALA:HB2	17:S:79:LEU:HD22	2.00	0.44
1:A:473:A:H1'	1:A:489:G:N2	2.32	0.44
1:A:2073:U:H2'	1:A:2074:U:C6	2.52	0.44
1:A:2089:G:H2'	1:A:2090:C:C6	2.53	0.44
1:A:2090:C:H2'	1:A:2091:C:H6	1.83	0.44
16:R:54:ARG:HB2	16:R:57:ASN:HB2	2.00	0.44
18:T:59:VAL:HG22	18:T:101:ILE:HG23	2.00	0.44
22:X:131:ILE:HG12	22:X:184:VAL:HA	1.98	0.44
33:v:72:C:H2'	33:v:73:A:H8	1.83	0.44
1:A:654:G:N7	38:A:3341:HOH:O	2.36	0.44
1:A:803:U:H2'	1:A:804:C:H6	1.83	0.44
1:A:1081:G:H2'	1:A:1082:C:C6	2.53	0.44
1:A:1515:A:N6	1:A:1533:G:O2'	2.51	0.44
1:A:2006:A:H4'	17:S:34:VAL:HG21	1.99	0.44
1:A:2448:A:H2'	1:A:2449:C:C6	2.53	0.44
13:O:42:LEU:HG	13:O:97:ILE:HG13	2.00	0.44
18:T:24:LYS:HD3	18:T:92:TRP:HB3	1.99	0.44
1:A:458:G:OP1	29:6:33:ARG:NE	2.48	0.43
1:A:1253:G:O2'	1:A:1999:G:O6	2.24	0.43
1:A:1993:C:O2'	1:A:2810:A:N3	2.51	0.43
1:A:2091:C:H2'	1:A:2092:U:C6	2.52	0.43
1:A:2108:G:H2'	1:A:2109:U:C6	2.53	0.43
1:A:2376:G:H5''	1:A:2377:U:O4'	2.18	0.43
1:A:2885:U:O2'	10:L:134:ALA:O	2.33	0.43
12:N:85:VAL:HB	12:N:94:THR:HG22	2.00	0.43
33:v:67:G:H2'	33:v:68:G:C8	2.52	0.43
35:K:86:ILE:HD13	35:K:138:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:K:110:ALA:HB1	35:K:125:ALA:HB1	1.99	0.43
1:A:317:G:H2'	6:F:162:ASN:OD1	2.18	0.43
1:A:685:G:N7	38:A:3316:HOH:O	2.35	0.43
1:A:946:G:H2'	1:A:947:C:H2'	1.98	0.43
1:A:1911:C:H2'	1:A:1912:C:C6	2.53	0.43
1:A:1986:C:H5''	1:A:2710:C:O2'	2.18	0.43
1:A:2643:U:O2	1:A:2652:A:N7	2.50	0.43
3:C:53:ARG:HH21	33:v:62:U:H5'	1.84	0.43
1:A:570:U:H2'	1:A:571:C:H6	1.82	0.43
1:A:624:G:N7	12:N:74:ARG:NH1	2.65	0.43
1:A:840:U:H2'	1:A:841:C:H6	1.83	0.43
1:A:1381:U:H2'	1:A:1382:A:O4'	2.19	0.43
1:A:1914:A:H2'	1:A:1915:A:C8	2.53	0.43
1:A:2238:OMG:HM23	1:A:2238:OMG:H1'	1.70	0.43
14:P:17:ARG:HG2	14:P:21:PHE:CE2	2.52	0.43
14:P:35:LYS:HE3	14:P:100:CYS:SG	2.58	0.43
1:A:687:G:H2'	1:A:688:C:C6	2.53	0.43
1:A:1416:G:H2'	1:A:1417:G:H8	1.83	0.43
1:A:2169:G:H2'	1:A:2170:C:C6	2.54	0.43
1:A:2169:G:H2'	1:A:2170:C:H6	1.84	0.43
5:E:17:THR:O	16:R:80:PRO:HG2	2.19	0.43
6:F:31:VAL:HG13	6:F:177:VAL:HG22	2.01	0.43
1:A:228:C:N4	1:A:2394:A:N3	2.64	0.43
1:A:622:A:H2'	1:A:623:A:C8	2.53	0.43
1:A:1811:G:O2'	4:D:253:THR:HG21	2.18	0.43
1:A:2187:C:H5''	24:Z:35:HIS:O	2.17	0.43
1:A:2456:A:H4'	13:O:56:ARG:HD2	1.99	0.43
3:C:52:PRO:HG2	3:C:169:GLY:H	1.83	0.43
5:E:26:THR:HG21	5:E:193:VAL:HB	2.00	0.43
32:9:17:LEU:HB2	32:9:51:LEU:HD23	1.99	0.43
1:A:1186:U:H2'	1:A:1187:C:H6	1.83	0.43
1:A:2163:A:H2'	1:A:2164:C:C6	2.53	0.43
1:A:2499:C:H2'	1:A:2500:A:O4'	2.17	0.43
1:A:2760:U:OP1	5:E:169:ARG:NE	2.47	0.43
4:D:16:VAL:HG22	4:D:206:GLY:HA3	1.99	0.43
34:J:23:LEU:N	34:J:85:SER:O	2.46	0.43
1:A:83:G:H1	1:A:102:G:HO2'	1.64	0.43
1:A:490:U:H2'	1:A:491:G:O4'	2.18	0.43
1:A:2161:C:H2'	1:A:2162:C:C6	2.53	0.43
1:A:2258:G:OP1	23:Y:18:SER:HB2	2.19	0.43
6:F:147:ILE:HD12	6:F:168:VAL:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:70:LYS:O	12:N:107:ARG:NH2	2.42	0.43
1:A:293:A:H8	1:A:293:A:OP2	2.01	0.43
1:A:719:G:C5	4:D:207:LYS:HB2	2.53	0.43
1:A:852:A:H2'	1:A:853:G:C8	2.54	0.43
1:A:1845:A:H2'	1:A:1846:U:O4'	2.18	0.43
1:A:2048:G:H2'	1:A:2488:C:O2'	2.19	0.43
1:A:2442:G:H2'	1:A:2443:C:C6	2.54	0.43
2:B:22:U:H2'	2:B:23:G:C8	2.54	0.43
2:B:48:U:H2'	2:B:49:C:C6	2.54	0.43
13:O:65:TRP:HB2	13:O:105:GLU:HB2	2.01	0.43
1:A:314:A:H4'	1:A:316:A:N7	2.33	0.43
1:A:349:U:O2'	1:A:350:G:H8	2.02	0.43
1:A:579:U:H2'	1:A:580:A:C8	2.53	0.43
1:A:583:U:H2'	1:A:584:U:C6	2.53	0.43
1:A:2304:C:H2'	1:A:2305:G:O4'	2.19	0.43
25:1:3:ALA:HA	25:1:6:LEU:HD12	2.01	0.43
1:A:23:G:OP1	1:A:495:U:N3	2.40	0.43
1:A:669:C:H2'	1:A:670:G:H8	1.83	0.43
1:A:1017:A:C2	1:A:2475:G:H5'	2.54	0.43
1:A:2326:G:H2'	1:A:2327:C:C6	2.54	0.43
2:B:37:C:O2	15:Q:99:HIS:NE2	2.34	0.43
3:C:25:GLU:HA	3:C:28:LYS:HG2	2.00	0.43
17:S:91:ASP:HB2	18:T:11:GLN:CD	2.43	0.43
1:A:586:A:H2'	1:A:587:G:C8	2.54	0.42
1:A:1037:G:N2	1:A:1100:G:O2'	2.52	0.42
1:A:1450:A:H2'	1:A:1451:A:C8	2.54	0.42
1:A:2336:G:OP1	30:7:44:ARG:NH2	2.51	0.42
1:A:2362:G:N2	1:A:2365:A:OP2	2.41	0.42
5:E:9:LYS:NZ	5:E:195:GLY:O	2.41	0.42
13:O:17:ASN:O	13:O:39:ARG:HD3	2.18	0.42
18:T:2:TYR:CD1	18:T:13:LYS:HE2	2.54	0.42
22:X:100:ASP:OD1	22:X:101:HIS:N	2.51	0.42
1:A:245:G:O2'	1:A:375:A:N1	2.40	0.42
1:A:484:G:O2'	19:U:7:LEU:HA	2.18	0.42
1:A:710:U:H2'	1:A:711:G:H8	1.84	0.42
1:A:1144:C:OP1	17:S:92:ARG:NH2	2.48	0.42
1:A:1158:U:H2'	1:A:1159:C:C6	2.54	0.42
1:A:1532:C:H2'	1:A:1533:G:O4'	2.19	0.42
1:A:1856:G:N2	1:A:1859:A:OP2	2.33	0.42
1:A:1971:G:N7	38:A:3347:HOH:O	2.37	0.42
3:C:21:TYR:HB2	3:C:222:LEU:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:LYS:HG3	3:C:29:LEU:N	2.33	0.42
1:A:2038:U:H5'	1:A:2565:G:O4'	2.18	0.42
1:A:2156:A:C6	33:v:56:C:C4	3.08	0.42
1:A:2334:C:H2'	1:A:2335:U:C6	2.55	0.42
35:K:81:LYS:O	35:K:85:GLY:N	2.51	0.42
1:A:3:U:H2'	1:A:4:C:C6	2.54	0.42
1:A:443:G:OP1	6:F:51:VAL:HG13	2.19	0.42
1:A:535:C:H2'	1:A:536:U:H5''	2.02	0.42
1:A:555:C:H2'	1:A:556:U:O4'	2.18	0.42
1:A:624:G:H2'	1:A:625:C:C6	2.54	0.42
1:A:1154:G:OP1	18:T:24:LYS:NZ	2.43	0.42
1:A:1722:C:H2'	1:A:1723:G:O4'	2.19	0.42
4:D:24:LEU:HD13	4:D:83:TYR:HB2	2.01	0.42
7:G:22:LEU:HD22	7:G:27:GLU:HB3	2.00	0.42
1:A:227:A:C2	1:A:2394:A:H1'	2.54	0.42
1:A:248:G:O5'	1:A:249:C:H5''	2.20	0.42
1:A:1393:U:H2'	1:A:1394:C:C6	2.54	0.42
1:A:2578:C:H2'	1:A:2579:G:H8	1.84	0.42
1:A:2624:U:H2'	1:A:2625:G:O4'	2.20	0.42
15:Q:35:HIS:ND1	15:Q:54:THR:OG1	2.47	0.42
1:A:1594:C:O2'	1:A:1600:A:N1	2.48	0.42
5:E:121:THR:HB	5:E:127:PHE:CD2	2.55	0.42
10:L:90:GLU:OE2	10:L:91:LYS:HG3	2.20	0.42
13:O:33:ALA:HB2	13:O:105:GLU:HG2	2.02	0.42
16:R:2:THR:HG22	16:R:7:GLN:HG3	2.01	0.42
22:X:138:CYS:HB3	22:X:171:VAL:HA	2.00	0.42
1:A:151:C:H2'	1:A:152:U:C6	2.54	0.42
1:A:272:A:H2'	1:A:273:A:C8	2.54	0.42
1:A:1256:A:H2'	1:A:1257:C:C6	2.55	0.42
1:A:1530:G:H2'	1:A:1531:A:C8	2.54	0.42
1:A:1657:G:O2'	1:A:1978:U:O4	2.32	0.42
1:A:1693:G:H2'	1:A:1694:U:C6	2.54	0.42
1:A:2232:U:H5''	38:A:4241:HOH:O	2.19	0.42
3:C:14:LYS:C	3:C:14:LYS:HD3	2.45	0.42
4:D:7:LYS:HA	4:D:8:PRO:HD3	1.91	0.42
6:F:1:MET:HG3	6:F:13:VAL:HG23	2.01	0.42
11:M:8:LEU:HD11	11:M:84:ALA:HB2	2.01	0.42
16:R:40:ARG:NH2	32:9:84:ASP:OD1	2.52	0.42
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.42
1:A:1460:U:H2'	1:A:1461:G:O4'	2.19	0.42
15:Q:91:PHE:HB2	15:Q:116:PHE:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:9:27:VAL:HG12	32:9:30:LYS:HD2	2.02	0.42
35:K:25:GLY:HA2	35:K:35:ILE:HD13	2.01	0.42
1:A:2544:G:H2'	1:A:2545:C:C6	2.55	0.42
1:A:2614:G:O2'	1:A:2768:A:N1	2.52	0.42
15:Q:26:ARG:HH21	15:Q:41:ILE:HD12	1.85	0.42
17:S:28:ARG:NH1	38:S:306:HOH:O	2.47	0.42
21:W:12:VAL:HG22	21:W:69:VAL:HG12	2.01	0.42
33:v:15:G:H4'	33:v:16:C:C5	2.55	0.42
1:A:664:G:H1'	6:F:68:ARG:HE	1.84	0.42
1:A:1405:G:N2	1:A:1569:A:N7	2.68	0.42
1:A:1433:C:H2'	1:A:1434:U:C6	2.54	0.42
1:A:2182:U:H2'	1:A:2183:C:C6	2.54	0.42
1:A:2351:C:H2'	1:A:2352:G:O4'	2.19	0.42
4:D:164:LEU:HD12	4:D:164:LEU:HA	1.78	0.42
15:Q:93:ARG:HD2	15:Q:96:PHE:O	2.19	0.42
1:A:78:U:H2'	1:A:79:C:H6	1.83	0.41
1:A:584:U:H2'	1:A:585:C:C6	2.54	0.41
1:A:622:A:H5'	12:N:68:SER:HB2	2.01	0.41
1:A:699:U:H2'	1:A:700:U:O4'	2.19	0.41
1:A:731:U:H2'	1:A:732:C:C6	2.55	0.41
1:A:2151:C:H2'	1:A:2152:C:O4'	2.20	0.41
1:A:2158:A:H1'	1:A:2159:U:C6	2.55	0.41
1:A:2181:U:H2'	1:A:2182:U:C6	2.55	0.41
4:D:5:LYS:HB2	4:D:5:LYS:HE2	1.87	0.41
4:D:25:HIS:CG	4:D:80:ARG:HD2	2.54	0.41
5:E:23:ILE:HG23	5:E:190:LYS:HG3	2.02	0.41
10:L:105:VAL:HG11	10:L:122:LEU:HD22	2.01	0.41
16:R:8:GLN:O	16:R:12:GLU:HG3	2.20	0.41
33:v:28:C:H2'	33:v:29:U:C6	2.55	0.41
1:A:364:U:H2'	1:A:365:A:H8	1.85	0.41
1:A:634:A:H2'	1:A:636:A:N7	2.35	0.41
1:A:732:C:H2'	1:A:733:C:C6	2.56	0.41
1:A:1078:A:H2'	1:A:1078:A:N3	2.35	0.41
1:A:1372:A:H1'	1:A:1373:C:C6	2.54	0.41
1:A:2171:A:H2'	1:A:2172:U:C6	2.54	0.41
3:C:55:SER:CB	33:v:53:G:O2'	2.68	0.41
5:E:84:ARG:HD2	5:E:84:ARG:HA	1.89	0.41
6:F:16:ARG:NH1	6:F:199:LEU:O	2.52	0.41
35:K:106:LEU:HD22	35:K:129:ILE:HG22	2.02	0.41
1:A:898:A:H2'	1:A:901:C:C5	2.55	0.41
1:A:2124:C:H2'	1:A:2125:G:H8	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:U:H1'	2:B:45:A:H61	1.85	0.41
6:F:1:MET:HE3	6:F:19:GLY:HA3	2.02	0.41
11:M:104:ARG:CZ	16:R:33:VAL:HG11	2.50	0.41
19:U:18:ARG:HG3	19:U:76:VAL:HB	2.02	0.41
1:A:1912:C:H2'	1:A:1913:U:O4'	2.21	0.41
1:A:2009:U:O2'	1:A:2604:U:H5'	2.20	0.41
1:A:2501:U:H2'	1:A:2502:C:C6	2.56	0.41
2:B:93:C:H5''	22:X:24:ARG:CZ	2.49	0.41
7:G:104:LEU:HD23	7:G:108:LEU:HD12	2.01	0.41
10:L:13:ARG:HH22	10:L:49:ASP:HB3	1.84	0.41
19:U:3:VAL:HG21	19:U:58:ALA:HA	2.02	0.41
33:v:40:C:H2'	33:v:41:A:H8	1.84	0.41
34:J:64:VAL:HG11	34:J:76:PHE:HZ	1.85	0.41
1:A:30:G:H2'	1:A:31:C:C6	2.56	0.41
1:A:150:U:H2'	1:A:151:C:H6	1.85	0.41
1:A:466:C:O2	1:A:470:A:N6	2.42	0.41
1:A:677:C:H2'	1:A:678:U:O4'	2.21	0.41
1:A:987:G:OP1	17:S:92:ARG:HB2	2.21	0.41
1:A:1770:A:H5'	1:A:2595:G:H4'	2.02	0.41
2:B:14:U:O3'	2:B:107:U:O2'	2.32	0.41
4:D:133:ARG:HB2	4:D:186:ALA:HB1	2.01	0.41
6:F:28:HIS:O	6:F:32:VAL:HG23	2.20	0.41
7:G:56:ASP:OD2	7:G:150:ARG:NH1	2.53	0.41
1:A:387:G:H1'	24:Z:29:PHE:HB3	2.01	0.41
1:A:1045:G:H1	1:A:1094:C:H42	1.68	0.41
1:A:1456:A:H2'	1:A:1457:A:H8	1.86	0.41
1:A:1773:A:H1'	1:A:1925:A:N6	2.35	0.41
1:A:2086:U:H2'	1:A:2087:G:C8	2.54	0.41
7:G:147:ASP:OD1	7:G:147:ASP:N	2.53	0.41
12:N:78:ARG:HG3	12:N:111:MET:HE3	2.03	0.41
1:A:601:C:H2'	1:A:602:G:O4'	2.20	0.41
1:A:1048:G:C6	1:A:1049:G:C6	3.08	0.41
1:A:1114:G:O2'	31:8:37:GLN:HG2	2.21	0.41
1:A:1144:C:H5'	17:S:76:TYR:HE2	1.86	0.41
1:A:1174:G:H5''	18:T:83:HIS:NE2	2.35	0.41
1:A:1250:U:C4	1:A:1251:G:C6	3.09	0.41
1:A:1621:G:N1	1:A:1624:A:OP2	2.41	0.41
1:A:1795:A:H3'	1:A:1796:A:C8	2.56	0.41
1:A:2358:G:O2'	28:5:42:HIS:ND1	2.39	0.41
12:N:48:PRO:HB3	30:7:59:ARG:HG2	2.03	0.41
20:V:93:ASP:OD1	20:V:93:ASP:N	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:G:H1'	1:A:445:A:C4	2.56	0.41
1:A:151:C:H2'	1:A:152:U:H6	1.86	0.41
1:A:2121:A:H2'	1:A:2122:A:C8	2.55	0.41
1:A:2318:G:O2'	1:A:2323:A:N1	2.53	0.41
5:E:30:VAL:O	5:E:185:ASN:HB3	2.21	0.41
15:Q:55:LEU:HA	15:Q:60:ARG:HD2	2.02	0.41
1:A:301:G:N1	1:A:304:A:OP2	2.46	0.41
1:A:578:U:H2'	1:A:579:U:C6	2.56	0.41
1:A:851:G:H2'	1:A:852:A:O4'	2.21	0.41
1:A:949:A:H2'	1:A:950:A:C8	2.55	0.41
1:A:1296:G:H4'	29:6:7:PRO:HB2	2.02	0.41
1:A:1419:G:H2'	1:A:1420:A:H8	1.84	0.41
1:A:1635:G:H5''	1:A:1636:C:H5'	2.02	0.41
1:A:1673:C:H2'	1:A:1674:A:H8	1.86	0.41
1:A:2080:G:O2'	9:I:25:TYR:CB	2.68	0.41
1:A:2112:G:H22	1:A:2159:U:P	2.43	0.41
1:A:2173:G:H2'	1:A:2174:C:C6	2.56	0.41
1:A:2228:A:H2'	1:A:2229:G:C8	2.56	0.41
1:A:2674:U:H2'	1:A:2675:G:O4'	2.20	0.41
1:A:2743:U:H4'	1:A:2744:A:OP1	2.19	0.41
6:F:163:LEU:HD12	6:F:163:LEU:HA	1.95	0.41
7:G:43:ALA:HB1	7:G:50:ILE:HD11	2.03	0.41
11:M:113:LYS:HD3	32:9:77:TRP:CE3	2.55	0.41
14:P:20:MET:HE2	14:P:20:MET:HB3	1.94	0.41
15:Q:52:ALA:HB3	15:Q:77:VAL:HB	2.02	0.41
22:X:22:LEU:HD22	22:X:28:LEU:HD12	2.03	0.41
24:Z:21:ALA:HB3	24:Z:23:ASN:HD21	1.85	0.41
28:5:21:LYS:HE3	28:5:21:LYS:HB3	1.93	0.41
32:9:95:ARG:HH21	32:9:101:GLU:CD	2.29	0.41
33:v:62:U:H2'	33:v:63:C:C6	2.56	0.41
1:A:809:A:H5''	1:A:963:A:N1	2.36	0.41
1:A:847:G:N3	1:A:2255:A:H2'	2.36	0.41
1:A:1265:G:O2'	14:P:27:SER:HB3	2.20	0.41
1:A:1850:G:H4'	1:A:2398:A:H4'	2.02	0.41
1:A:2087:G:H1	1:A:2176:U:H3	1.67	0.41
1:A:2102:G:C2	1:A:2104:A:C8	3.09	0.41
1:A:2143:G:N7	1:A:2144:G:N1	2.69	0.41
1:A:2366:G:H4'	15:Q:22:LEU:HD11	2.03	0.41
1:A:2665:A:H2'	1:A:2666:A:C8	2.55	0.41
2:B:58:A:H2'	2:B:59:A:O4'	2.21	0.41
10:L:114:LEU:HD12	10:L:114:LEU:HA	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:8:LYS:NZ	25:1:25:GLN:OE1	2.48	0.41
33:v:65:U:H2'	33:v:66:U:H6	1.86	0.41
1:A:614:C:O2'	1:A:647:U:OP1	2.38	0.40
1:A:938:C:H1'	1:A:974:A:C8	2.56	0.40
1:A:1740:G:N7	38:A:3346:HOH:O	2.36	0.40
1:A:1998:U:H2'	1:A:1999:G:O4'	2.21	0.40
1:A:2360:A:H2'	1:A:2361:C:C6	2.56	0.40
4:D:107:PRO:HG2	4:D:110:VAL:HG21	2.02	0.40
4:D:205:LEU:HB3	4:D:210:ALA:HB3	2.02	0.40
5:E:121:THR:HG21	5:E:143:PRO:HB3	2.03	0.40
6:F:17:THR:HA	6:F:105:ARG:HG2	2.03	0.40
33:v:24:G:H2'	33:v:25:C:C6	2.56	0.40
1:A:467:G:N1	1:A:470:A:OP2	2.43	0.40
1:A:471:A:H5''	21:W:41:ILE:HD12	2.03	0.40
1:A:1157:G:H2'	1:A:1158:U:C6	2.56	0.40
1:A:1424:C:H2'	1:A:1425:U:H6	1.85	0.40
1:A:1658:A:O2'	1:A:1664:G:N7	2.41	0.40
1:A:1933:U:H2'	1:A:1934:C:C6	2.57	0.40
1:A:2378:G:O6	1:A:2412:A:H8	2.05	0.40
6:F:167:ASP:HB2	6:F:182:TYR:OH	2.21	0.40
7:G:143:TYR:HE1	7:G:149:LEU:HD21	1.85	0.40
20:V:91:ASP:OD1	20:V:92:LEU:N	2.54	0.40
22:X:6:LEU:HG	22:X:53:LEU:HD22	2.03	0.40
1:A:2065:C:H2'	1:A:2066:U:C6	2.55	0.40
1:A:2806:G:H2'	1:A:2808:A:N7	2.37	0.40
18:T:5:ILE:HG12	18:T:14:VAL:HG21	2.02	0.40
1:A:317:G:H1'	1:A:1192:A:N1	2.36	0.40
1:A:1845:A:H61	1:A:1871:G:H1'	1.86	0.40
1:A:2100:U:H2'	1:A:2101:A:O4'	2.22	0.40
1:A:2233:G:H2'	1:A:2234:A:H8	1.86	0.40
2:B:9:G:C2	2:B:10:A:C8	3.10	0.40
6:F:3:LEU:HD23	6:F:3:LEU:HA	1.92	0.40
9:I:79:LEU:HD23	9:I:79:LEU:H	1.87	0.40
33:v:28:C:H2'	33:v:29:U:H6	1.86	0.40
33:v:69:C:H2'	33:v:70:U:C6	2.57	0.40
1:A:152:U:H2'	1:A:153:U:C6	2.56	0.40
1:A:355:G:OP2	1:A:356:A:O2'	2.28	0.40
1:A:456:G:H2'	1:A:457:A:C8	2.56	0.40
1:A:906:A:H5''	1:A:2255:A:H61	1.87	0.40
1:A:1081:G:H2'	1:A:1082:C:H6	1.86	0.40
1:A:2111:G:H21	3:C:217:THR:HG22	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2472:G:O3'	13:O:126:PRO:HB3	2.22	0.40
1:A:2592:U:H2'	1:A:2593:C:C6	2.57	0.40
2:B:20:G:H2'	2:B:21:U:C6	2.56	0.40
24:Z:34:GLN:HB3	38:Z:101:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	115/231 (50%)	113 (98%)	2 (2%)	0	100	100
4	D	270/273 (99%)	265 (98%)	5 (2%)	0	100	100
5	E	206/211 (98%)	200 (97%)	6 (3%)	0	100	100
6	F	198/200 (99%)	198 (100%)	0	0	100	100
7	G	177/179 (99%)	175 (99%)	2 (1%)	0	100	100
8	H	172/177 (97%)	171 (99%)	1 (1%)	0	100	100
9	I	107/148 (72%)	104 (97%)	3 (3%)	0	100	100
10	L	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
11	M	120/122 (98%)	120 (100%)	0	0	100	100
12	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
13	O	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
14	P	117/129 (91%)	115 (98%)	2 (2%)	0	100	100
15	Q	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	R	112/116 (97%)	109 (97%)	3 (3%)	0	100	100
17	S	115/118 (98%)	115 (100%)	0	0	100	100
18	T	101/103 (98%)	101 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
20	V	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
21	W	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
22	X	188/204 (92%)	187 (100%)	1 (0%)	0	100	100
23	Y	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
24	Z	75/78 (96%)	75 (100%)	0	0	100	100
25	1	59/63 (94%)	59 (100%)	0	0	100	100
26	2	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
27	4	52/60 (87%)	52 (100%)	0	0	100	100
28	5	49/51 (96%)	49 (100%)	0	0	100	100
29	6	42/44 (96%)	42 (100%)	0	0	100	100
30	7	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
31	8	36/38 (95%)	36 (100%)	0	0	100	100
32	9	102/118 (86%)	100 (98%)	2 (2%)	0	100	100
34	J	109/166 (66%)	105 (96%)	4 (4%)	0	100	100
35	K	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
All	All	3672/4031 (91%)	3619 (99%)	53 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	102/180 (57%)	102 (100%)	0	100	100
4	D	212/213 (100%)	211 (100%)	1 (0%)	81	90
5	E	160/162 (99%)	160 (100%)	0	100	100
6	F	157/158 (99%)	157 (100%)	0	100	100
7	G	153/153 (100%)	153 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	137/141 (97%)	137 (100%)	0	100	100
9	I	85/107 (79%)	84 (99%)	1 (1%)	63	79
10	L	119/119 (100%)	118 (99%)	1 (1%)	73	86
11	M	102/102 (100%)	102 (100%)	0	100	100
12	N	106/106 (100%)	105 (99%)	1 (1%)	70	84
13	O	110/110 (100%)	110 (100%)	0	100	100
14	P	98/104 (94%)	98 (100%)	0	100	100
15	Q	86/87 (99%)	86 (100%)	0	100	100
16	R	96/98 (98%)	96 (100%)	0	100	100
17	S	87/88 (99%)	86 (99%)	1 (1%)	65	81
18	T	86/86 (100%)	86 (100%)	0	100	100
19	U	87/87 (100%)	87 (100%)	0	100	100
20	V	79/82 (96%)	79 (100%)	0	100	100
21	W	81/88 (92%)	81 (100%)	0	100	100
22	X	154/164 (94%)	153 (99%)	1 (1%)	78	89
23	Y	57/61 (93%)	57 (100%)	0	100	100
24	Z	66/67 (98%)	66 (100%)	0	100	100
25	1	54/55 (98%)	53 (98%)	1 (2%)	50	69
26	2	48/49 (98%)	48 (100%)	0	100	100
27	4	47/52 (90%)	47 (100%)	0	100	100
28	5	47/47 (100%)	46 (98%)	1 (2%)	47	66
29	6	37/37 (100%)	35 (95%)	2 (5%)	20	29
30	7	54/55 (98%)	54 (100%)	0	100	100
31	8	34/34 (100%)	34 (100%)	0	100	100
32	9	90/101 (89%)	89 (99%)	1 (1%)	65	81
34	J	82/122 (67%)	82 (100%)	0	100	100
35	K	110/110 (100%)	110 (100%)	0	100	100
All	All	3023/3225 (94%)	3012 (100%)	11 (0%)	81	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	180	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	27	ARG
10	L	111	LYS
12	N	92	LEU
17	S	6	ARG
22	X	109	LEU
25	1	7	ARG
28	5	21	LYS
29	6	41	ARG
29	6	42	LEU
32	9	8	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	47	ASN
4	D	22	GLN
4	D	90	HIS
4	D	200	HIS
4	D	226	ASN
5	E	65	GLN
5	E	126	ASN
5	E	148	GLN
5	E	150	GLN
6	F	28	HIS
8	H	22	GLN
8	H	73	ASN
8	H	111	HIS
9	I	11	ASN
11	M	91	GLN
12	N	104	HIS
12	N	106	GLN
14	P	9	HIS
14	P	89	ASN
18	T	69	HIS
18	T	102	GLN
19	U	23	GLN
20	V	61	ASN
20	V	87	GLN
21	W	48	ASN
22	X	161	HIS
23	Y	29	GLN
24	Z	23	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Z	34	GLN
24	Z	35	HIS
25	1	39	GLN
25	1	58	ASN
27	4	5	GLN
29	6	26	ASN
32	9	20	GLN
34	J	73	ASN
35	K	30	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2827/2892 (97%)	310 (10%)	6 (0%)
2	B	118/121 (97%)	14 (11%)	0
33	v	75/76 (98%)	13 (17%)	0
All	All	3020/3089 (97%)	337 (11%)	6 (0%)

All (337) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	34	U
1	A	45	G
1	A	51	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	85	G
1	A	97	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	131	A
1	A	142	C
1	A	163	C
1	A	165	A
1	A	166	U
1	A	181	A
1	A	196	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	199	A
1	A	205	G
1	A	216	A
1	A	220	G
1	A	221	A
1	A	222	A
1	A	242	G
1	A	248	G
1	A	265	A
1	A	270	U
1	A	271	U
1	A	293	A
1	A	294	A
1	A	305	A
1	A	315	U
1	A	318	U
1	A	323	G
1	A	324	A
1	A	337	C
1	A	350	G
1	A	356	A
1	A	359	U
1	A	376	C
1	A	377	G
1	A	387	G
1	A	402	G
1	A	407	U
1	A	434	A
1	A	445	A
1	A	447	C
1	A	472	G
1	A	481	A
1	A	482	G
1	A	485	G
1	A	495	U
1	A	496	A
1	A	499	A
1	A	520	A
1	A	521	G
1	A	522	C
1	A	523	A
1	A	536	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	537	U
1	A	538	G
1	A	553	A
1	A	563	U
1	A	565	A
1	A	593	A
1	A	603	U
1	A	604	A
1	A	622	A
1	A	627	A
1	A	635	U
1	A	636	A
1	A	660	A
1	A	676	U
1	A	700	U
1	A	716	G
1	A	719	G
1	A	720	A
1	A	737	U
1	A	754	A
1	A	765	G
1	A	766	G
1	A	772	A
1	A	774	G
1	A	775	G
1	A	779	A
1	A	795	G
1	A	802	C
1	A	813	C
1	A	817	U
1	A	818	U
1	A	836	U
1	A	848	G
1	A	855	A
1	A	860	U
1	A	899	A
1	A	904	C
1	A	921	C
1	A	922	G
1	A	936	C
1	A	951	C
1	A	964	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	973	A
1	A	979	G
1	A	986	A
1	A	1002	U
1	A	1003	U
1	A	1016	U
1	A	1023	U
1	A	1035	U
1	A	1037	G
1	A	1050	U
1	A	1060	A
1	A	1078	A
1	A	1080	A
1	A	1090	C
1	A	1101	A
1	A	1102	G
1	A	1120	U
1	A	1122	U
1	A	1123	A
1	A	1125	C
1	A	1126	G
1	A	1133	A
1	A	1148	G
1	A	1162	G
1	A	1193	G
1	A	1199	G
1	A	1223	G
1	A	1240	A
1	A	1243	G
1	A	1258	G
1	A	1259	A
1	A	1287	A
1	A	1288	A
1	A	1308	A
1	A	1316	U
1	A	1339	U
1	A	1347	G
1	A	1352	A
1	A	1365	A
1	A	1366	U
1	A	1379	A
1	A	1381	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1403	G
1	A	1404	C
1	A	1414	A
1	A	1415	C
1	A	1439	G
1	A	1447	U
1	A	1469	G
1	A	1495	A
1	A	1496	A
1	A	1511	G
1	A	1556	A
1	A	1559	A
1	A	1568	U
1	A	1572	C
1	A	1573	U
1	A	1598	A
1	A	1624	A
1	A	1636	C
1	A	1637	U
1	A	1638	U
1	A	1664	G
1	A	1712	G
1	A	1717	U
1	A	1732	G
1	A	1736	G
1	A	1743	G
1	A	1751	G
1	A	1760	A
1	A	1769	U
1	A	1771	A
1	A	1773	A
1	A	1787	C
1	A	1788	A
1	A	1795	A
1	A	1803	C
1	A	1816	A
1	A	1835	A
1	A	1845	A
1	A	1871	G
1	A	1872	A
1	A	1893	G
1	A	1914	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1916	G
1	A	1917	G
1	A	1918	U
1	A	1923	A
1	A	1925	A
1	A	1942	U
1	A	1950	U
1	A	1952	C
1	A	1954	C
1	A	1957	A
1	A	1958	U
1	A	1959	G
1	A	1978	U
1	A	1979	G
1	A	1980	U
1	A	2008	A
1	A	2010	C
1	A	2017	6MZ
1	A	2018	A
1	A	2020	A
1	A	2030	U
1	A	2042	C
1	A	2043	G
1	A	2047	A
1	A	2048	G
1	A	2049	A
1	A	2056	7MG
1	A	2080	G
1	A	2114	G
1	A	2120	G
1	A	2139	G
1	A	2143	G
1	A	2144	G
1	A	2146	G
1	A	2149	A
1	A	2176	U
1	A	2185	A
1	A	2191	G
1	A	2198	A
1	A	2201	C
1	A	2212	A
1	A	2225	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2226	G
1	A	2266	G
1	A	2270	U
1	A	2274	A
1	A	2292	U
1	A	2295	G
1	A	2298	A
1	A	2306	C
1	A	2308	G
1	A	2309	A
1	A	2312	A
1	A	2323	A
1	A	2332	G
1	A	2337	C
1	A	2341	A
1	A	2348	C
1	A	2358	G
1	A	2359	U
1	A	2370	G
1	A	2371	U
1	A	2372	C
1	A	2379	A
1	A	2393	U
1	A	2412	A
1	A	2416	G
1	A	2417	A
1	A	2422	A
1	A	2428	U
1	A	2432	2MG
1	A	2435	A
1	A	2460	U
1	A	2462	C
1	A	2481	G
1	A	2489	G
1	A	2492	G
1	A	2493	U
1	A	2505	A
1	A	2516	G
1	A	2517	A
1	A	2522	G
1	A	2534	A
1	A	2553	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2554	G
1	A	2559	A
1	A	2569	G
1	A	2589	A
1	A	2596	U
1	A	2600	U
1	A	2602	U
1	A	2616	U
1	A	2633	C
1	A	2648	G
1	A	2676	U
1	A	2677	U
1	A	2701	G
1	A	2713	U
1	A	2720	A
1	A	2731	G
1	A	2735	A
1	A	2744	A
1	A	2750	G
1	A	2752	A
1	A	2765	A
1	A	2767	G
1	A	2786	G
1	A	2787	A
1	A	2795	G
1	A	2805	C
1	A	2806	G
1	A	2807	A
1	A	2808	A
1	A	2822	A
1	A	2823	U
1	A	2836	U
1	A	2859	A
1	A	2860	A
1	A	2867	C
1	A	2871	U
1	A	2872	U
1	A	2873	G
2	B	9	G
2	B	13	A
2	B	19	C
2	B	24	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	41	C
2	B	53	A
2	B	56	G
2	B	73	A
2	B	89	U
2	B	90	C
2	B	105	G
2	B	109	A
2	B	116	A
2	B	117	G
33	v	10	G
33	v	16	C
33	v	17	U
33	v	18	G
33	v	19	G
33	v	20	G
33	v	21	A
33	v	46	G
33	v	47	U
33	v	48	C
33	v	59	U
33	v	61	C
33	v	74	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	221	A
1	A	635	U
1	A	774	G
1	A	1871	G
1	A	2516	G
1	A	2743	U

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

14 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	2MA	A	2490	1,36	22,25,26	1.70	5 (22%)	32,37,40	3.47	13 (40%)
1	OMC	A	2485	1,36	19,22,23	0.56	0	25,31,34	0.68	0
1	5MU	A	1926	1	19,22,23	0.46	0	27,32,35	0.62	0
1	2MG	A	2432	1	23,26,27	0.57	0	33,38,41	0.50	0
1	5MC	A	1949	1	19,22,23	0.58	0	26,32,35	0.61	0
1	OMG	A	2238	1	23,26,27	0.52	0	32,38,41	0.45	0
33	5MU	v	54	33	19,22,23	0.36	0	27,32,35	0.58	0
1	2MG	A	1822	1	23,26,27	0.49	0	33,38,41	0.49	0
33	PSU	v	55	33	18,21,22	1.15	1 (5%)	21,30,33	1.89	4 (19%)
1	6MZ	A	2017	1	22,25,26	2.36	5 (22%)	29,36,39	2.32	12 (41%)
1	6MZ	A	1608	1	22,25,26	2.40	4 (18%)	29,36,39	2.36	10 (34%)
1	7MG	A	2056	1	23,26,27	1.12	1 (4%)	27,39,42	0.92	2 (7%)
1	1MG	A	735	1	23,26,27	3.05	8 (34%)	33,39,42	1.85	8 (24%)
1	OMU	A	2539	1	19,22,23	2.97	7 (36%)	25,31,34	1.83	5 (20%)

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	2MA	A	2490	1,36	-	1/7/25/26	0/3/3/3
1	OMC	A	2485	1,36	-	0/9/27/28	0/2/2/2
1	5MU	A	1926	1	-	0/7/25/26	0/2/2/2
1	2MG	A	2432	1	-	2/9/27/28	0/3/3/3
1	5MC	A	1949	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2238	1	-	1/9/27/28	0/3/3/3
33	5MU	v	54	33	-	0/7/25/26	0/2/2/2
1	2MG	A	1822	1	-	2/9/27/28	0/3/3/3
33	PSU	v	55	33	-	0/7/25/26	0/2/2/2
1	6MZ	A	2017	1	-	2/9/27/28	0/3/3/3
1	6MZ	A	1608	1	-	0/9/27/28	0/3/3/3
1	7MG	A	2056	1	-	0/7/37/38	0/3/3/3
1	1MG	A	735	1	-	0/7/25/26	0/3/3/3
1	OMU	A	2539	1	-	0/9/27/28	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1608	6MZ	C6-N6	9.41	1.45	1.34
1	A	735	1MG	C2-N3	9.25	1.48	1.33
1	A	2017	6MZ	C6-N6	9.04	1.44	1.34
1	A	2539	OMU	C2-N1	7.65	1.50	1.38
1	A	735	1MG	C4-N3	6.68	1.49	1.34
1	A	2539	OMU	C2-N3	6.44	1.49	1.38
1	A	735	1MG	C2-N2	5.93	1.44	1.34
1	A	2539	OMU	C6-C5	5.32	1.47	1.35
1	A	2490	2MA	C6-N6	5.29	1.47	1.34
1	A	2056	7MG	C5-N7	4.56	1.41	1.35
33	v	55	PSU	C6-C5	3.91	1.39	1.35
1	A	2017	6MZ	C5-C4	-3.32	1.33	1.39
1	A	1608	6MZ	C5-C4	-3.25	1.33	1.39
1	A	2539	OMU	C4-N3	3.12	1.44	1.38
1	A	735	1MG	C5-C6	3.10	1.53	1.45
1	A	2539	OMU	O4-C4	-3.08	1.18	1.24
1	A	2017	6MZ	C5-N7	-3.02	1.33	1.39
1	A	2490	2MA	C5-C4	-2.97	1.33	1.39
1	A	1608	6MZ	C5-N7	-2.96	1.33	1.39
1	A	2490	2MA	C5-N7	-2.91	1.33	1.39
1	A	735	1MG	O6-C6	-2.85	1.17	1.23
1	A	735	1MG	C2-N1	2.84	1.42	1.37
1	A	2539	OMU	O2-C2	-2.78	1.18	1.23
1	A	2539	OMU	C5-C4	2.74	1.49	1.43
1	A	2490	2MA	C6-N1	-2.69	1.31	1.35
1	A	2017	6MZ	C8-N9	-2.57	1.33	1.37
1	A	1608	6MZ	C8-N9	-2.57	1.33	1.37
1	A	2490	2MA	C8-N9	-2.50	1.33	1.37
1	A	735	1MG	C5-N7	-2.49	1.34	1.39
1	A	735	1MG	C6-N1	2.49	1.45	1.40
1	A	2017	6MZ	C4-N9	-2.05	1.33	1.37

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2490	2MA	C5-C4-N3	-8.74	117.97	127.18
1	A	2490	2MA	N6-C6-N1	-8.58	105.46	117.03
1	A	2490	2MA	CM2-C2-N3	7.73	128.70	117.13
1	A	2017	6MZ	N1-C2-N3	-5.88	119.69	128.58
1	A	1608	6MZ	N1-C2-N3	-5.82	119.77	128.58
1	A	2539	OMU	C4-N3-C2	-5.70	119.54	126.61
1	A	2490	2MA	N3-C4-N9	5.56	134.04	126.99
1	A	2490	2MA	C4-N9-C1'	-5.30	114.25	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2490	2MA	C1'-N9-C8	5.26	138.76	127.09
1	A	1608	6MZ	C5-C4-N3	-5.24	119.50	126.72
1	A	735	1MG	C5-C4-N3	-4.92	120.56	128.39
33	v	55	PSU	N1-C2-N3	4.79	120.22	115.17
33	v	55	PSU	C4-N3-C2	-4.68	119.93	126.37
1	A	2017	6MZ	C5-C4-N3	-4.60	120.39	126.72
1	A	2017	6MZ	C9-N6-C6	-4.40	118.77	122.85
1	A	2490	2MA	C5-C6-N6	4.34	134.03	123.29
1	A	2017	6MZ	N9-C8-N7	-4.04	108.20	113.94
1	A	1608	6MZ	N9-C8-N7	-4.02	108.23	113.94
1	A	1608	6MZ	C4-C5-C6	3.91	120.03	116.78
1	A	2490	2MA	CM2-C2-N1	-3.89	111.30	117.13
1	A	2539	OMU	N3-C2-N1	3.82	119.87	114.89
1	A	735	1MG	C1'-N9-C4	-3.73	115.47	126.49
1	A	2539	OMU	C5-C4-N3	3.72	120.01	114.80
1	A	735	1MG	C2-N3-C4	3.61	120.09	111.98
1	A	1608	6MZ	C9-N6-C6	-3.59	119.52	122.85
1	A	1608	6MZ	C2-N3-C4	3.58	120.56	111.83
1	A	2490	2MA	N9-C8-N7	-3.54	108.92	113.94
1	A	735	1MG	C1'-N9-C8	3.39	136.37	126.73
1	A	2017	6MZ	C2-N3-C4	3.35	120.02	111.83
1	A	2490	2MA	N3-C2-N1	-3.27	120.00	125.77
1	A	1608	6MZ	N3-C4-N9	3.22	132.65	127.17
1	A	2017	6MZ	C4-C5-C6	3.20	119.44	116.78
1	A	735	1MG	N9-C8-N7	-2.96	107.92	113.40
1	A	2539	OMU	O4-C4-C5	-2.95	120.08	125.16
1	A	1608	6MZ	C5-N7-C8	2.85	107.93	103.45
1	A	2490	2MA	C5-N7-C8	2.85	107.93	103.45
33	v	55	PSU	O2-C2-N1	-2.81	119.89	122.79
1	A	735	1MG	N9-C4-N3	2.77	131.49	125.95
1	A	2017	6MZ	C5-N7-C8	2.75	107.77	103.45
1	A	735	1MG	C5-C6-N1	2.74	120.08	115.02
33	v	55	PSU	C6-N1-C2	-2.58	120.30	122.69
1	A	2017	6MZ	N3-C4-N9	2.56	131.51	127.17
1	A	2490	2MA	C6-C5-C4	2.53	120.64	117.18
1	A	2056	7MG	C4-C5-N7	2.35	108.15	105.38
1	A	2017	6MZ	C4-C5-N7	-2.23	108.04	110.58
1	A	2056	7MG	C5-C4-N9	2.21	109.17	106.33
1	A	2017	6MZ	C4-N9-C1'	-2.18	121.52	126.63
1	A	1608	6MZ	C4-C5-N7	-2.18	108.09	110.58
1	A	2539	OMU	O2-C2-N1	-2.10	120.06	122.80
1	A	2017	6MZ	C5-C4-N9	2.10	108.10	105.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2490	2MA	C4-C5-N7	-2.10	108.18	110.58
1	A	2017	6MZ	C4-N9-C8	2.05	107.89	105.74
1	A	1608	6MZ	C4-N9-C8	2.05	107.89	105.74
1	A	735	1MG	C8-N7-C5	2.04	107.89	104.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2238	OMG	C1'-C2'-O2'-CM2
1	A	2432	2MG	C3'-C4'-C5'-O5'
1	A	2017	6MZ	O4'-C4'-C5'-O5'
1	A	2432	2MG	O4'-C4'-C5'-O5'
1	A	2017	6MZ	C3'-C4'-C5'-O5'
1	A	1822	2MG	O4'-C4'-C5'-O5'
1	A	1822	2MG	C3'-C4'-C5'-O5'
1	A	2490	2MA	C4'-C5'-O5'-P

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1926	5MU	1	0
1	A	2432	2MG	1	0
1	A	2238	OMG	1	0
1	A	1822	2MG	1	0
1	A	2017	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 203 ligands modelled in this entry, 203 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

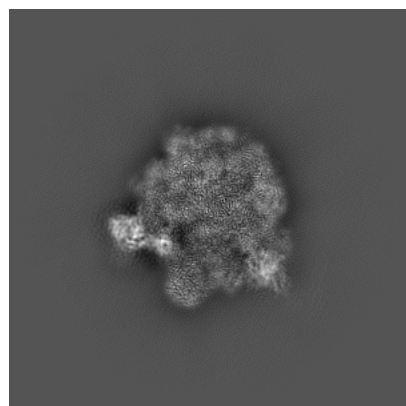
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72219. These allow visual inspection of the internal detail of the map and identification of artifacts.

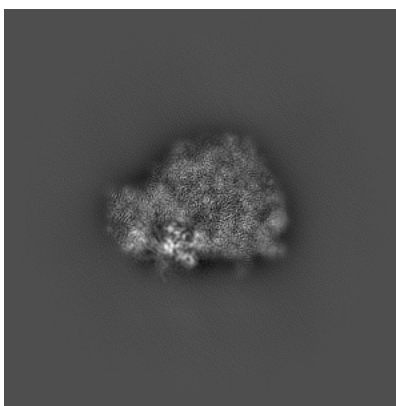
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

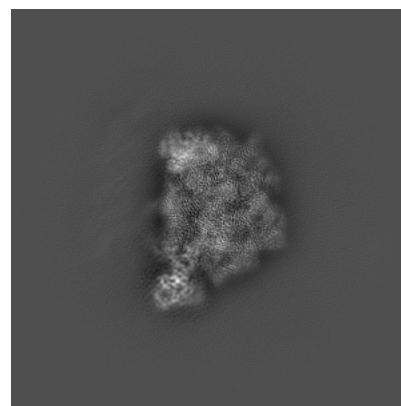
6.1.1 Primary map



X

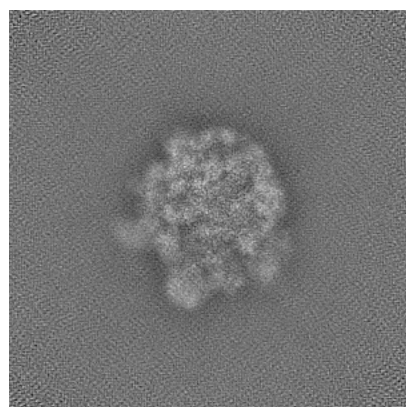


Y

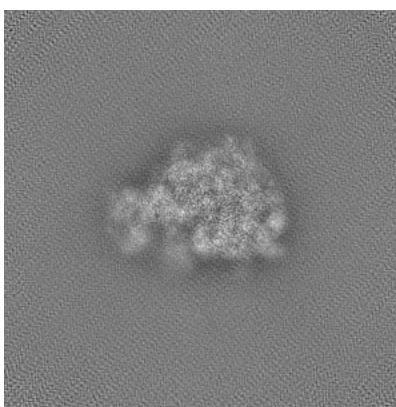


Z

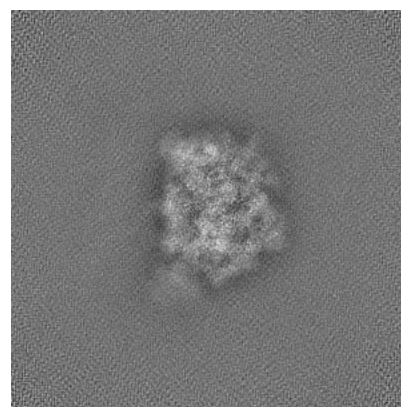
6.1.2 Raw map



X



Y

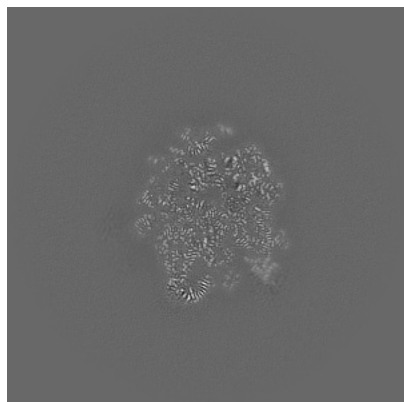


Z

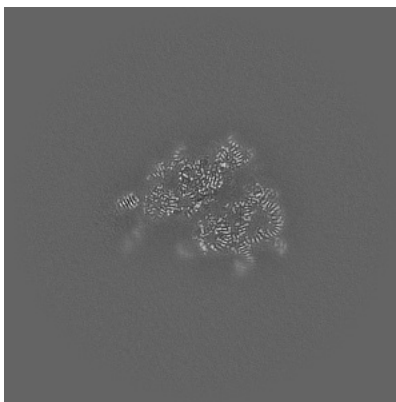
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

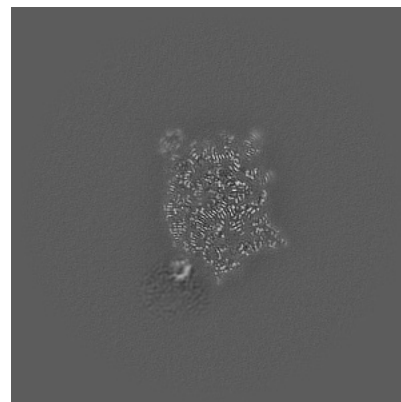
6.2.1 Primary map



X Index: 348

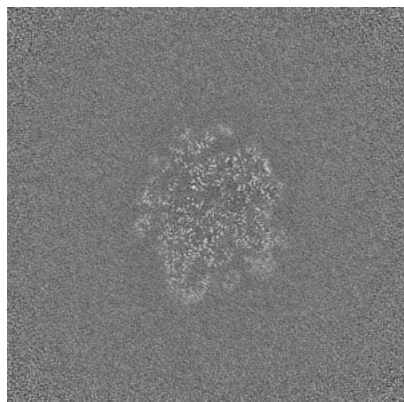


Y Index: 348

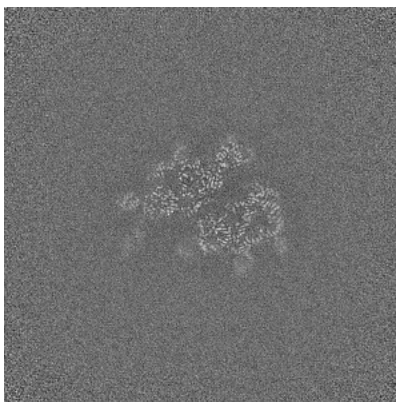


Z Index: 348

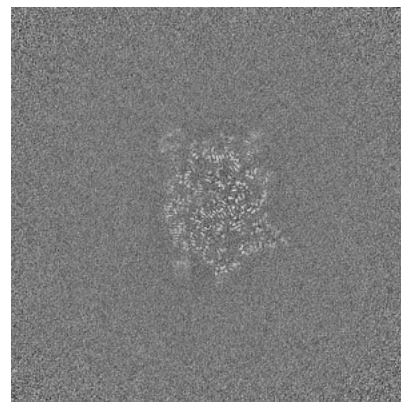
6.2.2 Raw map



X Index: 348



Y Index: 348

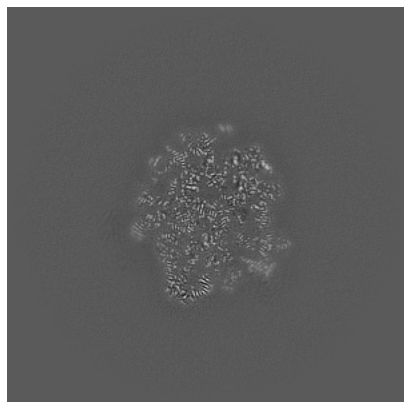


Z Index: 348

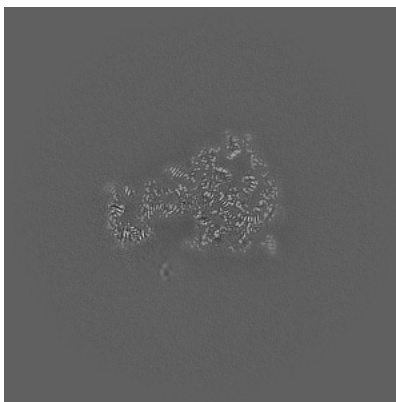
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

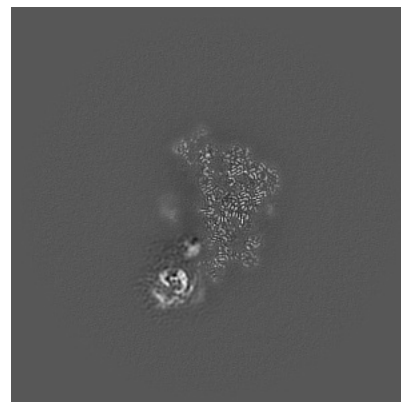
6.3.1 Primary map



X Index: 353

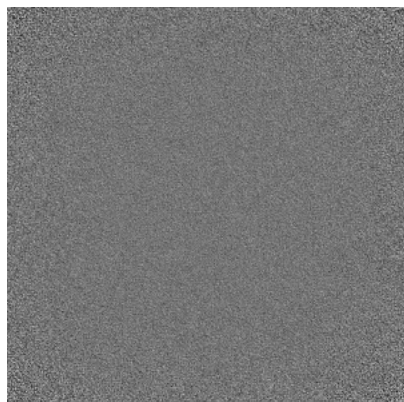


Y Index: 319

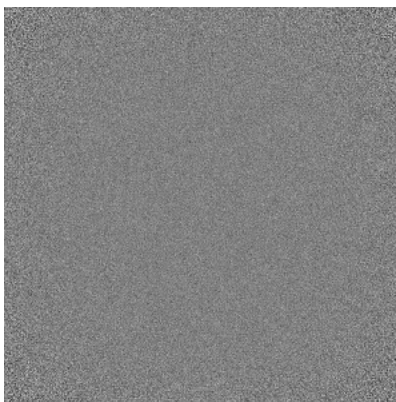


Z Index: 313

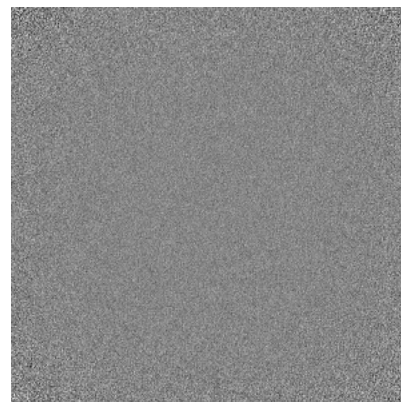
6.3.2 Raw map



X Index: 0



Y Index: 0

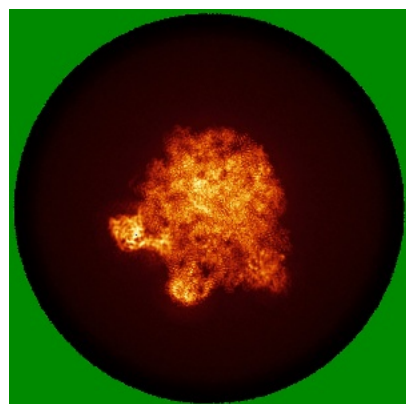


Z Index: 0

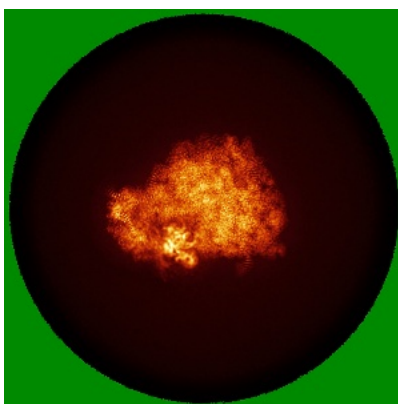
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

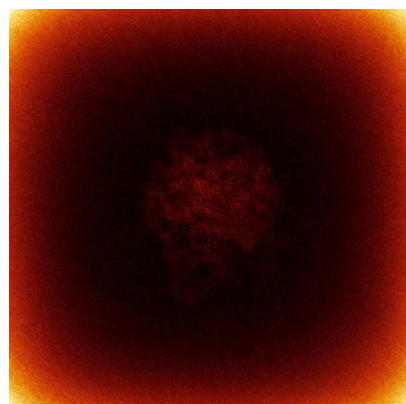


Y

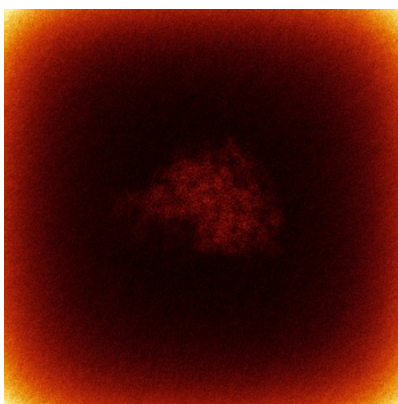


Z

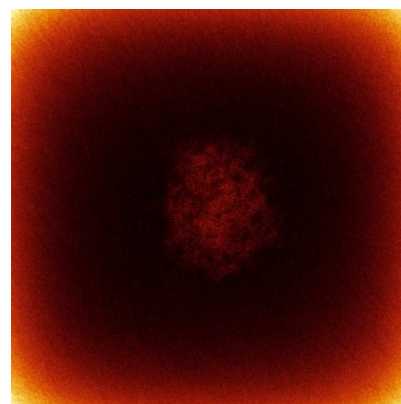
6.4.2 Raw map



X



Y

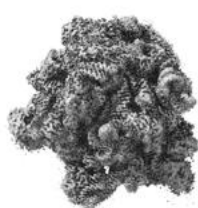


Z

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



X



Y



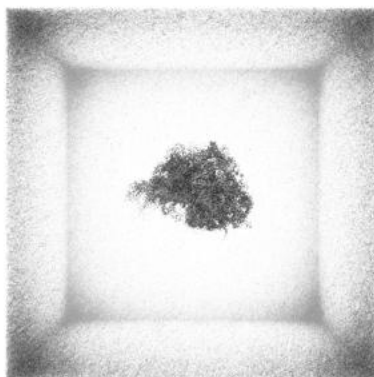
Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

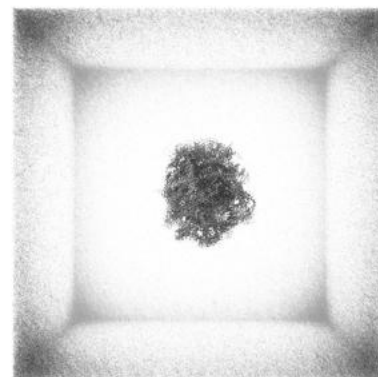
6.5.2 Raw map



X



Y



Z

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

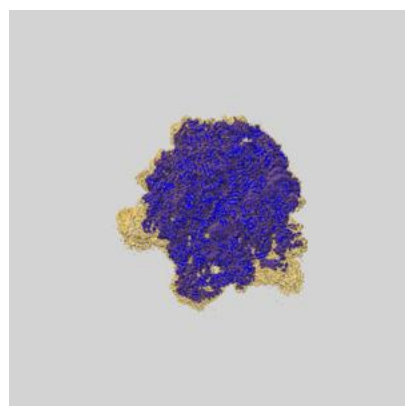
6.6 Mask visualisation [i](#)

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

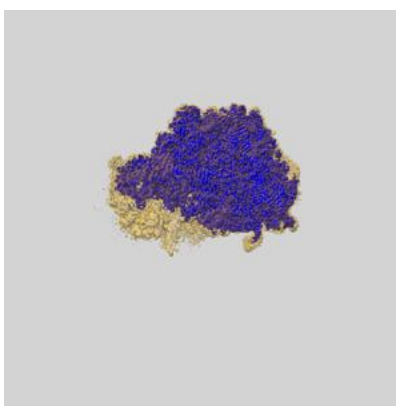
A mask typically either:

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

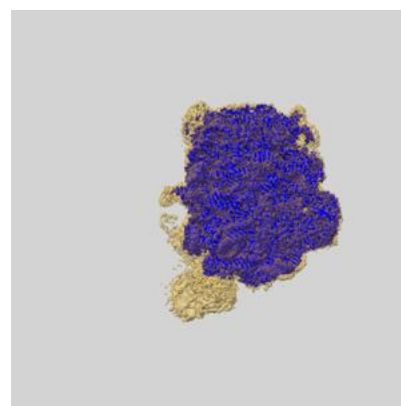
6.6.1 emd_72219_msk_1.map [i](#)



X



Y

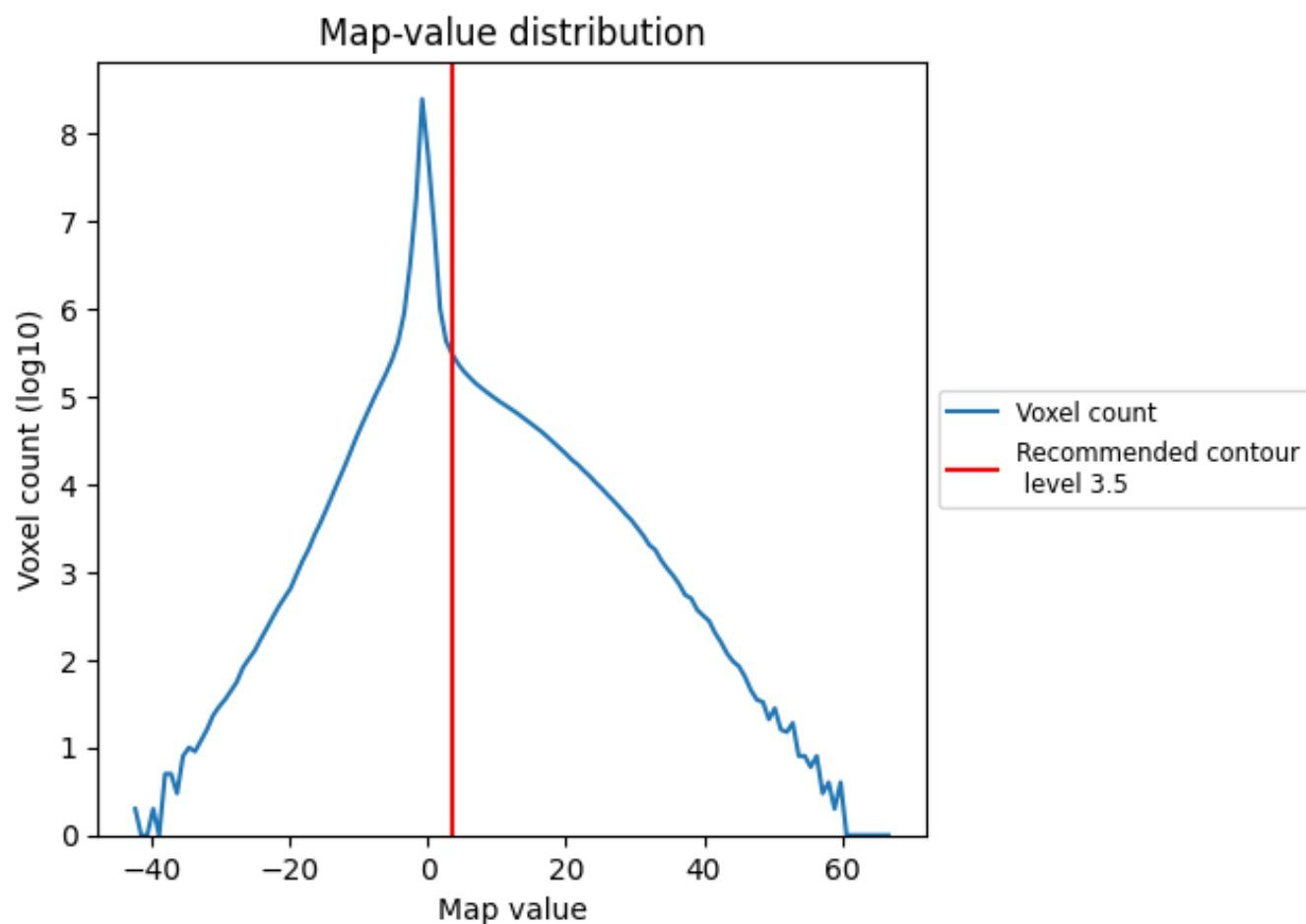


Z

7 Map analysis [i](#)

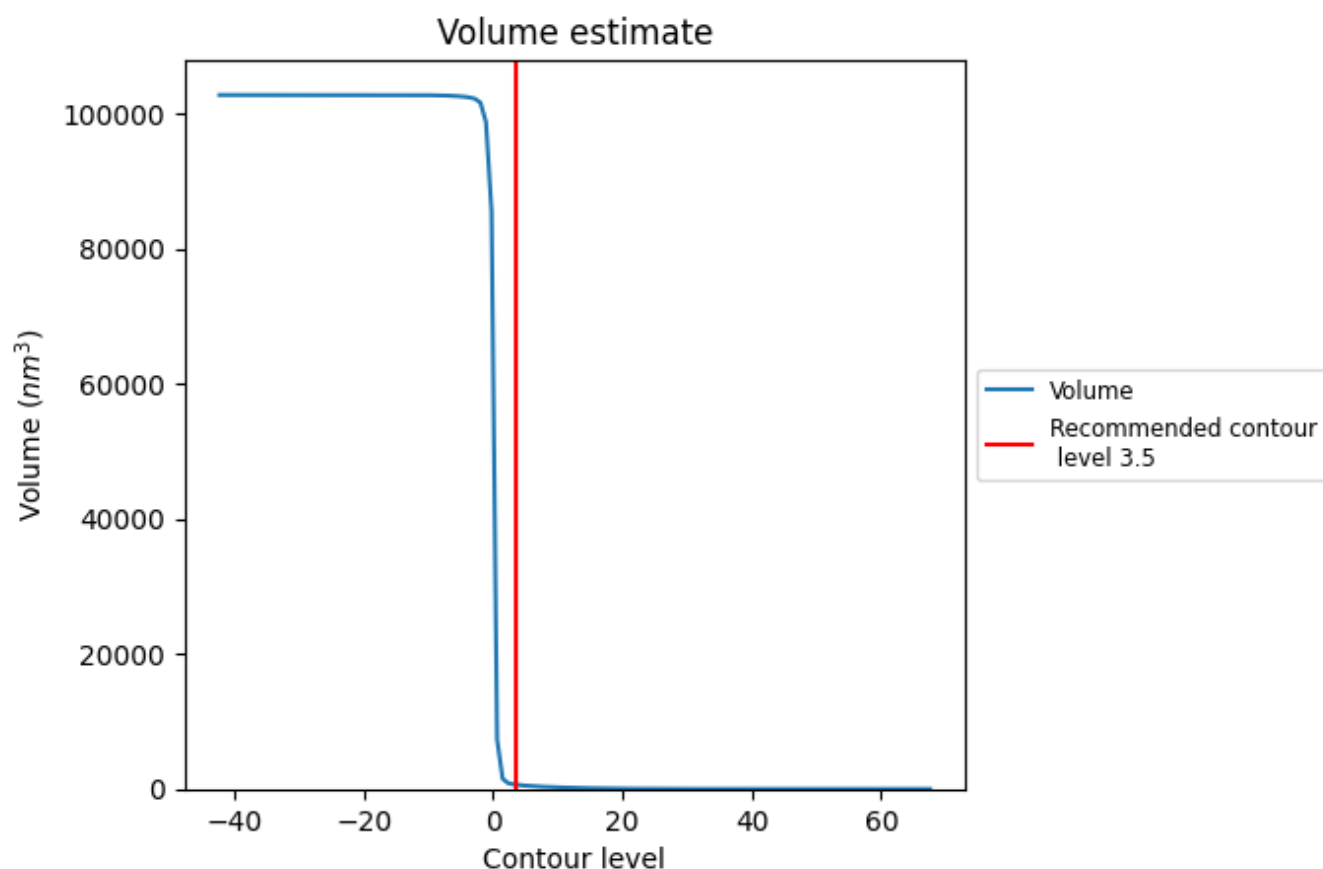
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

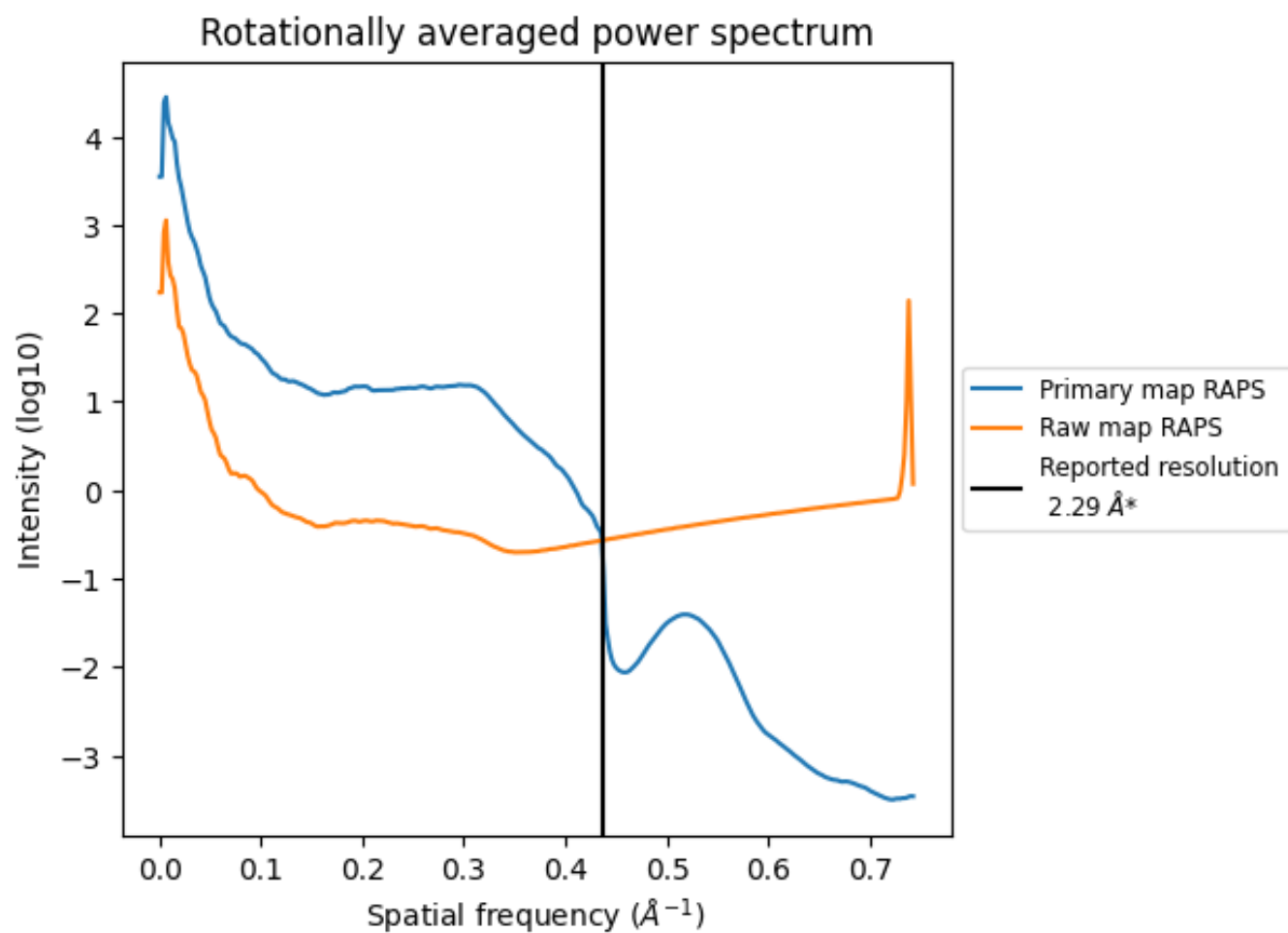
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 649 nm^3 ; this corresponds to an approximate mass of 587 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 ⓘ

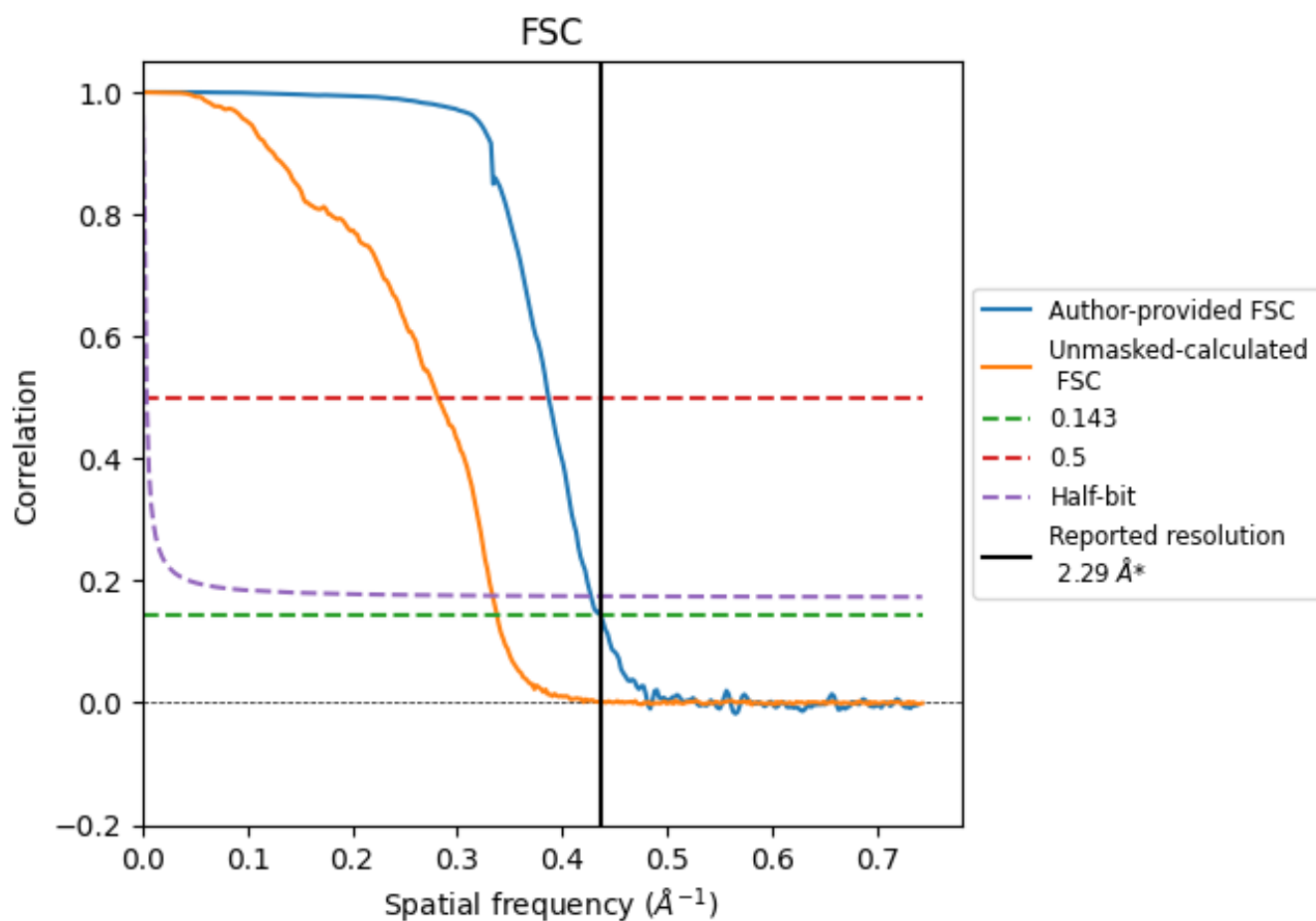


*Reported resolution corresponds to spatial frequency of 0.437 $\text{\AA}^{-1}$

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 0.437 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

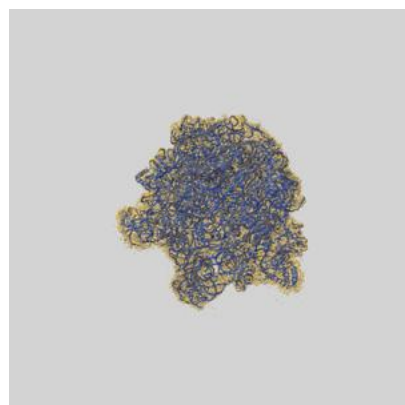
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.29	2.58	2.34
Unmasked-calculated*	2.96	3.55	3.00

*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 2.96 differs from the reported value 2.29 by more than 10 %

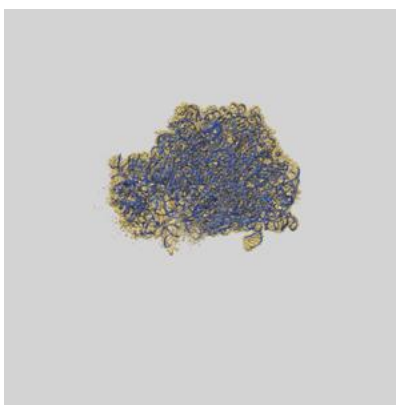
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72219 and PDB model 9Q43. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

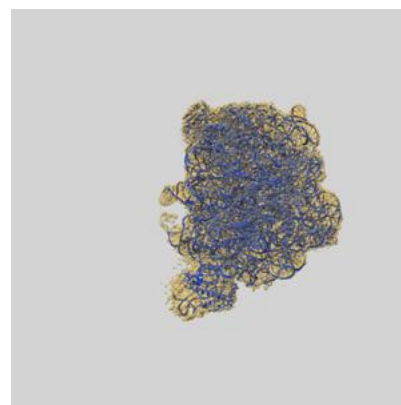
9.1 Map-model overlay [i](#)



X



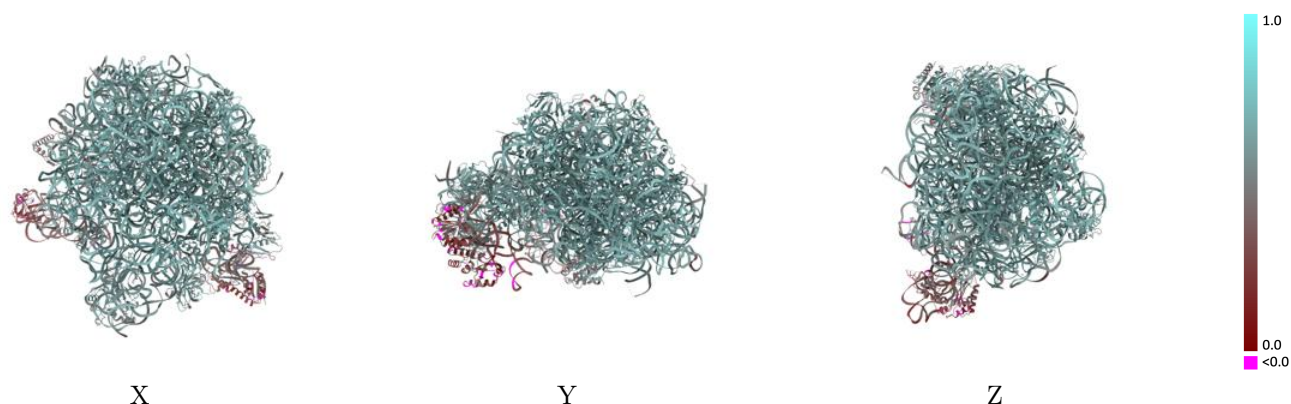
Y



Z

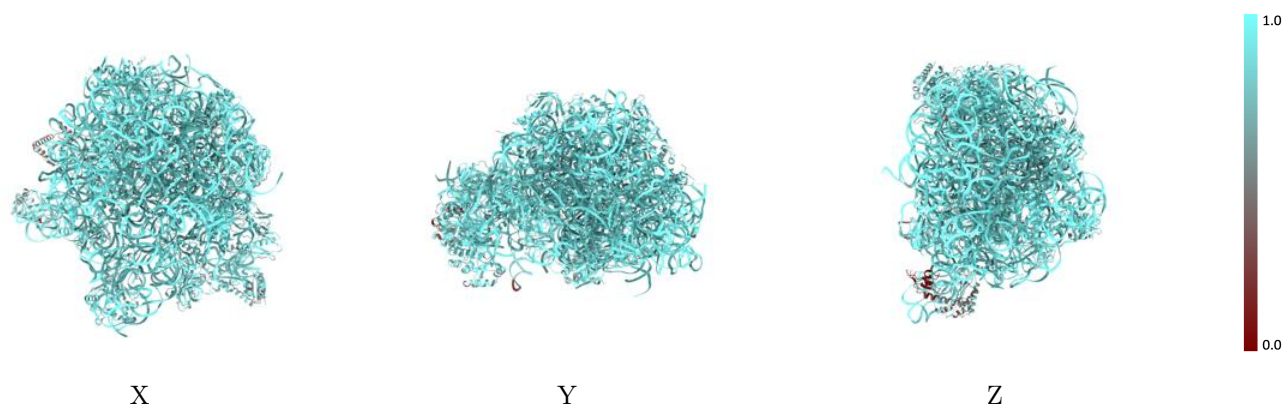
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



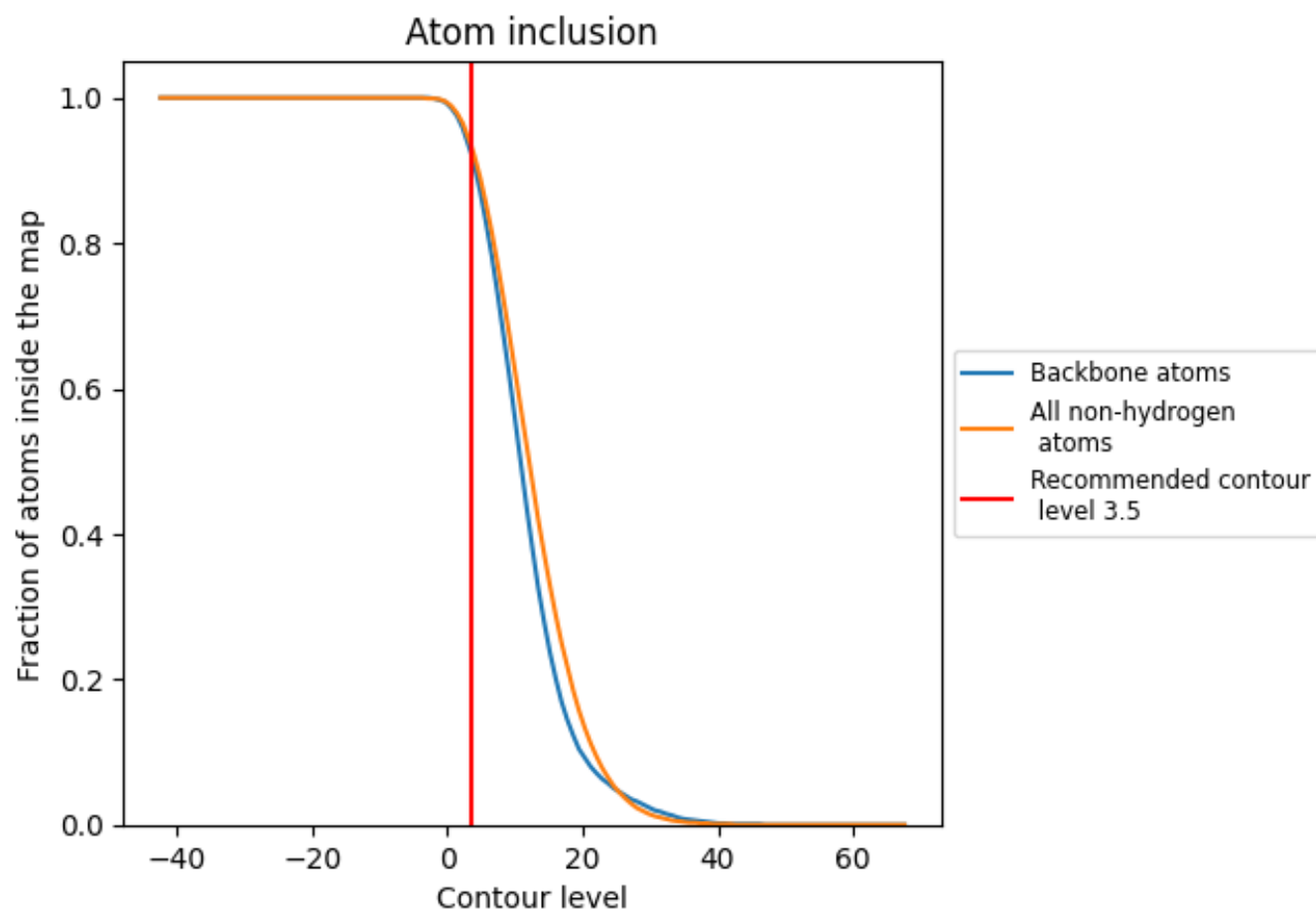
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 94% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.6020
1	 0.8900	 0.6060
2	 0.9320	 0.6350
4	 0.9110	 0.6280
5	 0.7950	 0.5740
6	 0.9390	 0.6590
7	 0.9370	 0.6570
8	 0.9290	 0.6220
9	 0.7680	 0.4890
A	 0.9690	 0.6270
B	 0.9540	 0.5980
C	 0.7190	 0.2090
D	 0.9420	 0.6540
E	 0.9320	 0.6450
F	 0.9200	 0.6260
G	 0.8460	 0.5260
H	 0.8350	 0.5540
I	 0.4070	 0.4090
J	 0.7410	 0.2410
K	 0.8210	 0.2000
L	 0.9290	 0.6450
M	 0.8870	 0.6210
N	 0.9240	 0.6400
O	 0.8970	 0.6370
P	 0.9510	 0.6530
Q	 0.9000	 0.5930
R	 0.8700	 0.6190
S	 0.9530	 0.6540
T	 0.9220	 0.6220
U	 0.8880	 0.6340
V	 0.8800	 0.6060
W	 0.8760	 0.5790
X	 0.8490	 0.5760
Y	 0.9190	 0.6410
Z	 0.9060	 0.6400
v	 0.8880	 0.2590

