



Full wwPDB EM Validation Report ⓘ

Feb 22, 2025 – 01:17 PM EST

PDB ID : 9HA6
EMDB ID : EMD-51978
Title : mature 50S subunit supplemented with Api137
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.
Deposited on : 2024-11-01
Resolution : 3.08 Å(reported)

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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

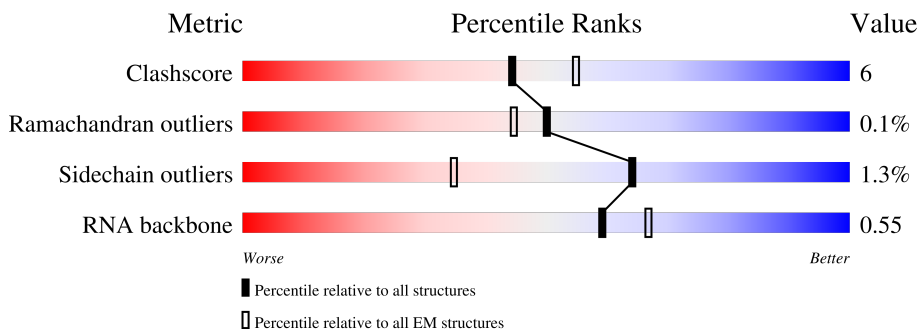
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	50	
3	2	46	
4	3	64	
5	4	38	
6	B	120	
7	C	271	

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Mol	Chain	Length	Quality of chain
8	D	209	
9	E	201	
10	F	177	
11	G	176	
12	H	149	
13	J	142	
14	K	122	
15	L	143	
16	M	136	
17	N	120	
18	O	116	
19	P	114	
20	Q	117	
21	R	103	
22	S	110	
23	T	93	
24	U	102	
25	V	94	
26	W	75	
27	X	77	
28	Y	63	
29	Z	58	
30	A	2904	
31	y	17	
31	z	17	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 90242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1402434313

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

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

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

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 12 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 17 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	110	Total	C	N	O	S	1
			868	538	170	157	3	0

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 25 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 26 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 27 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 30 is a RNA chain called 23S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A	2900	Total	C	N	O	P	1	0
			62281	27783	11461	20136	2901		

- Molecule 31 is a protein called Apidaecins type 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	z	17	Total	C	N	O	0	0
			148	94	33	21		
31	y	17	Total	C	N	O	0	0
			148	94	33	21		

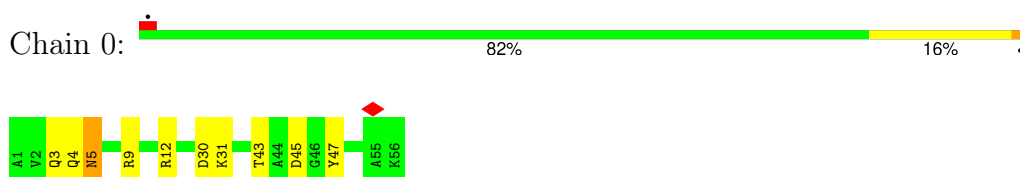
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	10	ARG	GLN	conflict	UNP P35581
y	10	ARG	GLN	conflict	UNP P35581

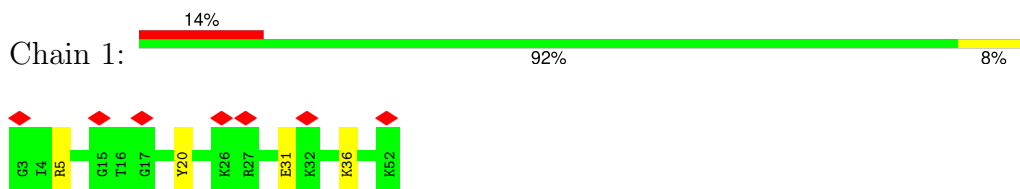
3 Residue-property plots [i](#)

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

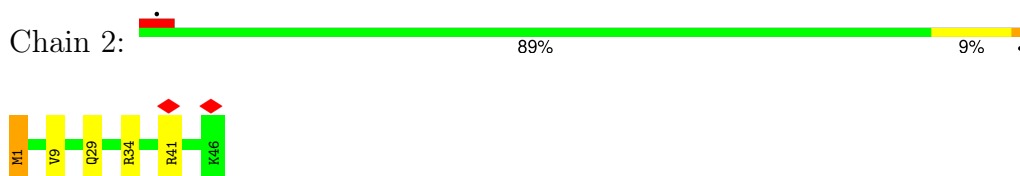
- Molecule 1: Large ribosomal subunit protein bL32



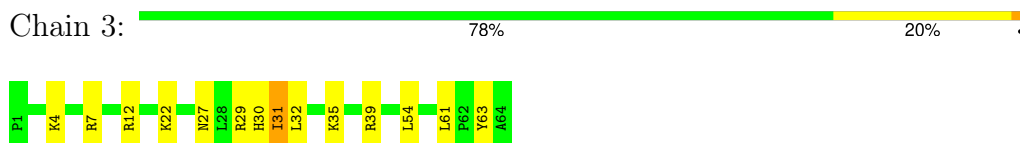
- Molecule 2: Large ribosomal subunit protein bL33



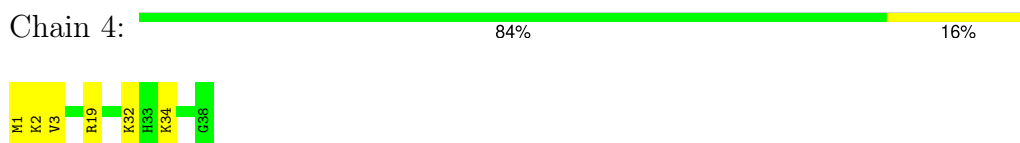
- Molecule 3: Large ribosomal subunit protein bL34




- Molecule 4: Large ribosomal subunit protein bL35

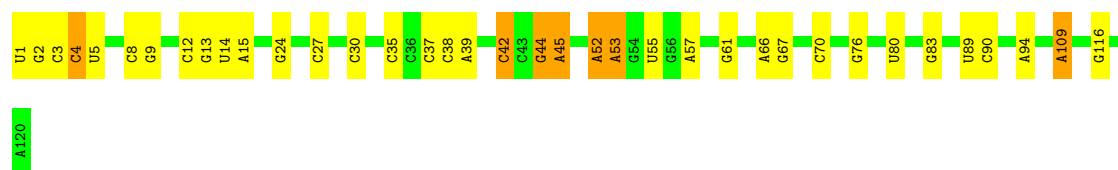


- Molecule 5: Large ribosomal subunit protein bL36A




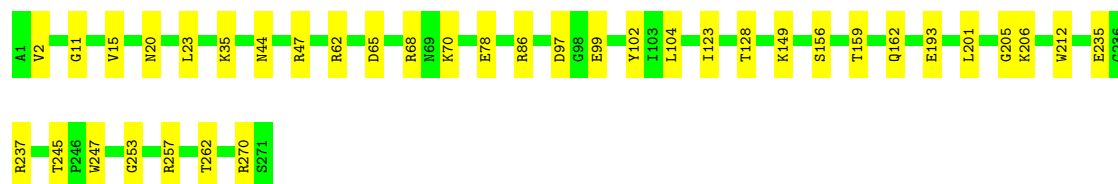
- Molecule 6: 5S ribosomal RNA

Chain B: 




- Molecule 7: Large ribosomal subunit protein uL2

Chain C: 




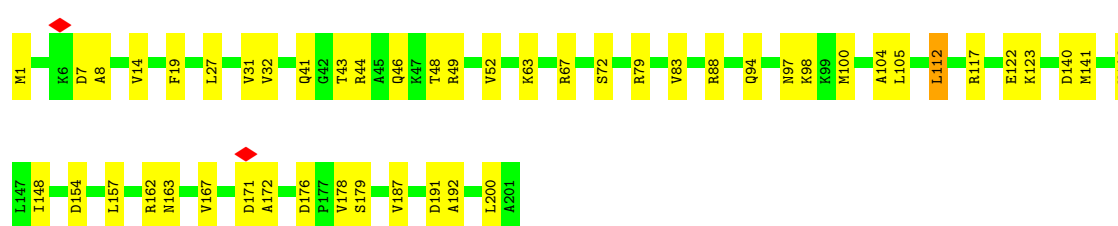
- Molecule 8: 50S ribosomal protein L3

Chain D: 




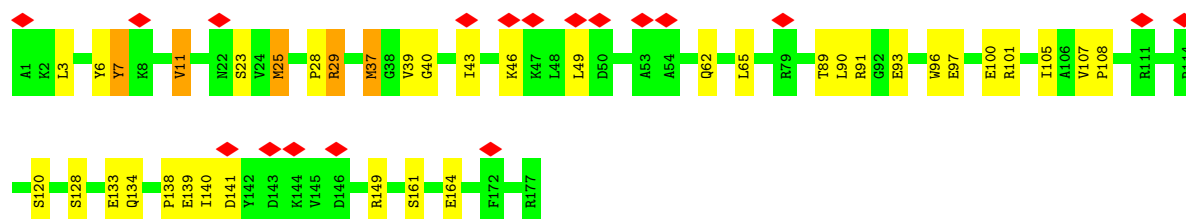
- Molecule 9: Large ribosomal subunit protein uL4

Chain E: 

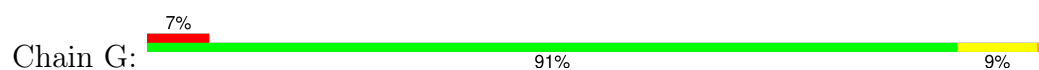


- Molecule 10: Large ribosomal subunit protein uL5

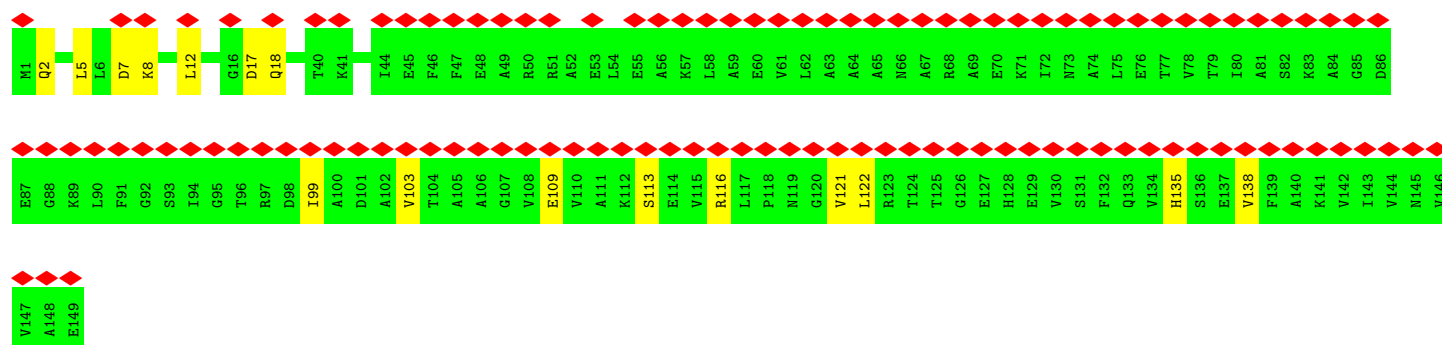
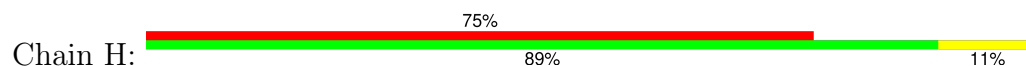
Chain F: 



- Molecule 11: Large ribosomal subunit protein uL6



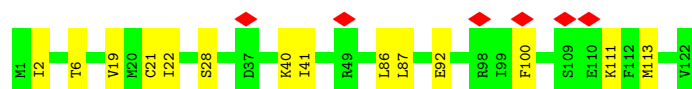
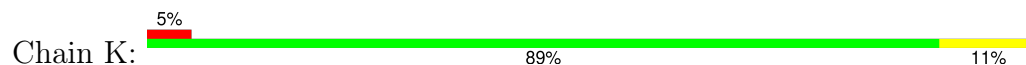
- Molecule 12: Large ribosomal subunit protein bL9



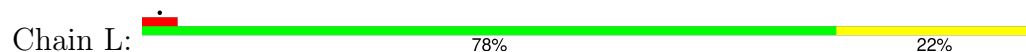
- Molecule 13: Large ribosomal subunit protein uL13



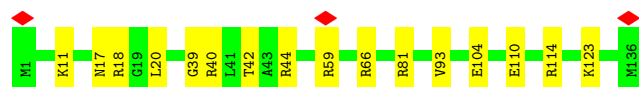
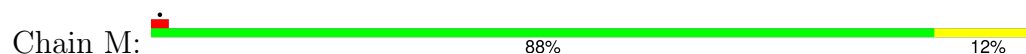
- Molecule 14: Large ribosomal subunit protein uL14




- Molecule 15: Large ribosomal subunit protein uL15

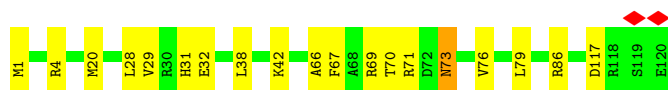


- Molecule 16: 50S ribosomal protein L16




- Molecule 17: Large ribosomal subunit protein bL17

Chain N:  84% 15%




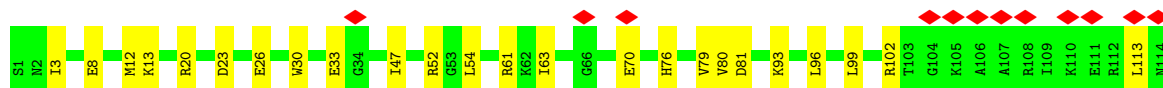
- Molecule 18: Large ribosomal subunit protein uL18

Chain O:  84% 16%




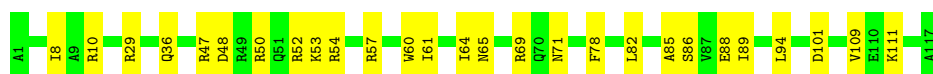
- Molecule 19: Large ribosomal subunit protein bL19

Chain P:  11% 79% 21%




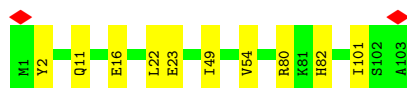
- Molecule 20: Large ribosomal subunit protein bL20

Chain Q:  77% 23%




- Molecule 21: Large ribosomal subunit protein bL21

Chain R:  90% 10%




- Molecule 22: Large ribosomal subunit protein uL22

Chain S:  82% 17%

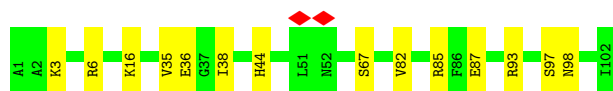
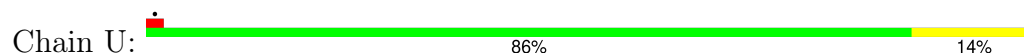


- Molecule 23: Large ribosomal subunit protein uL23

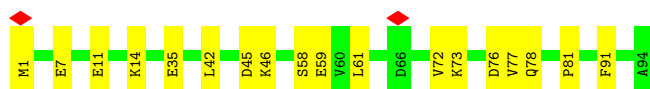
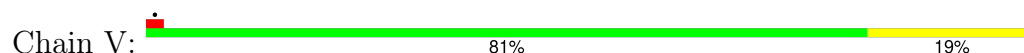
Chain T:  82% 18%



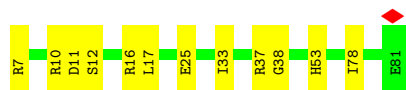
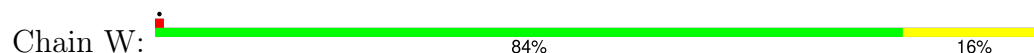
- Molecule 24: Large ribosomal subunit protein uL24



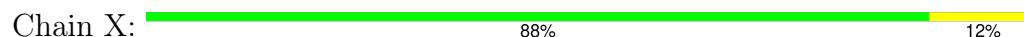
- Molecule 25: Large ribosomal subunit protein bL25



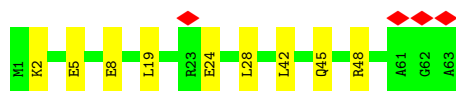
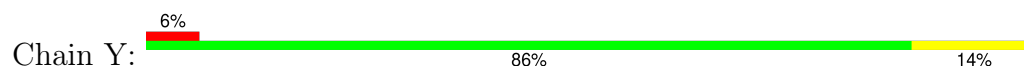
- Molecule 26: Large ribosomal subunit protein bL27



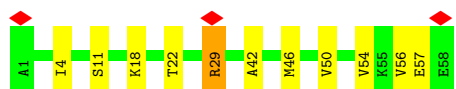
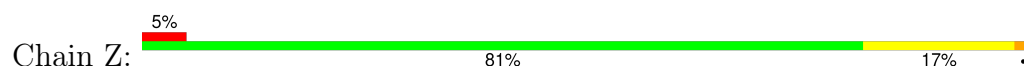
- Molecule 27: Large ribosomal subunit protein bL28



- Molecule 28: Large ribosomal subunit protein uL29



- Molecule 29: Large ribosomal subunit protein uL30

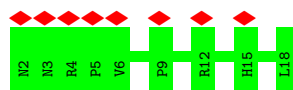


- Molecule 30: 23S ribosomal rRNA

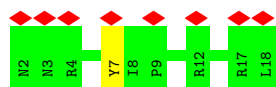
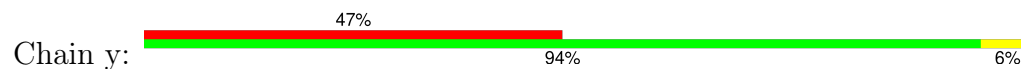


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U2891	A2764	G2661	C2559	A2469	C2379	G2279	A2163	C2103	C2021	A1901	A1781	G1681	A1545
G2894	A2765	A2662	A2564	U2474	C2380	C2381	C2164	C2104	U2022	G1906	U1782	U1683	G1546
C2901	A2776	A2679	A2565	C2475	G2382	C2283	C2165	U2105	C2023	G1907	A1783	C1684	C1550
C2902	G2777	A2682	A2567	C2476	C2383	A2284	U2166	G2107	G2024	C1908	A1784	C1685	U1559
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	A2809	U2707	G2596	G2495	G2410	C2326	U2180	G2120	A2052	G1930	A1802	A1713	C1585
	G2816	G2708	A2598	C2497	U2419	A2327	U2181	U2122	C2055	A1937	A1808	G1715	G1601
	U2817	C2710	U2600	U2498	U2419	G2330	U2182	G2123	G2056	A1936	A1809	U1717	U1602
	U2818	G2711	A2601	U2500	C2422	U2334	A2183	G2124	G2057	U1940	U1812	U1720	A1603
	G2819	G2714	G2602	C2501	U2423	U2334	A2184	G2125	A2058	C1941	G1813	G1721	C1604
	A2820	C2717	U2609	G2502	A2424	A2335	U2189	G2126	A2059	U1942	G1814	G1724	A1608
	A2821	G2718	C2610	U2503	A2425	A2336	A2198	A2126	A2060	U1943	A1815		A1609
	G2822	U2719	C2611	U2504	C2426	G2337	A2199	G2127	A2061	U1953	G1816	U1729	A1610
	A2823	U2720	C2612	U2505	G2427	G2337	G2200	G2128	A2062	G1954	U1818	C1730	G1622
	U2833	A2721	U2613	U2506	G2428	U2343	G2201	C2129	C2063	U1955	A1819	G1731	A1634
	U2845	G2722	A2614	G2509	G2429	U2344	G2204	U2130	G2069	C1962	U1820	C1732	C1638
	G2846	C2723	U2615	A2513	U2431	A2345	G2204	U2131	A2070	U1963	G1826	G1733	G1645
	U2847	A2726	C2618	U2514	A2432	C2347	C2208	U2132	A2071	G1964	U1827	A1735	C1646
	G2848	G2729	C2619	C2515	A2434	U2348	A2211	G2133	C2073	C1967	G1828	U1736	U1647
	U2849	C2732	C2620	A2518	A2435	C2349	A2212	A2134	U2074	A1970	A1829	G1737	U1648
	G2852	A2733	C2628	U2519	A2439	G2351	U2213	A2135	U2075	U1971	C1833	A1739	G1649
	G2857	U2739	U2629	C2520	U2441	G2351	G2214	G2136	A2077	G1972	G1835	A1744	A1654
	A2860	G2743	A2635	U2522	C2442	C2357	C2215	U2137	U2079	A1977	C1837	A1754	G1659
	U2865	G2744	C2636	G2526	C2443	G2360	A2225	G2138	U2085	G1983	C1843	A1755	U1662
	U2866	G2747	G2638	C2527	G2444	C2361	C2226	U2139	C2089	U1991	G1857	A1757	G1663
	G2867	A2748	G2645	U2528	G2445	C2362	G2230	G2140	A2090	G1992	A1858	C1764	A1664
	A2868	A2749	C2646	C2529	G2446	G2363	G2234	A2141	G2093	U1995	U1864	U1769	A1665
	U2871	A2750	U2647	A2530	G2447	G2365	G2234	A2142	C2096	U1996	U1865	G1770	G1666
	A2872	G2751	C2652	G2535	A2451	A2369	G2238	G2144	C2096	C1997	A1866	A1771	G1667
	C2874	C2755	A2653	A2547	G2454	G2373	G2239	C2145	U2099	A1998	A1867	C1772	A1668
		U2756	G2655	U2552	U2457	G2375	G2250	C2146	G2100	C1999	G1869	A1773	A1669
							G2251	A2147					
							C2258	G2148					
							A2266	U2149					
							A2267	C2150					
								U2151					
								G2152					
								C2153					
								A2154					
								U2155					
								G2156					
								U2157					
								A2158					
								C2159					
								G2160					

- Molecule 31: Apidaecins type 22



- Molecule 31: Apidaecins type 22



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41476	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.850	Depositor
Minimum map value	-0.385	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	399.6, 399.6, 399.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.332, 1.332, 1.332	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.23	0/450	0.54	0/599
2	1	0.24	0/416	0.48	0/554
3	2	0.25	0/380	0.64	0/498
4	3	0.23	0/513	0.52	0/676
5	4	0.26	0/303	0.56	0/397
6	B	0.24	1/2876 (0.0%)	0.70	0/4483
7	C	0.24	0/2121	0.55	0/2852
8	D	0.25	0/1586	0.50	0/2134
9	E	0.24	0/1571	0.48	0/2113
10	F	0.25	0/1434	0.53	0/1926
11	G	0.24	0/1343	0.48	0/1816
12	H	0.24	0/1122	0.48	0/1515
13	J	0.24	0/1152	0.49	0/1551
14	K	0.24	0/947	0.55	0/1268
15	L	0.25	0/1054	0.57	0/1403
16	M	0.25	0/1093	0.54	0/1460
17	N	0.25	0/973	0.59	0/1301
18	O	0.24	0/902	0.53	0/1209
19	P	0.25	0/929	0.55	0/1242
20	Q	0.24	0/960	0.52	0/1278
21	R	0.25	0/829	0.53	0/1107
22	S	0.24	0/875	0.52	0/1170
23	T	0.29	0/744	0.51	0/994
24	U	0.25	0/787	0.51	0/1051
25	V	0.25	0/766	0.48	0/1025
26	W	0.25	0/582	0.53	0/769
27	X	0.24	0/635	0.56	0/848
28	Y	0.24	0/510	0.49	0/677
29	Z	0.24	0/453	0.53	0/605
30	A	0.16	1/69755 (0.0%)	0.72	8/108820 (0.0%)
31	y	0.27	0/155	0.62	0/212
31	z	0.22	0/155	0.58	0/212
All	All	0.19	2/98371 (0.0%)	0.68	8/147765 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	T	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	1	G	OP3-P	-10.58	1.48	1.61
6	B	1	U	OP3-P	-10.57	1.48	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1913	A	OP1-P-O3'	-10.68	81.70	105.20
30	A	1913	A	OP2-P-O3'	-10.06	83.07	105.20
30	A	1914	C	OP1-P-OP2	7.08	130.22	119.60
30	A	2474	U	C2-N1-C1'	5.71	124.55	117.70
30	A	2321	U	C2-N1-C1'	5.58	124.40	117.70
30	A	62	U	C2-N1-C1'	5.48	124.28	117.70
30	A	1313	U	C2-N1-C1'	5.16	123.89	117.70
30	A	2704	C	N1-C2-O2	5.02	121.91	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	T	73	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	7	0
2	1	409	0	440	4	0
3	2	377	0	418	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	504	0	574	11	0
5	4	302	0	343	6	0
6	B	2572	0	1302	22	0
7	C	2082	0	2157	30	0
8	D	1565	0	1616	20	0
9	E	1552	0	1619	35	0
10	F	1410	0	1447	29	0
11	G	1323	0	1374	11	0
12	H	1111	0	1148	12	0
13	J	1129	0	1162	9	0
14	K	938	0	1012	10	0
15	L	1045	0	1117	27	0
16	M	1074	0	1157	11	0
17	N	960	0	1000	15	0
18	O	892	0	923	14	0
19	P	917	0	965	16	0
20	Q	947	0	1022	23	0
21	R	816	0	839	8	0
22	S	868	0	934	15	0
23	T	738	0	807	11	0
24	U	779	0	834	11	0
25	V	753	0	780	15	0
26	W	575	0	592	10	0
27	X	625	0	655	8	0
28	Y	509	0	543	6	0
29	Z	449	0	491	10	0
30	A	62281	0	31323	520	0
31	y	148	0	152	0	0
31	z	148	0	150	0	0
All	All	90242	0	59357	788	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 (788) 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)
30:A:727:A:OP2	30:A:1431:A:O2'	1.88	0.91
30:A:177:G:OP2	30:A:177:G:N2	2.05	0.89
15:L:93:ASN:O	15:L:94:THR:OG1	1.91	0.88
30:A:1837:C:O2'	30:A:1927:A:N3	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:2343:U:HO2'	30:A:2373:G:HO2'	1.12	0.87
30:A:2258:C:O2'	30:A:2427:C:OP2	1.92	0.87
30:A:959:A:N3	30:A:2457:U:O2'	2.09	0.85
30:A:1681:G:OP2	30:A:1757:A:N6	2.09	0.85
30:A:2576:G:O2'	30:A:2579:C:OP2	1.93	0.85
30:A:1798:U:O2'	30:A:1802:A:N3	2.10	0.85
30:A:948:C:O2	30:A:984:A:O2'	1.96	0.84
7:C:253:GLY:O	30:A:1843:C:O2'	1.96	0.84
30:A:2522:U:O2'	30:A:2647:U:OP1	1.93	0.84
30:A:2530:A:OP2	30:A:2535:G:N2	2.11	0.83
18:O:117:PHE:O	30:A:2377:A:O2'	1.95	0.83
30:A:1447:C:O2'	30:A:1544:A:N3	2.09	0.83
6:B:5:U:OP1	6:B:61:G:O2'	1.96	0.83
30:A:1826:G:O2'	30:A:1971:U:OP2	1.97	0.83
30:A:275:C:O2	30:A:362:A:N6	2.12	0.82
30:A:612:G:N2	30:A:614:A:O2'	2.12	0.82
30:A:1962:C:O2'	30:A:1964:G:OP2	1.97	0.82
30:A:1942:C:OP2	30:A:1943:U:O2'	1.96	0.82
30:A:227:A:O2'	30:A:228:C:O5'	1.97	0.82
30:A:463:G:N2	30:A:466:A:OP2	2.14	0.81
20:Q:52:ARG:NH2	30:A:994:C:OP1	2.13	0.81
2:1:5:ARG:NH1	30:A:2285:C:OP2	2.13	0.81
30:A:2326:C:O2'	30:A:2327:A:OP1	1.98	0.80
15:L:55:MET:O	15:L:60:ARG:NH1	2.14	0.80
30:A:698:C:O2'	30:A:734:A:N6	2.14	0.80
29:Z:29:ARG:NE	30:A:1184:U:OP1	2.14	0.80
21:R:80:ARG:NH2	30:A:572:A:OP2	2.15	0.80
30:A:2144:G:O2'	30:A:2147:A:N1	2.15	0.80
30:A:234:U:O4	30:A:263:G:N2	2.15	0.79
30:A:2645:G:OP2	30:A:2645:G:N2	2.13	0.79
30:A:200:U:O2	30:A:386:G:N2	2.15	0.79
30:A:2857:G:N2	30:A:2860:A:OP2	2.14	0.79
7:C:149:LYS:NZ	30:A:1801:A:OP2	2.15	0.79
30:A:1779:U:OP2	30:A:1784:A:N6	2.16	0.79
1:0:4:GLN:OE1	30:A:2056:G:O2'	2.00	0.79
16:M:66:ARG:NH1	16:M:104:GLU:OE2	2.15	0.79
19:P:102:ARG:NH2	30:A:1754:A:O2'	2.17	0.78
25:V:11:GLU:N	25:V:11:GLU:OE1	2.17	0.78
30:A:1907:G:O6	30:A:1924:C:N4	2.16	0.78
30:A:1953:A:O2'	30:A:2559:C:O2	2.00	0.78
9:E:63:LYS:NZ	30:A:2061:G:OP2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:22:ASN:OD1	30:A:2079:U:O2'	2.01	0.78
30:A:191:A:O2'	30:A:678:C:O2	2.00	0.78
30:A:675:A:N3	30:A:2443:C:O2'	2.16	0.78
17:N:86:ARG:NH2	17:N:117:ASP:OD2	2.16	0.77
2:1:20:TYR:HH	30:A:2347:C:HO2'	1.32	0.77
4:3:31:ILE:O	4:3:35:LYS:NZ	2.17	0.77
11:G:29:ASN:ND2	11:G:77:GLY:O	2.18	0.77
25:V:58:SER:OG	25:V:59:GLU:OE1	2.03	0.77
29:Z:11:SER:OG	30:A:989:G:OP2	2.03	0.76
15:L:41:ARG:NH2	30:A:807:U:OP2	2.18	0.76
9:E:163:ASN:ND2	30:A:320:A:N3	2.33	0.76
23:T:36:LYS:NZ	30:A:57:C:O2'	2.19	0.76
9:E:67:ARG:NE	30:A:1257:C:OP1	2.19	0.76
26:W:37:ARG:NH2	30:A:2387:U:O2'	2.19	0.76
30:A:2816:G:N3	30:A:2883:A:O2'	2.19	0.75
30:A:570:G:O4'	30:A:983:A:N6	2.20	0.75
6:B:14:U:OP2	6:B:70:C:O2'	2.04	0.75
30:A:2006:C:O2'	30:A:2823:A:N3	2.18	0.75
30:A:2595:G:O2'	30:A:2597:G:O6	2.03	0.75
30:A:2115:G:N2	30:A:2118:U:OP2	2.19	0.75
30:A:1668:A:N3	30:A:1670:C:N4	2.34	0.74
20:Q:101:ASP:OD2	21:R:2:TYR:OH	2.04	0.74
30:A:2063:C:N4	30:A:2501:C:O2	2.21	0.74
28:Y:48:ARG:NH1	30:A:76:C:OP1	2.21	0.74
30:A:248:G:O2'	30:A:2432:A:OP1	2.05	0.74
30:A:725:G:O2'	30:A:726:G:O4'	2.04	0.74
30:A:2469:A:N6	30:A:2481:G:O2'	2.21	0.74
30:A:2646:C:OP2	30:A:2732:G:O2'	2.06	0.73
30:A:647:G:N2	30:A:2350:C:O2'	2.21	0.73
30:A:542:C:N4	30:A:543:G:O6	2.20	0.73
3:2:34:ARG:NH2	3:2:41:ARG:O	2.21	0.73
5:4:19:ARG:NE	30:A:2756:U:OP2	2.20	0.73
30:A:2564:A:O2'	30:A:2565:A:O4'	2.01	0.73
4:3:63:TYR:HH	30:A:592:A:HO2'	1.35	0.73
21:R:11:GLN:N	21:R:11:GLN:OE1	2.21	0.73
10:F:25:MET:O	10:F:29:ARG:NH1	2.22	0.72
15:L:77:ILE:HD11	15:L:108:ALA:HB1	1.71	0.72
16:M:40:ARG:NH2	30:A:958:U:OP1	2.21	0.72
30:A:1936:A:OP2	30:A:1962:C:N4	2.22	0.72
30:A:240:C:OP2	30:A:241:A:O2'	2.03	0.72
30:A:1209:U:O2'	30:A:1237:A:N1	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:115:GLY:N	30:A:2821:A:OP2	2.22	0.72
18:O:8:ILE:O	18:O:12:THR:HG23	1.89	0.72
30:A:1724:G:O6	30:A:1737:G:N2	2.23	0.72
30:A:2865:U:OP2	30:A:2866:U:O2'	2.06	0.71
30:A:1834:U:O2'	30:A:1970:A:OP2	2.08	0.71
30:A:249:C:OP2	30:A:2394:C:O2'	2.05	0.71
30:A:372:G:O2'	30:A:373:U:O5'	2.09	0.71
30:A:603:A:N6	30:A:655:A:O4'	2.23	0.71
9:E:44:ARG:NH1	30:A:1248:G:OP1	2.24	0.71
16:M:81:ARG:NH1	30:A:2251:G:OP1	2.23	0.71
30:A:571:U:O2'	30:A:573:U:OP2	2.08	0.70
30:A:807:U:O2'	30:A:2060:A:N1	2.22	0.70
30:A:963:U:O4'	30:A:2250:G:N2	2.24	0.70
30:A:1062:G:O2'	30:A:1063:G:O4'	2.06	0.70
7:C:70:LYS:NZ	7:C:99:GLU:OE2	2.25	0.70
30:A:1048:A:OP2	30:A:1110:G:N2	2.24	0.70
30:A:1638:C:O2	30:A:2698:U:O2'	2.09	0.70
15:L:99:ASN:ND2	30:A:621:A:OP2	2.25	0.70
4:3:39:ARG:NH2	30:A:2362:C:OP1	2.25	0.70
25:V:45:ASP:OD1	25:V:46:LYS:N	2.24	0.70
30:A:227:A:HO2'	30:A:228:C:P	2.15	0.70
30:A:584:C:N4	30:A:585:G:O6	2.25	0.70
6:B:76:G:O2'	25:V:78:GLN:OE1	2.09	0.69
30:A:18:U:O2'	30:A:554:U:OP1	2.10	0.69
30:A:219:A:N3	30:A:234:U:O2'	2.25	0.69
1:0:5:ASN:ND2	30:A:2022:U:O4	2.24	0.69
18:O:31:THR:OG1	18:O:33:ARG:O	2.10	0.69
30:A:2705:A:O2'	30:A:2852:G:OP1	2.09	0.69
10:F:134:GLN:NE2	10:F:149:ARG:O	2.25	0.69
7:C:86:ARG:NH2	30:A:1817:G:OP1	2.26	0.69
30:A:1125:G:OP2	30:A:1126:A:O2'	2.10	0.69
30:A:1129:A:O2'	30:A:2515:C:O2	2.10	0.69
30:A:1264:A:OP2	30:A:1265:A:O2'	2.08	0.69
30:A:1426:G:OP2	30:A:1427:A:O2'	2.11	0.69
19:P:30:TRP:NE1	19:P:81:ASP:OD2	2.26	0.69
30:A:28:A:HO2'	30:A:582:A:HO2'	1.41	0.69
30:A:1019:U:OP1	30:A:1035:U:O2'	2.07	0.69
30:A:1682:G:OP2	30:A:1699:G:N2	2.26	0.69
30:A:1218:G:N1	30:A:1232:G:N7	2.41	0.68
30:A:1869:G:N2	30:A:1872:A:OP2	2.26	0.68
8:D:70:LYS:NZ	30:A:2786:U:OP1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:113:SER:O	12:H:116:ARG:NH1	2.25	0.68
30:A:514:A:N3	30:A:581:C:O2'	2.26	0.68
30:A:743:A:O2'	30:A:1659:G:OP1	2.09	0.68
30:A:2788:C:O2'	30:A:2809:A:N3	2.24	0.68
8:D:118:PHE:O	30:A:1654:A:O2'	2.11	0.68
20:Q:57:ARG:HE	20:Q:61:ILE:HD11	1.59	0.68
30:A:1696:G:N2	30:A:1977:A:O2'	2.22	0.68
10:F:89:THR:OG1	10:F:91:ARG:NH2	2.27	0.68
27:X:36:ARG:NH2	30:A:2199:A:OP1	2.27	0.68
30:A:1528:A:OP2	30:A:1543:G:N2	2.27	0.68
23:T:19:LYS:NZ	30:A:1340:U:OP1	2.27	0.67
30:A:239:C:O2'	30:A:622:G:O2'	2.12	0.67
4:3:4:LYS:O	15:L:48:ARG:NH1	2.27	0.67
7:C:156:SER:HG	7:C:159:THR:HG1	1.29	0.67
30:A:1712:U:OP2	30:A:1713:A:O2'	2.02	0.67
30:A:1363:C:O2'	30:A:1809:A:N3	2.26	0.67
7:C:62:ARG:NH2	30:A:1568:G:OP2	2.28	0.67
30:A:1361:G:HO2'	30:A:2215:C:HO2'	1.38	0.67
30:A:2595:G:N2	30:A:2598:A:OP2	2.25	0.67
3:2:29:GLN:NE2	30:A:210:C:OP1	2.28	0.67
22:S:25:ARG:NH1	22:S:74:ILE:O	2.28	0.66
30:A:1021:A:H61	30:A:1142:A:H61	1.43	0.66
30:A:2659:G:N2	30:A:2662:A:OP2	2.29	0.66
30:A:1721:G:O2'	30:A:1739:A:N6	2.28	0.66
22:S:49:LYS:NZ	30:A:488:G:O3'	2.28	0.66
30:A:1536:C:O2'	30:A:1537:G:N2	2.29	0.66
13:J:37:ARG:NH1	30:A:1007:C:OP1	2.29	0.66
29:Z:46:MET:O	29:Z:50:VAL:HG22	1.95	0.66
30:A:693:A:O2'	30:A:1353:A:N3	2.26	0.66
9:E:97:ASN:OD1	9:E:98:LYS:N	2.29	0.65
10:F:133:GLU:OE1	10:F:133:GLU:N	2.29	0.65
30:A:1217:U:O2	30:A:1232:G:O6	2.14	0.65
9:E:46:GLN:O	9:E:88:ARG:NH2	2.29	0.65
30:A:482:A:O2'	30:A:497:A:N1	2.27	0.65
30:A:969:G:N2	30:A:984:A:O2'	2.28	0.65
30:A:1801:A:N6	30:A:2201:G:O2'	2.30	0.65
22:S:18:ARG:NH1	22:S:76:VAL:O	2.30	0.65
6:B:80:U:O4	25:V:14:LYS:NZ	2.30	0.65
30:A:569:U:O2'	30:A:983:A:N1	2.26	0.65
15:L:76:GLU:OE1	15:L:76:GLU:N	2.29	0.64
6:B:27:C:OP1	18:O:34:HIS:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1929:G:OP2	30:A:1929:G:N2	2.31	0.64
22:S:18:ARG:NH2	30:A:517:C:O2'	2.31	0.64
28:Y:8:GLU:N	28:Y:8:GLU:OE1	2.31	0.64
12:H:7:ASP:OD1	12:H:8:LYS:N	2.30	0.64
22:S:77:ASP:OD2	30:A:24:G:O2'	2.11	0.64
29:Z:18:LYS:O	29:Z:22:THR:HG23	1.97	0.64
15:L:33:ARG:NH2	30:A:587:C:O2	2.31	0.64
7:C:257:ARG:NH2	7:C:262:THR:OG1	2.31	0.63
20:Q:36:GLN:NE2	30:A:563:A:N3	2.46	0.63
30:A:577:G:O2'	30:A:1254:A:OP1	2.16	0.63
30:A:881:G:O6	30:A:895:U:O2	2.16	0.63
10:F:7:TYR:OH	10:F:28:PRO:O	2.16	0.63
9:E:148:ILE:HG21	9:E:157:LEU:HD21	1.81	0.63
18:O:48:LEU:O	18:O:85:LYS:NZ	2.30	0.63
25:V:76:ASP:OD1	25:V:77:VAL:N	2.31	0.63
30:A:1223:G:N2	30:A:1226:A:OP2	2.28	0.63
30:A:2594:C:N4	30:A:2595:G:O6	2.31	0.63
30:A:475:C:O2	30:A:479:A:N6	2.31	0.63
20:Q:48:ASP:OD2	30:A:534:U:O2'	2.05	0.63
29:Z:22:THR:HG22	30:A:850:U:O2'	1.98	0.63
17:N:71:ARG:NH2	30:A:2707:U:O2	2.32	0.63
30:A:271:G:O2'	30:A:272:A:OP2	2.13	0.63
9:E:1:MET:N	9:E:14:VAL:O	2.32	0.62
12:H:109:GLU:N	12:H:109:GLU:OE1	2.33	0.62
30:A:1697:G:OP2	30:A:1698:A:O2'	2.13	0.62
25:V:35:GLU:N	25:V:35:GLU:OE1	2.32	0.62
30:A:1550:C:OP1	30:A:1720:U:O2'	2.08	0.62
6:B:80:U:O2'	30:A:918:A:N3	2.31	0.62
30:A:2291:U:O2'	30:A:2374:C:O2	2.17	0.62
30:A:1060:U:O2'	30:A:1071:G:OP1	2.17	0.62
11:G:46:ASP:O	11:G:47:ASN:ND2	2.33	0.62
30:A:83:A:O2'	30:A:103:A:N6	2.33	0.62
1:O:9:ARG:NH2	30:A:516:C:OP1	2.33	0.61
30:A:345:A:N3	30:A:347:A:N6	2.47	0.61
30:A:966:G:H4'	30:A:2271:G:H22	1.64	0.61
30:A:2047:C:O2'	30:A:2823:A:N1	2.33	0.61
10:F:161:SER:N	10:F:164:GLU:OE2	2.34	0.61
17:N:73:ASN:OD1	30:A:1454:C:N4	2.33	0.61
27:X:40:GLU:OE1	27:X:40:GLU:N	2.34	0.61
30:A:1021:A:N6	30:A:1142:A:H61	1.98	0.61
3:2:1:MET:SD	3:2:1:MET:N	2.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:148:GLN:OE1	8:D:148:GLN:N	2.34	0.61
6:B:42:C:C5	10:F:65:LEU:HD13	2.36	0.60
17:N:42:LYS:NZ	30:A:2817:U:OP1	2.29	0.60
30:A:36:G:N3	30:A:450:G:O2'	2.34	0.60
25:V:58:SER:O	25:V:73:LYS:NZ	2.35	0.60
30:A:372:G:HO2'	30:A:373:U:P	2.24	0.60
30:A:1864:U:OP1	30:A:2410:G:O2'	2.19	0.60
20:Q:88:GLU:N	20:Q:88:GLU:OE1	2.35	0.60
6:B:52:A:O2'	6:B:53:A:OP2	2.17	0.60
23:T:13:ALA:O	23:T:33:LYS:N	2.35	0.60
30:A:2439:A:O2'	30:A:2600:A:OP1	2.18	0.60
8:D:131:ASP:O	8:D:136:ASN:ND2	2.34	0.59
27:X:56:ARG:NH2	30:A:372:G:O6	2.34	0.59
30:A:259:G:HO2'	30:A:621:A:HO2'	1.47	0.59
30:A:754:U:O2'	30:A:1272:A:N1	2.35	0.59
30:A:2032:G:OP2	30:A:2454:G:O2'	2.13	0.59
30:A:160:A:N3	30:A:2208:C:O2'	2.33	0.59
30:A:972:A:OP2	30:A:973:A:O2'	2.17	0.59
30:A:1771:C:O2'	30:A:1786:A:O4'	2.18	0.59
30:A:2090:A:N6	30:A:2230:G:O6	2.35	0.59
1:O:12:ARG:NH2	30:A:517:C:OP1	2.35	0.59
17:N:29:VAL:HG21	17:N:79:LEU:HD11	1.82	0.59
28:Y:5:GLU:OE1	28:Y:5:GLU:N	2.36	0.59
30:A:648:G:O2'	30:A:2351:G:OP1	2.13	0.59
12:H:135:HIS:HB3	12:H:138:VAL:HG12	1.85	0.59
22:S:79:GLY:N	22:S:100:THR:O	2.35	0.59
14:K:28:SER:OG	30:A:2566:A:N1	2.35	0.59
30:A:1130:U:N3	30:A:2025:C:OP1	2.35	0.59
9:E:97:ASN:ND2	30:A:606:U:OP1	2.36	0.58
11:G:66:THR:HG22	30:A:2747:G:O2'	2.03	0.58
8:D:16:THR:OG1	8:D:18:ASP:OD1	2.16	0.58
25:V:1:MET:SD	25:V:1:MET:N	2.77	0.58
9:E:43:THR:O	30:A:442:G:N2	2.33	0.58
10:F:120:SER:OG	10:F:128:SER:O	2.22	0.58
22:S:2:GLU:OE1	22:S:2:GLU:N	2.36	0.58
26:W:37:ARG:O	26:W:53:HIS:ND1	2.33	0.58
22:S:78:GLU:OE1	22:S:78:GLU:N	2.37	0.58
26:W:25:GLU:OE2	30:A:855:G:N2	2.37	0.58
30:A:726:G:O5'	30:A:1432:G:O2'	2.21	0.58
8:D:151:THR:OG1	30:A:2032:G:N2	2.37	0.58
20:Q:101:ASP:N	20:Q:101:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1131:G:O2'	30:A:2025:C:O2'	2.22	0.58
30:A:1068:G:N2	30:A:1095:A:O2'	2.36	0.58
9:E:49:ARG:NH2	9:E:72:SER:OG	2.36	0.58
9:E:122:GLU:OE1	9:E:123:LYS:N	2.37	0.58
5:4:1:MET:SD	5:4:34:LYS:NZ	2.77	0.57
22:S:77:ASP:O	22:S:102:HIS:N	2.35	0.57
30:A:644:A:O2'	30:A:645:C:O5'	2.14	0.57
30:A:2580:U:O2'	30:A:2581:G:O4'	2.20	0.57
10:F:37:MET:SD	10:F:37:MET:N	2.78	0.57
30:A:1040:A:N6	30:A:1116:G:O6	2.37	0.57
7:C:235:GLU:N	7:C:235:GLU:OE1	2.37	0.57
10:F:97:GLU:OE1	10:F:101:ARG:NE	2.37	0.57
30:A:324:A:N6	30:A:339:U:O4'	2.37	0.57
30:A:2324:U:O2'	30:A:2337:G:OP1	2.21	0.57
6:B:37:C:O2	18:O:100:HIS:NE2	2.37	0.57
15:L:95:LEU:HD11	15:L:100:ILE:HD11	1.85	0.57
30:A:629:G:N3	30:A:639:U:O2'	2.38	0.57
30:A:1326:U:HO2'	30:A:2010:G:HO2'	1.52	0.57
7:C:99:GLU:N	7:C:99:GLU:OE1	2.37	0.57
23:T:54:GLU:OE1	23:T:54:GLU:N	2.37	0.57
24:U:3:LYS:O	24:U:93:ARG:NH1	2.37	0.57
24:U:6:ARG:N	30:A:85:G:OP1	2.37	0.57
10:F:93:GLU:OE1	10:F:93:GLU:N	2.37	0.57
4:3:30:HIS:NE2	30:A:2392:A:OP2	2.37	0.57
7:C:270:ARG:NH2	30:A:1798:U:OP2	2.33	0.57
30:A:2692:G:N3	30:A:2847:U:O2'	2.38	0.57
8:D:123:LYS:NZ	30:A:1999:C:OP1	2.38	0.57
16:M:20:LEU:HD21	25:V:81:PRO:HG2	1.87	0.56
29:Z:57:GLU:N	29:Z:57:GLU:OE1	2.38	0.56
9:E:162:ARG:NH2	30:A:340:A:O2'	2.38	0.56
9:E:154:ASP:OD1	9:E:154:ASP:N	2.38	0.56
9:E:176:ASP:N	9:E:176:ASP:OD1	2.35	0.56
11:G:87:GLN:OE1	11:G:87:GLN:N	2.39	0.56
30:A:586:A:OP2	30:A:1251:C:N4	2.38	0.56
10:F:62:GLN:OE1	10:F:62:GLN:N	2.39	0.56
10:F:7:TYR:HA	10:F:11:VAL:HG12	1.88	0.56
30:A:1205:A:O2'	30:A:1206:G:OP1	2.22	0.56
20:Q:85:ALA:O	20:Q:86:SER:OG	2.21	0.56
26:W:7:ARG:O	26:W:10:ARG:NH1	2.38	0.56
30:A:527:C:OP2	30:A:2779:U:N3	2.35	0.56
30:A:2528:U:O2'	30:A:2530:A:OP1	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:25:THR:OG1	8:D:191:GLY:O	2.14	0.55
8:D:114:LYS:NZ	30:A:2723:C:OP1	2.39	0.55
15:L:111:ILE:HD11	30:A:627:A:C5	2.40	0.55
20:Q:47:ARG:NH2	30:A:560:C:O2	2.39	0.55
25:V:61:LEU:N	25:V:72:VAL:O	2.39	0.55
4:3:32:LEU:HD22	30:A:2419:U:OP2	2.06	0.55
30:A:2637:U:O4	30:A:2776:A:N7	2.40	0.55
16:M:11:LYS:O	30:A:911:A:N6	2.39	0.55
2:1:31:GLU:OE1	2:1:31:GLU:N	2.39	0.55
24:U:16:LYS:N	30:A:329:G:O6	2.39	0.55
27:X:57:VAL:HG12	30:A:372:G:H3'	1.89	0.55
30:A:84:A:N1	30:A:98:G:O2'	2.31	0.55
30:A:1353:A:OP2	30:A:1377:G:N1	2.36	0.55
24:U:85:ARG:NE	24:U:87:GLU:OE2	2.40	0.55
30:A:976:G:O2'	30:A:1155:A:O2'	2.14	0.55
30:A:2451:A:OP1	30:A:2497:A:N6	2.39	0.55
18:O:116:GLN:OE1	18:O:116:GLN:N	2.39	0.54
30:A:1007:C:OP2	30:A:1008:A:O2'	2.12	0.54
7:C:78:GLU:N	7:C:78:GLU:OE1	2.40	0.54
30:A:184:C:O2'	30:A:217:A:N3	2.41	0.54
30:A:793:A:OP2	30:A:2071:A:O2'	2.25	0.54
30:A:2349:G:O6	30:A:2369:A:N6	2.40	0.54
30:A:2776:A:O2'	30:A:2782:G:N7	2.37	0.54
19:P:13:LYS:NZ	19:P:76:HIS:O	2.41	0.54
30:A:222:A:H61	30:A:232:G:H1'	1.71	0.54
12:H:2:GLN:N	12:H:2:GLN:OE1	2.39	0.54
13:J:138:GLN:OE1	13:J:138:GLN:N	2.37	0.54
14:K:6:THR:HG23	30:A:1666:G:H4'	1.89	0.54
30:A:2075:U:O2'	30:A:2077:A:OP2	2.15	0.54
30:A:2509:G:N1	30:A:2580:U:O4	2.41	0.54
4:3:12:ARG:NE	15:L:61:LEU:O	2.39	0.54
30:A:1341:G:OP1	30:A:1397:U:N3	2.40	0.54
30:A:1999:C:O2	30:A:2687:U:O2'	2.23	0.54
30:A:1084:A:N6	30:A:1085:A:N1	2.56	0.54
30:A:2133:G:N2	30:A:2157:G:O6	2.41	0.54
8:D:155:VAL:HG21	30:A:2618:G:H21	1.73	0.54
19:P:33:GLU:N	19:P:33:GLU:OE1	2.40	0.54
30:A:48:G:H22	30:A:177:G:P	2.31	0.54
30:A:462:C:N4	30:A:463:G:O6	2.41	0.54
30:A:954:G:O2'	30:A:2274:A:N1	2.38	0.54
30:A:1018:U:O3'	30:A:1120:G:N2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:2468:A:O2'	30:A:2469:A:O4'	2.25	0.54
30:A:2751:G:OP1	30:A:2751:G:N2	2.37	0.53
19:P:93:LYS:NZ	30:A:2848:G:OP1	2.40	0.53
9:E:79:ARG:NE	30:A:448:U:O4'	2.41	0.53
15:L:91:ASP:OD1	15:L:92:LEU:N	2.41	0.53
30:A:245:G:O2'	30:A:384:A:N1	2.37	0.53
30:A:1048:A:O2'	30:A:1112:G:N2	2.41	0.53
30:A:1662:U:O2'	30:A:2687:U:OP1	2.24	0.53
30:A:1779:U:O2	30:A:1783:A:N6	2.41	0.53
30:A:2099:U:O2'	30:A:2100:G:O5'	2.20	0.53
13:J:135:GLN:NE2	30:A:6:A:N3	2.56	0.53
30:A:575:A:OP2	30:A:2055:C:N4	2.42	0.53
30:A:2077:A:N3	30:A:2434:A:O2'	2.40	0.53
30:A:453:A:N3	30:A:457:A:O2'	2.42	0.53
26:W:11:ASP:OD1	26:W:12:SER:N	2.40	0.53
4:3:7:ARG:NH1	30:A:243:U:OP1	2.42	0.53
10:F:139:GLU:OE1	10:F:139:GLU:N	2.40	0.53
19:P:12:MET:HB2	19:P:54:LEU:HD11	1.91	0.53
26:W:25:GLU:N	26:W:25:GLU:OE1	2.42	0.53
30:A:370:G:O2'	30:A:424:G:OP1	2.26	0.53
30:A:2506[A]:U:OP2	30:A:2576:G:N1	2.39	0.53
9:E:32:VAL:HG23	9:E:178:VAL:HG22	1.89	0.52
17:N:1:MET:N	30:A:1654:A:OP2	2.42	0.52
30:A:630:G:N2	30:A:633:A:OP2	2.41	0.52
9:E:140:ASP:OD1	9:E:141:MET:N	2.42	0.52
30:A:799:G:OP2	30:A:800:A:O2'	2.22	0.52
9:E:146:VAL:HG21	9:E:187:VAL:HG13	1.90	0.52
25:V:72:VAL:HG21	25:V:91:PHE:HB3	1.91	0.52
30:A:2250:G:O2'	30:A:2496:C:OP1	2.27	0.52
30:A:212:G:H2'	30:A:213:A:C8	2.45	0.52
30:A:477:A:N6	30:A:501:A:OP1	2.43	0.52
30:A:1020:A:H1'	30:A:1021:A:OP2	2.09	0.52
30:A:966:G:O4'	30:A:2267:A:N6	2.43	0.52
30:A:2628:C:O2'	30:A:2782:G:OP1	2.22	0.52
10:F:134:GLN:N	10:F:134:GLN:OE1	2.42	0.52
19:P:26:GLU:N	19:P:26:GLU:OE1	2.42	0.52
19:P:47:ILE:HG22	19:P:99:LEU:HD12	1.91	0.52
25:V:7:GLU:N	25:V:7:GLU:OE1	2.42	0.52
30:A:981:A:OP2	30:A:982:C:N4	2.37	0.52
30:A:2468:A:P	30:A:2476:A:H61	2.33	0.52
28:Y:24:GLU:HA	28:Y:28:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:974:G:O4'	30:A:990:A:N6	2.43	0.52
13:J:14:ASP:OD1	13:J:15:TRP:N	2.43	0.52
21:R:22:LEU:HD12	21:R:23:GLU:O	2.10	0.52
9:E:171:ASP:OD1	9:E:172:ALA:N	2.41	0.51
30:A:45:G:N7	30:A:215:G:O2'	2.43	0.51
30:A:644:A:HO2'	30:A:645:C:P	2.31	0.51
30:A:59:U:O2'	30:A:74:A:OP2	2.19	0.51
30:A:1026:G:OP2	30:A:1134:A:O2'	2.27	0.51
15:L:29:LYS:O	15:L:30:THR:OG1	2.17	0.51
22:S:18:ARG:NH2	22:S:78:GLU:OE2	2.43	0.51
30:A:28:A:O2'	30:A:582:A:O2'	2.17	0.51
9:E:48:THR:O	9:E:52:VAL:HG23	2.11	0.51
30:A:1205:A:HO2'	30:A:1206:G:P	2.33	0.51
1:O:43:THR:OG1	1:O:45:ASP:OD1	2.18	0.51
5:4:2:LYS:NZ	30:A:2478:A:OP2	2.42	0.51
7:C:47:ARG:NH1	30:A:774:G:OP1	2.44	0.51
30:A:574:A:N6	30:A:2034:U:OP1	2.41	0.51
20:Q:8:ILE:HD12	20:Q:8:ILE:H	1.76	0.51
22:S:109:ASP:OD1	22:S:110:ARG:N	2.43	0.51
15:L:82:LEU:O	15:L:82:LEU:HD23	2.11	0.51
30:A:1255:U:O4'	30:A:2502:G:N2	2.43	0.51
19:P:79:VAL:HG13	19:P:80:VAL:HG13	1.93	0.51
30:A:1447:C:N4	30:A:1448:G:O6	2.43	0.51
30:A:2637:U:H3	30:A:2776:A:H62	1.57	0.51
15:L:79:LEU:HD21	15:L:131:ALA:HB1	1.93	0.50
30:A:2076:U:OP2	30:A:2238:G:N2	2.41	0.50
20:Q:54:ARG:NH2	30:A:1155:A:O3'	2.44	0.50
30:A:378:C:N4	30:A:379:G:O6	2.44	0.50
24:U:67:SER:O	30:A:335:C:O2'	2.25	0.50
30:A:1141:U:O2	30:A:1142:A:N6	2.44	0.50
7:C:62:ARG:NH2	30:A:1567:G:O2'	2.45	0.50
30:A:1733:G:C2	30:A:1734:G:N7	2.79	0.50
30:A:2638:G:O2'	30:A:2778:A:N6	2.44	0.50
30:A:1275:A:N1	30:A:1295:C:O2'	2.37	0.50
6:B:52:A:O2'	6:B:53:A:P	2.70	0.50
30:A:308:G:O2'	30:A:329:G:N2	2.45	0.50
30:A:951:C:N4	30:A:952:G:O6	2.44	0.50
18:O:61:GLN:OE1	18:O:61:GLN:N	2.44	0.50
30:A:1018:U:O2'	30:A:1120:G:N2	2.36	0.50
22:S:67:ASP:OD1	22:S:68:ASP:N	2.45	0.49
30:A:1688:U:O2'	30:A:1700:A:N7	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:8:C:OP1	18:O:15:ARG:NH2	2.45	0.49
9:E:191:ASP:OD1	9:E:192:ALA:N	2.45	0.49
24:U:44:HIS:N	30:A:481:G:OP2	2.39	0.49
30:A:724:U:C2'	30:A:725:G:O5'	2.60	0.49
30:A:837:C:N3	30:A:941:A:N6	2.61	0.49
30:A:1022:G:H4'	30:A:1023:U:O5'	2.12	0.49
30:A:2743:U:OP2	30:A:2755:C:N4	2.45	0.49
7:C:123:ILE:O	7:C:123:ILE:HG22	2.11	0.49
30:A:259:G:O2'	30:A:621:A:O2'	2.20	0.49
30:A:1664:A:H61	30:A:1996:C:N4	2.10	0.49
30:A:1814:G:OP2	30:A:1815:A:O2'	2.26	0.49
30:A:2808:G:O2'	30:A:2809:A:N7	2.45	0.49
30:A:2577:A:O4'	30:A:2612:C:N4	2.45	0.49
7:C:245:THR:HG23	7:C:247:TRP:H	1.77	0.49
22:S:80:PRO:O	22:S:100:THR:OG1	2.28	0.49
30:A:220:G:N1	30:A:428:A:OP2	2.44	0.49
30:A:1282:U:O4	30:A:1286:A:N7	2.45	0.49
20:Q:53:LYS:NZ	30:A:994:C:OP2	2.45	0.49
26:W:38:GLY:HA2	30:A:2330:G:H21	1.76	0.49
29:Z:4:ILE:HD11	29:Z:56:VAL:CG2	2.42	0.49
14:K:22:ILE:HD11	14:K:40:LYS:HG2	1.95	0.49
30:A:451:U:O2	30:A:453:A:N6	2.46	0.49
30:A:1288:G:OP2	30:A:1288:G:N2	2.33	0.49
30:A:2474:U:H2'	30:A:2474:U:O2	2.12	0.49
10:F:25:MET:SD	10:F:25:MET:N	2.84	0.49
10:F:90:LEU:HD23	10:F:90:LEU:H	1.77	0.49
7:C:237:ARG:NH2	30:A:1787:A:OP1	2.46	0.49
30:A:728:G:O2'	30:A:730:A:O4'	2.31	0.49
30:A:1794:A:N6	30:A:1826:G:O6	2.45	0.49
8:D:3:GLY:C	8:D:4:LEU:HD12	2.34	0.48
14:K:19:VAL:HG11	14:K:41:ILE:HD12	1.94	0.48
20:Q:10:ARG:NH2	30:A:513:A:N3	2.59	0.48
30:A:357:C:C2	30:A:358:U:C5	3.01	0.48
30:A:864:G:H21	30:A:866:A:H62	1.61	0.48
7:C:20:ASN:O	7:C:23:LEU:HD22	2.12	0.48
9:E:7:ASP:OD1	9:E:8:ALA:N	2.46	0.48
17:N:67:PHE:HA	17:N:76:VAL:HG11	1.94	0.48
20:Q:65:ASN:OD1	20:Q:69:ARG:NE	2.45	0.48
24:U:3:LYS:NZ	24:U:82:VAL:O	2.46	0.48
30:A:1275:A:O2'	30:A:1645:G:N3	2.46	0.48
16:M:110:GLU:OE2	16:M:114:ARG:NE	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:549:G:HO2'	30:A:550:C:P	2.37	0.48
6:B:38:C:O4'	18:O:100:HIS:NE2	2.46	0.48
30:A:549:G:O2'	30:A:550:C:P	2.72	0.48
30:A:1270:C:N4	30:A:1648:U:O4	2.47	0.48
9:E:176:ASP:OD1	9:E:179:SER:OG	2.12	0.48
12:H:12:LEU:H	12:H:12:LEU:HD23	1.79	0.48
13:J:36:LEU:HD21	13:J:122:LEU:HD13	1.95	0.48
30:A:225:C:N3	30:A:231:A:N6	2.61	0.48
30:A:1276:A:N6	30:A:1645:G:O6	2.46	0.48
30:A:1638:C:OP1	30:A:2710:C:O2'	2.32	0.48
19:P:8:GLU:HB2	19:P:54:LEU:HD13	1.95	0.48
15:L:82:LEU:HD23	15:L:90:VAL:HG21	1.96	0.48
30:A:27:G:O2'	30:A:28:A:OP2	2.24	0.48
30:A:2720:U:C2	30:A:2721:A:C8	3.01	0.48
6:B:83:G:O6	6:B:94:A:N6	2.47	0.48
8:D:8:LYS:HA	8:D:27:ILE:HD12	1.96	0.48
30:A:1289:C:C2	30:A:1290:C:C5	3.02	0.48
30:A:2581:G:N2	30:A:2581:G:OP2	2.47	0.48
30:A:2699:C:N4	30:A:2700:A:H62	2.12	0.48
7:C:193:GLU:N	7:C:193:GLU:OE1	2.46	0.47
8:D:129:THR:OG1	30:A:1997:C:O5'	2.26	0.47
25:V:59:GLU:OE1	25:V:59:GLU:N	2.43	0.47
6:B:15:A:N3	6:B:109:A:N6	2.61	0.47
30:A:1754:A:N6	30:A:2717:C:O4'	2.46	0.47
19:P:61:ARG:NH1	19:P:70:GLU:OE2	2.43	0.47
30:A:1288:G:OP1	30:A:1289:C:N4	2.47	0.47
15:L:82:LEU:CD2	15:L:90:VAL:HG21	2.44	0.47
30:A:2679:A:N6	30:A:2729:G:O6	2.48	0.47
7:C:15:VAL:HG22	7:C:205:GLY:HA3	1.95	0.47
7:C:206:LYS:NZ	30:A:729:G:O4'	2.39	0.47
23:T:37:ASP:OD1	23:T:38:ALA:N	2.47	0.47
11:G:154:GLU:OE1	11:G:156:TYR:N	2.48	0.47
12:H:17:ASP:OD1	12:H:18:GLN:N	2.48	0.47
30:A:641:U:O2'	30:A:2350:C:OP1	2.17	0.47
6:B:45:A:O4'	10:F:91:ARG:NH1	2.48	0.47
16:M:44:ARG:NH2	30:A:2484:G:OP2	2.47	0.47
30:A:299:A:N6	30:A:322:A:O2'	2.45	0.47
30:A:555:G:HO2'	30:A:556:A:H8	1.60	0.47
30:A:2286:G:N2	30:A:2344:U:O2	2.48	0.47
30:A:2655:G:O2'	30:A:2656:U:O5'	2.33	0.47
30:A:1857:G:HO2'	30:A:1858:A:H8	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:27:ASN:ND2	30:A:2361:G:O3'	2.48	0.46
9:E:31:VAL:HG21	9:E:104:ALA:CB	2.45	0.46
17:N:66:ALA:O	17:N:69:ARG:O	2.33	0.46
23:T:70:HIS:HD2	30:A:64:A:C2	2.33	0.46
26:W:17:LEU:HD21	26:W:37:ARG:HD3	1.98	0.46
30:A:727:A:H2'	30:A:728:G:O4'	2.15	0.46
30:A:780:G:O2'	30:A:783:A:N6	2.42	0.46
8:D:14:ILE:HD13	8:D:178:VAL:CG1	2.45	0.46
15:L:3:LEU:HD21	30:A:1202:G:O2'	2.14	0.46
23:T:82:LYS:NZ	30:A:1339:G:OP1	2.49	0.46
24:U:36:GLU:O	24:U:38:ILE:HD12	2.14	0.46
30:A:2652:C:H2'	30:A:2653:U:O4'	2.16	0.46
15:L:43:GLY:N	30:A:671:C:OP1	2.42	0.46
20:Q:29:ARG:NH1	30:A:18:U:OP1	2.42	0.46
5:4:3:VAL:HG12	5:4:3:VAL:O	2.14	0.46
6:B:116:G:H4'	18:O:54:VAL:HG12	1.98	0.46
8:D:124:ARG:NH1	30:A:2620:C:O2'	2.44	0.46
9:E:27:LEU:HD13	9:E:100:MET:CE	2.45	0.46
20:Q:71:ASN:OD1	20:Q:109:VAL:HG11	2.16	0.46
30:A:971:G:O2'	30:A:983:A:N3	2.32	0.46
30:A:1432:G:H2'	30:A:1433:A:C8	2.50	0.46
7:C:65:ASP:N	7:C:102:TYR:O	2.45	0.46
10:F:3:LEU:HD21	10:F:96:TRP:HB3	1.96	0.46
14:K:92:GLU:OE1	14:K:92:GLU:N	2.45	0.46
16:M:123:LYS:O	30:A:2484:G:O2'	2.34	0.46
7:C:44:ASN:N	30:A:1812:U:O2'	2.46	0.46
30:A:969:G:H22	30:A:984:A:HO2'	1.61	0.46
30:A:1290:C:C2	30:A:1291:C:C5	3.04	0.46
7:C:104:LEU:H	7:C:104:LEU:HD12	1.81	0.46
14:K:2:ILE:HG23	14:K:6:THR:HG21	1.98	0.46
16:M:17:ASN:ND2	16:M:39:GLY:O	2.48	0.46
20:Q:89:ILE:HD12	20:Q:94:LEU:HD21	1.98	0.46
30:A:1497:U:OP2	30:A:1498:C:N4	2.42	0.46
10:F:105:ILE:HD12	10:F:138:PRO:HG2	1.98	0.46
30:A:24:G:C2	30:A:25:U:C5	3.04	0.46
30:A:1734:G:C2	30:A:1735:A:N7	2.84	0.46
5:4:1:MET:N	30:A:2526:G:N3	2.64	0.46
30:A:723:C:C2	30:A:724:U:C5	3.03	0.46
30:A:1342:A:O2'	30:A:1344:U:OP1	2.29	0.46
23:T:7:LEU:O	23:T:10:VAL:HG12	2.16	0.45
30:A:2564:A:C2	30:A:2647:U:H4'	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:105:LEU:HD23	9:E:200:LEU:HD21	1.97	0.45
30:A:1022:G:H1'	30:A:1023:U:OP2	2.16	0.45
30:A:1344:U:H3'	30:A:1345:C:H5'	1.98	0.45
30:A:1797:G:HO2'	30:A:1798:U:H5'	1.81	0.45
30:A:2777:G:OP2	30:A:2781:A:O2'	2.24	0.45
1:O:3:GLN:NE2	30:A:1263:U:O2'	2.42	0.45
30:A:2506[B]:U:OP2	30:A:2576:G:N2	2.43	0.45
30:A:2848:G:O2'	30:A:2868:A:N6	2.47	0.45
24:U:35:VAL:HB	24:U:38:ILE:HD13	1.99	0.45
30:A:51:G:HO2'	30:A:52:A:P	2.39	0.45
30:A:729:G:O2'	30:A:763:G:H4'	2.17	0.45
9:E:148:ILE:N	9:E:148:ILE:HD12	2.32	0.45
14:K:21:CYS:HA	14:K:41:ILE:HG22	1.99	0.45
15:L:127:VAL:HG23	15:L:131:ALA:HB3	1.97	0.45
21:R:16:GLU:OE2	21:R:101:ILE:N	2.49	0.45
27:X:44:ARG:NH1	30:A:166:U:O2'	2.50	0.45
30:A:29:U:C2	30:A:30:G:C8	3.05	0.45
30:A:1141:U:H4'	30:A:1142:A:O4'	2.16	0.45
30:A:1378:A:C4'	30:A:1379:U:OP1	2.65	0.45
10:F:3:LEU:HD22	10:F:100:GLU:HG2	1.98	0.45
30:A:639:U:C2	30:A:640:C:C5	3.05	0.45
30:A:2120:G:N1	30:A:2121:G:O6	2.50	0.45
14:K:113:MET:SD	14:K:113:MET:N	2.90	0.45
30:A:526:A:O2'	30:A:2043:C:O2	2.27	0.45
30:A:725:G:HO2'	30:A:726:G:C4'	2.27	0.45
30:A:1203:U:OP2	30:A:1204:A:O2'	2.13	0.45
30:A:1272:A:O2'	30:A:1274:A:OP1	2.35	0.45
15:L:77:ILE:HD12	15:L:109:LYS:O	2.17	0.45
17:N:38:LEU:HD11	17:N:42:LYS:HZ1	1.81	0.45
30:A:1378:A:O2'	30:A:1380:G:OP2	2.29	0.45
30:A:1702:G:C6	30:A:1703:G:N7	2.85	0.45
30:A:2552:U:O2'	30:A:2553:G:N7	2.41	0.45
20:Q:78:PHE:CE2	20:Q:82:LEU:HD11	2.52	0.45
30:A:532:A:N7	30:A:2021:C:O2'	2.40	0.45
30:A:554:U:H2'	30:A:555:G:O4'	2.17	0.45
30:A:1224:U:H4'	30:A:1225:G:OP1	2.18	0.45
30:A:1827:U:OP1	30:A:1971:U:O2'	2.35	0.45
19:P:20:ARG:NH1	30:A:2849:U:O4	2.50	0.44
30:A:48:G:N2	30:A:177:G:OP2	2.50	0.44
30:A:58:G:O2'	30:A:73:A:N1	2.45	0.44
30:A:1058:U:H2'	30:A:1059:G:C4	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:2552:U:H3'	30:A:2552:U:O2	2.17	0.44
6:B:39:A:C2	6:B:44:G:C2	3.05	0.44
23:T:2:ILE:HD11	30:A:144:A:H4'	1.99	0.44
30:A:724:U:H2'	30:A:725:G:O5'	2.16	0.44
30:A:1425:G:H2'	30:A:1426:G:O4'	2.17	0.44
30:A:2756:U:H4'	30:A:2757:A:OP1	2.17	0.44
11:G:36:LEU:HD23	11:G:37:ASN:H	1.83	0.44
21:R:23:GLU:OE2	30:A:1161:C:O2'	2.31	0.44
30:A:1663:G:O2'	30:A:1664:A:O5'	2.32	0.44
30:A:1769:U:O2	30:A:1983:G:O6	2.35	0.44
9:E:31:VAL:HG21	9:E:104:ALA:HB2	1.99	0.44
21:R:82:HIS:ND1	21:R:82:HIS:O	2.50	0.44
30:A:247:G:N2	30:A:251:A:OP2	2.49	0.44
30:A:1477:A:N6	30:A:1514:G:O2'	2.49	0.44
9:E:41:GLN:NE2	30:A:442:G:O4'	2.51	0.44
15:L:111:ILE:HD12	30:A:636:G:N2	2.33	0.44
30:A:2050:C:H2'	30:A:2051:A:O4'	2.17	0.44
7:C:11:GLY:O	7:C:15:VAL:HG23	2.18	0.44
11:G:36:LEU:HD23	11:G:37:ASN:N	2.32	0.44
30:A:725:G:H2'	30:A:726:G:C4	2.52	0.44
12:H:122:LEU:O	12:H:122:LEU:HD12	2.18	0.44
18:O:46:GLU:OE1	18:O:46:GLU:N	2.51	0.44
22:S:13:SER:O	22:S:17:VAL:HG23	2.18	0.44
30:A:1129:A:N6	30:A:2491:U:OP1	2.50	0.44
30:A:1142:A:C4	30:A:1144:A:N7	2.86	0.44
30:A:1145:C:C2	30:A:1146:C:C5	3.05	0.44
30:A:1313:U:O2'	30:A:1332:G:O4'	2.34	0.44
30:A:1737:G:O3'	30:A:1738:G:O4'	2.35	0.44
30:A:1790:C:H2'	30:A:1791:A:C8	2.53	0.44
7:C:2:VAL:HG21	7:C:201:LEU:HG	1.99	0.44
9:E:112:LEU:HD13	9:E:117:ARG:HB2	1.98	0.44
10:F:107:VAL:N	10:F:108:PRO:CD	2.81	0.44
20:Q:89:ILE:CD1	20:Q:94:LEU:HD21	2.48	0.44
29:Z:42:ALA:O	30:A:851:C:O2'	2.35	0.44
30:A:213:A:H2'	30:A:214:G:C8	2.52	0.44
30:A:754:U:C2	30:A:755:U:C5	3.06	0.44
9:E:27:LEU:HD13	9:E:100:MET:HE2	1.99	0.44
20:Q:111:LYS:NZ	21:R:49:ILE:O	2.39	0.44
24:U:97:SER:O	24:U:98:ASN:OD1	2.36	0.44
30:A:216:A:C8	30:A:432:A:N6	2.86	0.44
30:A:549:G:C2'	30:A:550:C:O5'	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:579:G:C6	30:A:1262:A:N6	2.86	0.44
7:C:68:ARG:NH1	7:C:128:THR:OG1	2.51	0.43
18:O:9:ARG:NH2	30:A:2296:U:OP2	2.51	0.43
30:A:582:A:N6	30:A:1259:G:O6	2.51	0.43
30:A:640:C:N4	30:A:649:G:O6	2.50	0.43
2:1:20:TYR:OH	30:A:2347:C:O2'	2.13	0.43
10:F:23:SER:OG	10:F:25:MET:SD	2.76	0.43
13:J:120:ARG:NE	30:A:2780:G:OP2	2.51	0.43
30:A:1071:G:N3	30:A:1089:A:O2'	2.47	0.43
30:A:1164:C:O2'	30:A:1224:U:C4	2.72	0.43
30:A:2375:G:N1	30:A:2379:G:O6	2.51	0.43
17:N:69:ARG:O	17:N:70:THR:OG1	2.31	0.43
26:W:16:ARG:NE	30:A:2357:G:OP1	2.44	0.43
30:A:2700:A:N6	30:A:2708:G:O6	2.51	0.43
4:3:22:LYS:NZ	30:A:630:G:OP1	2.41	0.43
10:F:140:ILE:N	10:F:140:ILE:HD12	2.33	0.43
12:H:121:VAL:HG12	12:H:121:VAL:O	2.18	0.43
30:A:1139:G:O2'	30:A:1143:A:N1	2.46	0.43
30:A:2058:A:H61	30:A:2611:C:N4	2.16	0.43
30:A:2089:C:N4	30:A:2090:A:H62	2.17	0.43
14:K:86:LEU:O	14:K:87:LEU:HD12	2.18	0.43
30:A:723:C:N3	30:A:724:U:C5	2.86	0.43
30:A:1264:A:O5'	30:A:1265:A:H2'	2.19	0.43
30:A:2749:A:OP2	30:A:2750:A:O2'	2.20	0.43
14:K:92:GLU:OE2	14:K:111:LYS:NZ	2.34	0.43
15:L:112:LEU:HD21	30:A:627:A:N6	2.33	0.43
16:M:42:THR:HG22	16:M:93:VAL:HG12	1.99	0.43
19:P:52:ARG:NH1	30:A:2845:U:O3'	2.51	0.43
27:X:64:ASP:OD1	27:X:65:THR:N	2.52	0.43
30:A:28:A:C5	30:A:29:U:C5	3.07	0.43
30:A:2093:G:O2'	30:A:2198:A:N1	2.47	0.43
7:C:97:ASP:OD1	7:C:97:ASP:N	2.51	0.43
13:J:52:ASP:OD1	13:J:52:ASP:N	2.51	0.43
30:A:372:G:O2'	30:A:373:U:P	2.74	0.43
30:A:645:C:H2'	30:A:647:G:C8	2.53	0.43
30:A:711:G:C6	30:A:721:A:C6	3.07	0.43
16:M:18:ARG:NH1	30:A:952:G:OP1	2.52	0.43
17:N:4:ARG:NE	30:A:2874:C:OP1	2.50	0.43
30:A:447:A:N1	30:A:454:A:O2'	2.41	0.43
30:A:1287:A:C2'	30:A:1288:G:O5'	2.67	0.43
6:B:55:U:O2'	10:F:25:MET:SD	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:148:ILE:HD13	9:E:167:VAL:HG23	2.01	0.43
30:A:332:A:HO2'	30:A:334:C:P	2.42	0.43
30:A:1068:G:H2'	30:A:1069:A:O4'	2.19	0.43
30:A:2117:A:N1	30:A:2170:A:N6	2.64	0.43
30:A:29:U:O2	30:A:1215:G:O2'	2.37	0.43
30:A:543:G:O6	30:A:551:G:O6	2.36	0.43
6:B:42:C:C4	10:F:65:LEU:HD22	2.54	0.42
7:C:35:LYS:NZ	30:A:1353:A:O3'	2.50	0.42
26:W:33:ILE:HD11	26:W:78:ILE:HD11	2.00	0.42
30:A:442:G:C6	30:A:444:C:N4	2.87	0.42
30:A:458:G:O2'	30:A:459:U:P	2.77	0.42
30:A:488:G:H22	30:A:491:G:H5''	1.84	0.42
30:A:570:G:C1'	30:A:983:A:N6	2.82	0.42
30:A:1287:A:N6	30:A:1649:G:O2'	2.52	0.42
30:A:1995:U:OP2	30:A:1996:C:O2'	2.30	0.42
30:A:2345:G:O2'	30:A:2381:A:N3	2.44	0.42
30:A:2506[A]:U:OP2	30:A:2576:G:N2	2.51	0.42
10:F:43:ILE:HD12	10:F:43:ILE:N	2.35	0.42
11:G:62:ALA:O	11:G:66:THR:HG23	2.19	0.42
24:U:98:ASN:O	24:U:98:ASN:CG	2.58	0.42
28:Y:19:LEU:O	28:Y:19:LEU:HD23	2.19	0.42
8:D:7:LYS:N	8:D:28:GLU:O	2.42	0.42
30:A:1686:C:N4	30:A:1703:G:O6	2.53	0.42
3:2:9:VAL:HG12	30:A:1309:G:OP1	2.19	0.42
12:H:99:ILE:O	12:H:103:VAL:HG23	2.19	0.42
22:S:36:LEU:HD22	22:S:47:VAL:CG1	2.49	0.42
30:A:1663:G:O6	30:A:1998:A:N6	2.52	0.42
30:A:1684:G:C6	30:A:1705:A:N6	2.87	0.42
30:A:1992:G:N2	30:A:1996:C:O2'	2.48	0.42
9:E:97:ASN:HB3	9:E:100:MET:HG2	2.01	0.42
28:Y:42:LEU:HD13	28:Y:45:GLN:OE1	2.20	0.42
20:Q:60:TRP:O	20:Q:64:ILE:HG12	2.20	0.42
12:H:5:LEU:HD12	12:H:5:LEU:N	2.34	0.42
19:P:3:ILE:N	19:P:3:ILE:HD12	2.35	0.42
30:A:827:U:OP2	30:A:828:U:N3	2.53	0.42
30:A:1425:G:N2	30:A:1574:C:C4	2.88	0.42
30:A:2487:G:C2	30:A:2488:G:C5	3.08	0.42
23:T:37:ASP:O	23:T:81:LYS:NZ	2.50	0.42
29:Z:4:ILE:HD11	29:Z:56:VAL:HG21	2.01	0.42
30:A:1268:A:H1'	30:A:2013:A:H61	1.84	0.42
30:A:1466:U:O3'	30:A:1546:G:O2'	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1788:C:C2	30:A:1789:A:C8	3.07	0.42
29:Z:50:VAL:O	29:Z:54:VAL:HG22	2.19	0.42
30:A:379:G:C6	30:A:396:G:O6	2.73	0.42
6:B:2:G:H2'	6:B:3:C:C6	2.55	0.42
6:B:30:C:H1'	6:B:57:A:H61	1.85	0.42
30:A:2028:U:O4	30:A:2033:A:N7	2.53	0.42
7:C:156:SER:OG	7:C:159:THR:OG1	2.06	0.41
30:A:619:G:O5'	30:A:620:G:N2	2.53	0.41
30:A:1386:C:H2'	30:A:1387:A:C8	2.55	0.41
30:A:1604:C:O2'	30:A:1610:A:N1	2.42	0.41
4:3:29:ARG:NH2	15:L:63:LYS:O	2.52	0.41
8:D:81:GLU:OE1	30:A:2635:A:O2'	2.37	0.41
23:T:11:LEU:HD23	23:T:12:ARG:N	2.35	0.41
30:A:464:U:C2'	30:A:465:G:O5'	2.68	0.41
30:A:1024:G:H1'	30:A:1144:A:O2'	2.19	0.41
30:A:1186:G:H2'	30:A:1187:G:O4'	2.20	0.41
6:B:3:C:H3'	6:B:4:C:H5''	2.02	0.41
11:G:51:PHE:CZ	11:G:71:LEU:HD22	2.55	0.41
30:A:619:G:H3'	30:A:620:G:H21	1.85	0.41
30:A:619:G:OP2	30:A:620:G:N2	2.53	0.41
30:A:2058:A:H61	30:A:2611:C:H42	1.67	0.41
30:A:2074:U:O2'	30:A:2597:G:H1'	2.20	0.41
30:A:2464:G:C6	30:A:2487:G:C6	3.07	0.41
8:D:33:ARG:HD2	8:D:73:VAL:HG13	2.01	0.41
11:G:47:ASN:O	11:G:48:THR:HG23	2.20	0.41
12:H:12:LEU:HD23	12:H:12:LEU:N	2.35	0.41
13:J:43:GLU:N	13:J:43:GLU:OE1	2.53	0.41
15:L:23:ILE:N	30:A:813:U:OP2	2.53	0.41
20:Q:78:PHE:CZ	20:Q:82:LEU:HD11	2.56	0.41
30:A:202:U:H2'	30:A:203:A:O4'	2.20	0.41
30:A:633:A:O2'	30:A:2404:U:OP1	2.38	0.41
30:A:2085:U:O2	30:A:2234:G:O6	2.38	0.41
30:A:2447:G:H2'	30:A:2500:U:OP2	2.21	0.41
17:N:28:LEU:C	17:N:28:LEU:HD23	2.41	0.41
30:A:2364:C:H2'	30:A:2365:G:O4'	2.21	0.41
30:A:2489:U:H2'	30:A:2490:G:O4'	2.20	0.41
19:P:96:LEU:HD12	19:P:96:LEU:N	2.35	0.41
30:A:45:G:H5''	30:A:46:G:H5'	2.02	0.41
30:A:458:G:O2'	30:A:459:U:O5'	2.38	0.41
30:A:512:G:OP1	30:A:1234:U:O2'	2.22	0.41
30:A:1164:C:O2'	30:A:1224:U:O4	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1425:G:N2	30:A:1574:C:N3	2.69	0.41
30:A:1664:A:H61	30:A:1996:C:H42	1.69	0.41
30:A:2125:G:N2	30:A:2170:A:O3'	2.50	0.41
30:A:2357:G:N1	30:A:2360:G:OP2	2.48	0.41
10:F:46:LYS:O	10:F:49:LEU:HD22	2.20	0.41
30:A:242:G:H4'	30:A:243:U:O5'	2.20	0.41
30:A:2028:U:H3	30:A:2033:A:H62	1.69	0.41
9:E:162:ARG:NE	30:A:322:A:OP1	2.41	0.41
13:J:100:VAL:HG23	13:J:101:ILE:N	2.36	0.41
17:N:28:LEU:HD23	17:N:28:LEU:O	2.21	0.41
19:P:63:ILE:HG23	19:P:63:ILE:O	2.20	0.41
30:A:725:G:O2'	30:A:726:G:C4'	2.67	0.41
5:4:2:LYS:NZ	5:4:32:LYS:O	2.49	0.41
15:L:127:VAL:HG21	15:L:132:ARG:N	2.35	0.41
17:N:31:HIS:O	17:N:32:GLU:HB2	2.20	0.41
18:O:72:ALA:O	18:O:76:LYS:HG2	2.21	0.41
25:V:72:VAL:HG22	25:V:73:LYS:N	2.36	0.41
30:A:196:A:H61	30:A:831:G:H21	1.69	0.41
30:A:499:U:H2'	30:A:500:G:O4'	2.21	0.41
30:A:1096:A:H3'	30:A:1097:U:H5''	2.03	0.41
30:A:1197:G:N2	30:A:1249:U:O2'	2.52	0.41
30:A:2585:U:O2	30:A:2585:U:O4'	2.38	0.41
10:F:39:VAL:HG13	10:F:40:GLY:N	2.36	0.41
11:G:157:LYS:NZ	30:A:2659:G:OP2	2.50	0.41
30:A:306:U:H2'	30:A:307:G:O4'	2.21	0.41
30:A:1215:G:O6	30:A:1235:G:C2	2.74	0.41
7:C:162:GLN:OE1	7:C:162:GLN:N	2.53	0.40
30:A:1394:U:H2'	30:A:1395:A:C4	2.56	0.40
30:A:2106:U:N3	30:A:2107:G:N7	2.69	0.40
1:O:30:ASP:OD1	1:O:31:LYS:N	2.54	0.40
20:Q:50:ARG:NH2	30:A:993:G:OP2	2.54	0.40
30:A:75:G:N3	30:A:75:G:H2'	2.36	0.40
30:A:285:G:C6	30:A:356:G:C5	3.09	0.40
30:A:1182:G:H2'	30:A:1183:U:O4'	2.22	0.40
30:A:1264:A:H4'	30:A:2615:U:H5'	2.03	0.40
30:A:1390:U:O4	30:A:1395:A:N7	2.54	0.40
30:A:2655:G:O2'	30:A:2656:U:P	2.78	0.40
8:D:130:GLN:NE2	30:A:2578:G:H21	2.19	0.40
27:X:2:ARG:NH1	30:A:1365:A:OP1	2.51	0.40
30:A:1196:C:C2	30:A:1197:G:C8	3.10	0.40
30:A:2553:G:H1'	30:A:2582:G:H21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:111:ILE:HD12	30:A:636:G:C2	2.57	0.40
17:N:70:THR:O	17:N:71:ARG:C	2.60	0.40
30:A:1601:G:H2'	30:A:1602:U:O4'	2.21	0.40
30:A:886:A:O4'	30:A:891:G:N1	2.55	0.40
30:A:2687:U:H2'	30:A:2688:G:O4'	2.21	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	
1	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
2	1	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
3	2	44/46 (96%)	44 (100%)	0	0	100	100
4	3	62/64 (97%)	60 (97%)	1 (2%)	1 (2%)	8	29
5	4	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	269/271 (99%)	258 (96%)	11 (4%)	0	100	100
8	D	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
9	E	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	25	55
10	F	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	G	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
12	H	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
13	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
14	K	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
15	L	141/143 (99%)	132 (94%)	9 (6%)	0	100	100
16	M	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
17	N	118/120 (98%)	109 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	O	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
19	P	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
20	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
21	R	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	13	40
22	S	109/110 (99%)	105 (96%)	4 (4%)	0	100	100
23	T	91/93 (98%)	88 (97%)	3 (3%)	0	100	100
24	U	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
25	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
26	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
27	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
28	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
29	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
31	y	15/17 (88%)	12 (80%)	3 (20%)	0	100	100
31	z	15/17 (88%)	15 (100%)	0	0	100	100
All	All	3197/3256 (98%)	3076 (96%)	118 (4%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	R	54	VAL
9	E	83	VAL
4	3	31	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	45 (96%)	2 (4%)	25	53
2	1	45/45 (100%)	44 (98%)	1 (2%)	47	68
3	2	38/38 (100%)	37 (97%)	1 (3%)	41	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	51/51 (100%)	49 (96%)	2 (4%)	27	56
5	4	34/34 (100%)	34 (100%)	0	100	100
7	C	216/216 (100%)	215 (100%)	1 (0%)	86	91
8	D	164/164 (100%)	164 (100%)	0	100	100
9	E	165/165 (100%)	162 (98%)	3 (2%)	54	74
10	F	148/148 (100%)	141 (95%)	7 (5%)	22	50
11	G	137/137 (100%)	135 (98%)	2 (2%)	60	78
12	H	114/114 (100%)	114 (100%)	0	100	100
13	J	116/116 (100%)	115 (99%)	1 (1%)	75	86
14	K	103/103 (100%)	102 (99%)	1 (1%)	73	85
15	L	102/102 (100%)	101 (99%)	1 (1%)	73	85
16	M	109/109 (100%)	108 (99%)	1 (1%)	75	86
17	N	100/100 (100%)	98 (98%)	2 (2%)	50	71
18	O	86/86 (100%)	85 (99%)	1 (1%)	67	82
19	P	99/99 (100%)	97 (98%)	2 (2%)	50	71
20	Q	89/89 (100%)	89 (100%)	0	100	100
21	R	84/84 (100%)	84 (100%)	0	100	100
22	S	94/93 (101%)	93 (99%)	1 (1%)	70	83
23	T	80/80 (100%)	79 (99%)	1 (1%)	65	80
24	U	83/83 (100%)	83 (100%)	0	100	100
25	V	78/78 (100%)	77 (99%)	1 (1%)	65	80
26	W	57/57 (100%)	57 (100%)	0	100	100
27	X	67/67 (100%)	67 (100%)	0	100	100
28	Y	55/55 (100%)	54 (98%)	1 (2%)	54	74
29	Z	48/48 (100%)	47 (98%)	1 (2%)	48	69
31	y	17/17 (100%)	16 (94%)	1 (6%)	16	42
31	z	17/17 (100%)	17 (100%)	0	100	100
All	All	2643/2642 (100%)	2609 (99%)	34 (1%)	64	80

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	5	ASN

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Mol	Chain	Res	Type
1	0	47	TYR
2	1	36	LYS
3	2	1	MET
4	3	54	LEU
4	3	61	LEU
7	C	212	TRP
9	E	19	PHE
9	E	94	GLN
9	E	112	LEU
10	F	6	TYR
10	F	7	TYR
10	F	11	VAL
10	F	25	MET
10	F	29	ARG
10	F	37	MET
10	F	141	ASP
11	G	36	LEU
11	G	98	LYS
13	J	96	ARG
14	K	100	PHE
15	L	27	LEU
16	M	59	ARG
17	N	20	MET
17	N	73	ASN
18	O	35	ILE
19	P	23	ASP
19	P	113	LEU
22	S	77	ASP
23	T	72	GLN
25	V	42	LEU
28	Y	2	LYS
29	Z	29	ARG
31	y	7	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	3	GLN
2	1	44	GLN
7	C	85	ASN
7	C	250	GLN
9	E	41	GLN

Continued on next page...

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Mol	Chain	Res	Type
9	E	163	ASN
11	G	47	ASN
17	N	18	GLN
20	Q	55	GLN
22	S	60	HIS
23	T	70	HIS
23	T	72	GLN
25	V	49	ASN
26	W	72	ASN
31	z	2	ASN
31	y	3	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	A	2897/2904 (99%)	462 (15%)	18 (0%)
6	B	119/120 (99%)	14 (11%)	2 (1%)
All	All	3016/3024 (99%)	476 (15%)	20 (0%)

All (476) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	4	C
6	B	9	G
6	B	12	C
6	B	13	G
6	B	24	G
6	B	35	C
6	B	42	C
6	B	44	G
6	B	45	A
6	B	53	A
6	B	67	G
6	B	89	U
6	B	90	C
6	B	109	A
30	A	10	A
30	A	27	G
30	A	28	A
30	A	34	U
30	A	35	G

Continued on next page...

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Mol	Chain	Res	Type
30	A	46	G
30	A	51	G
30	A	60	G
30	A	63	A
30	A	71	A
30	A	74	A
30	A	75	G
30	A	118	A
30	A	119	A
30	A	120	U
30	A	126	A
30	A	135	U
30	A	136	G
30	A	139	U
30	A	141	G
30	A	142	A
30	A	162	U
30	A	163	C
30	A	181	A
30	A	196	A
30	A	199	A
30	A	215	G
30	A	216	A
30	A	221	A
30	A	222	A
30	A	225	C
30	A	228	C
30	A	233	A
30	A	242	G
30	A	243	U
30	A	248	G
30	A	255	A
30	A	266	G
30	A	267	C
30	A	272	A
30	A	277	G
30	A	278	A
30	A	294	A
30	A	307	G
30	A	310	A
30	A	322	A
30	A	323	C

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Mol	Chain	Res	Type
30	A	324	A
30	A	329	G
30	A	330	A
30	A	345	A
30	A	356	G
30	A	362	A
30	A	371	A
30	A	372	G
30	A	373	U
30	A	386	G
30	A	387	U
30	A	404	A
30	A	406	G
30	A	411	G
30	A	417	C
30	A	424	G
30	A	429	A
30	A	435	C
30	A	446	G
30	A	456	C
30	A	457	A
30	A	458	G
30	A	459	U
30	A	465	G
30	A	473	G
30	A	480	A
30	A	481	G
30	A	491	G
30	A	505	A
30	A	509	C
30	A	528	A
30	A	530	G
30	A	531	C
30	A	532	A
30	A	533	G
30	A	543	G
30	A	544	C
30	A	545	U
30	A	547	A
30	A	550	C
30	A	563	A
30	A	573	U

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Mol	Chain	Res	Type
30	A	575	A
30	A	588	U
30	A	603	A
30	A	614	A
30	A	627	A
30	A	637	A
30	A	645	C
30	A	646	U
30	A	647	G
30	A	652	U
30	A	654	A
30	A	669	G
30	A	670	A
30	A	675	A
30	A	683	U
30	A	686	U
30	A	687	C
30	A	695	G
30	A	717	C
30	A	725	G
30	A	726	G
30	A	730	A
30	A	740	C
30	A	747	U
30	A	748	G
30	A	752	A
30	A	763	G
30	A	764	A
30	A	775	G
30	A	776	G
30	A	782	A
30	A	784	G
30	A	785	G
30	A	789	A
30	A	805	G
30	A	812	C
30	A	819	A
30	A	827	U
30	A	828	U
30	A	845	A
30	A	846	U
30	A	847	U

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Mol	Chain	Res	Type
30	A	856	G
30	A	857	G
30	A	869	G
30	A	877	A
30	A	878	A
30	A	885	C
30	A	891	G
30	A	896	A
30	A	897	C
30	A	907	G
30	A	910	A
30	A	941	A
30	A	946	C
30	A	953	G
30	A	961	C
30	A	973	A
30	A	974	G
30	A	980	A
30	A	983	A
30	A	984	A
30	A	985	C
30	A	995	C
30	A	996	A
30	A	1010	A
30	A	1011	G
30	A	1012	U
30	A	1013	C
30	A	1021	A
30	A	1022	G
30	A	1023	U
30	A	1026	G
30	A	1033	U
30	A	1040	A
30	A	1045	C
30	A	1046	A
30	A	1047	G
30	A	1053	C
30	A	1054	A
30	A	1057	A
30	A	1059	G
30	A	1060	U
30	A	1061	U

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Mol	Chain	Res	Type
30	A	1062	G
30	A	1065	U
30	A	1066	U
30	A	1068	G
30	A	1070	A
30	A	1073	A
30	A	1076	C
30	A	1079	C
30	A	1082	U
30	A	1083	U
30	A	1084	A
30	A	1088	A
30	A	1089	A
30	A	1097	U
30	A	1101	U
30	A	1104	C
30	A	1111	A
30	A	1119	U
30	A	1132	U
30	A	1135	C
30	A	1143	A
30	A	1157	G
30	A	1169	A
30	A	1171	G
30	A	1174	U
30	A	1175	A
30	A	1176	U
30	A	1180	U
30	A	1206	G
30	A	1212	G
30	A	1225	G
30	A	1236	G
30	A	1250	G
30	A	1253	A
30	A	1256	G
30	A	1271	G
30	A	1272	A
30	A	1273	U
30	A	1288	G
30	A	1300	G
30	A	1301	A
30	A	1306	C

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Mol	Chain	Res	Type
30	A	1314	C
30	A	1329	U
30	A	1341	G
30	A	1345	C
30	A	1359	A
30	A	1365	A
30	A	1378	A
30	A	1379	U
30	A	1383	A
30	A	1416	G
30	A	1419	A
30	A	1420	A
30	A	1421	G
30	A	1428	C
30	A	1437	C
30	A	1454	C
30	A	1458	U
30	A	1461	C
30	A	1475	G
30	A	1482	G
30	A	1490	A
30	A	1491	G
30	A	1508	A
30	A	1515	A
30	A	1524	G
30	A	1535	A
30	A	1536	C
30	A	1537	G
30	A	1559	U
30	A	1560	G
30	A	1563	U
30	A	1565	C
30	A	1566	A
30	A	1569	A
30	A	1578	U
30	A	1585	C
30	A	1608	A
30	A	1622	G
30	A	1634	A
30	A	1646	C
30	A	1647	U
30	A	1648	U

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Mol	Chain	Res	Type
30	A	1654	A
30	A	1664	A
30	A	1674	G
30	A	1699	G
30	A	1715	G
30	A	1729	U
30	A	1730	C
30	A	1731	G
30	A	1732	C
30	A	1733	G
30	A	1735	A
30	A	1737	G
30	A	1738	G
30	A	1744	A
30	A	1756	G
30	A	1764	C
30	A	1773	A
30	A	1776	G
30	A	1781	U
30	A	1800	C
30	A	1801	A
30	A	1808	A
30	A	1816	C
30	A	1819	A
30	A	1820	U
30	A	1829	A
30	A	1833	C
30	A	1835	G
30	A	1866	A
30	A	1871	A
30	A	1901	A
30	A	1906	G
30	A	1913	A
30	A	1917	U
30	A	1927	A
30	A	1929	G
30	A	1930	G
30	A	1937	A
30	A	1940	U
30	A	1941	C
30	A	1955	U
30	A	1963	U

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Mol	Chain	Res	Type
30	A	1967	C
30	A	1970	A
30	A	1971	U
30	A	1972	G
30	A	1991	U
30	A	1992	G
30	A	1997	C
30	A	2022	U
30	A	2023	C
30	A	2030	A
30	A	2031	A
30	A	2033	A
30	A	2043	C
30	A	2052	A
30	A	2055	C
30	A	2056	G
30	A	2059	A
30	A	2060	A
30	A	2061	G
30	A	2062	A
30	A	2069	G
30	A	2072	C
30	A	2093	G
30	A	2096	C
30	A	2100	G
30	A	2104	C
30	A	2110	G
30	A	2111	U
30	A	2112	G
30	A	2113	U
30	A	2118	U
30	A	2119	A
30	A	2120	G
30	A	2124	G
30	A	2125	G
30	A	2127	G
30	A	2131	U
30	A	2132	U
30	A	2133	G
30	A	2136	G
30	A	2137	U
30	A	2139	U

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Mol	Chain	Res	Type
30	A	2145	C
30	A	2162	G
30	A	2164	C
30	A	2172	U
30	A	2173	A
30	A	2184	A
30	A	2189	U
30	A	2199	A
30	A	2204	G
30	A	2211	A
30	A	2213	U
30	A	2225	A
30	A	2226	C
30	A	2238	G
30	A	2239	G
30	A	2250	G
30	A	2251	G
30	A	2266	A
30	A	2279	G
30	A	2283	C
30	A	2286	G
30	A	2287	A
30	A	2297	A
30	A	2305	U
30	A	2309	A
30	A	2325	G
30	A	2327	A
30	A	2333	A
30	A	2334	U
30	A	2335	A
30	A	2336	A
30	A	2345	G
30	A	2350	C
30	A	2357	G
30	A	2383	G
30	A	2385	C
30	A	2396	G
30	A	2402	U
30	A	2407	A
30	A	2422	C
30	A	2424	C
30	A	2425	A

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Mol	Chain	Res	Type
30	A	2428	G
30	A	2429	G
30	A	2430	A
30	A	2434	A
30	A	2435	A
30	A	2441	U
30	A	2445	G
30	A	2447	G
30	A	2448	A
30	A	2475	C
30	A	2476	A
30	A	2491	U
30	A	2492	U
30	A	2494	G
30	A	2497	A
30	A	2498	C
30	A	2502	G
30	A	2503	A
30	A	2504	U
30	A	2505	G
30	A	2513	A
30	A	2518	A
30	A	2520	C
30	A	2529	G
30	A	2530	A
30	A	2535	G
30	A	2547	A
30	A	2554	U
30	A	2564	A
30	A	2566	A
30	A	2567	G
30	A	2573	C
30	A	2582	G
30	A	2597	G
30	A	2602	A
30	A	2609	U
30	A	2610	C
30	A	2613	U
30	A	2614	A
30	A	2629	U
30	A	2655	G
30	A	2656	U

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Mol	Chain	Res	Type
30	A	2661	G
30	A	2682	A
30	A	2689	U
30	A	2690	U
30	A	2714	G
30	A	2718	G
30	A	2722	G
30	A	2726	A
30	A	2733	A
30	A	2739	U
30	A	2744	G
30	A	2748	A
30	A	2762	C
30	A	2764	A
30	A	2765	A
30	A	2778	A
30	A	2779	U
30	A	2780	G
30	A	2791	G
30	A	2799	A
30	A	2800	A
30	A	2809	A
30	A	2818	U
30	A	2820	A
30	A	2833	U
30	A	2849	U
30	A	2867	G
30	A	2868	A
30	A	2871	U
30	A	2872	A
30	A	2880	C
30	A	2883	A
30	A	2891	U
30	A	2894	G
30	A	2901	C
30	A	2902	C
30	A	2903	U

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	B	52	A

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Mol	Chain	Res	Type
6	B	66	A
30	A	227	A
30	A	242	G
30	A	372	G
30	A	458	G
30	A	549	G
30	A	644	A
30	A	784	G
30	A	1020	A
30	A	1022	G
30	A	1224	U
30	A	1358	G
30	A	1378	A
30	A	1663	G
30	A	1940	U
30	A	2058	A
30	A	2326	C
30	A	2655	G
30	A	2808	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

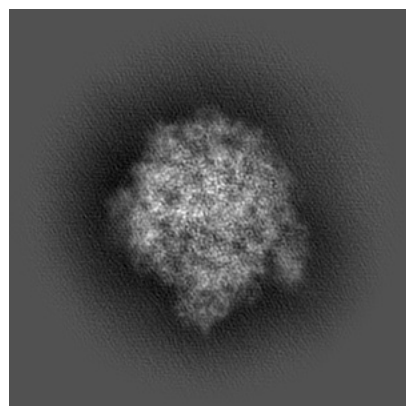
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51978. These allow visual inspection of the internal detail of the map and identification of artifacts.

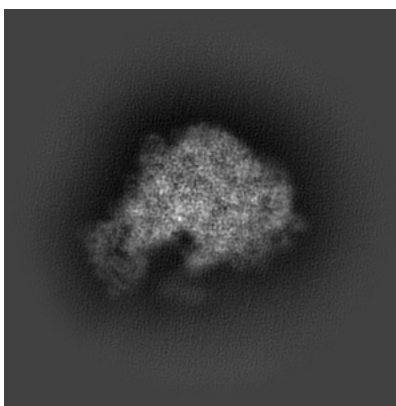
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

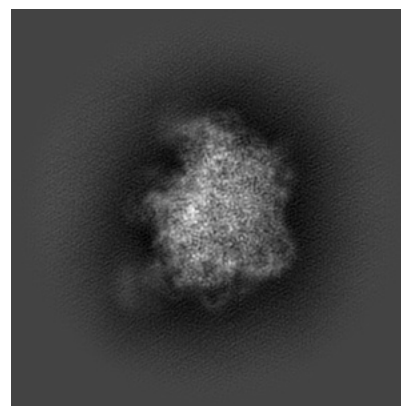
6.1.1 Primary map



X

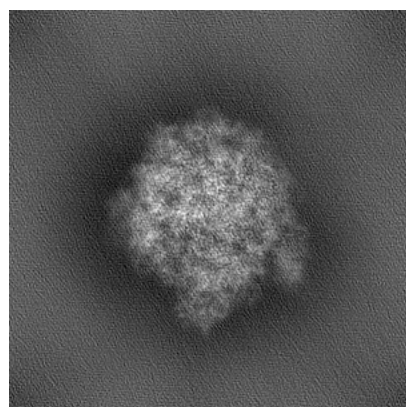


Y

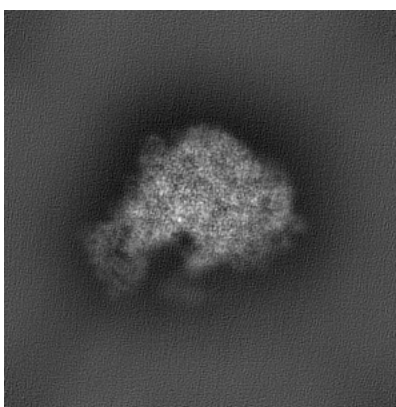


Z

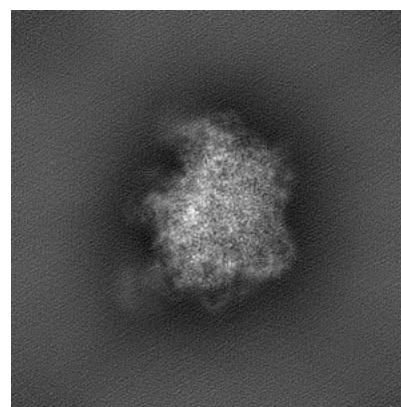
6.1.2 Raw map



X



Y

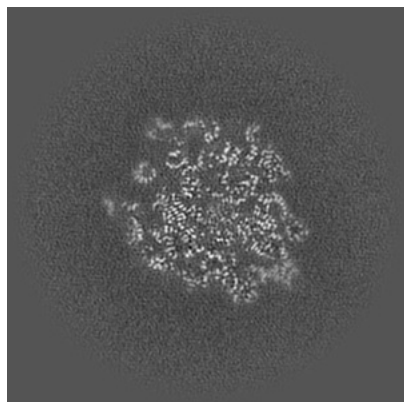


Z

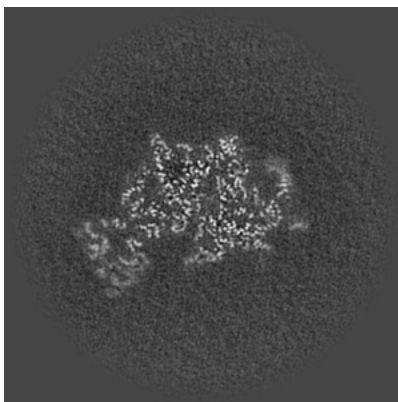
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

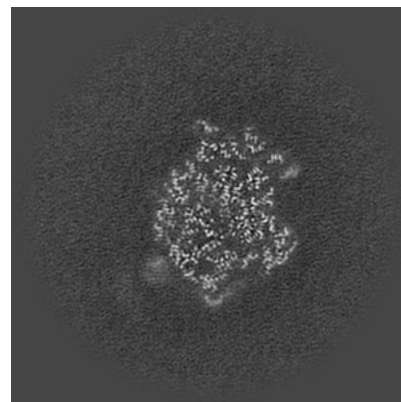
6.2.1 Primary map



X Index: 150

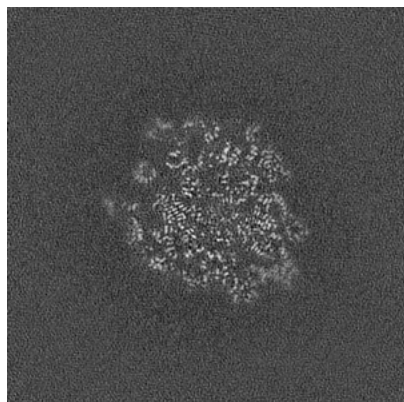


Y Index: 150

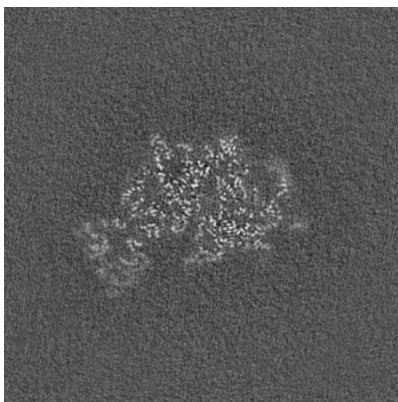


Z Index: 150

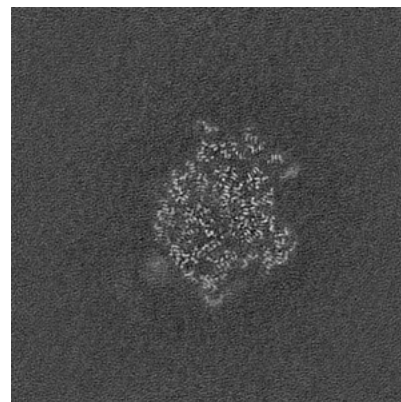
6.2.2 Raw map



X Index: 150



Y Index: 150

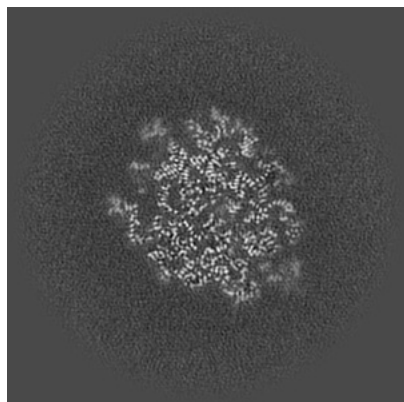


Z Index: 150

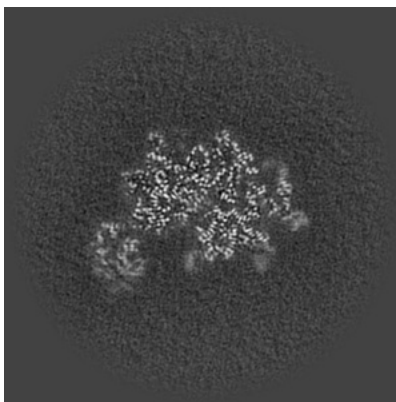
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

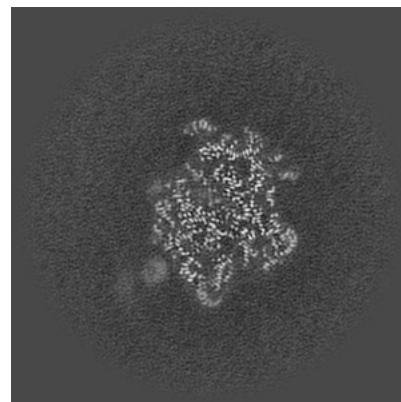
6.3.1 Primary map



X Index: 145

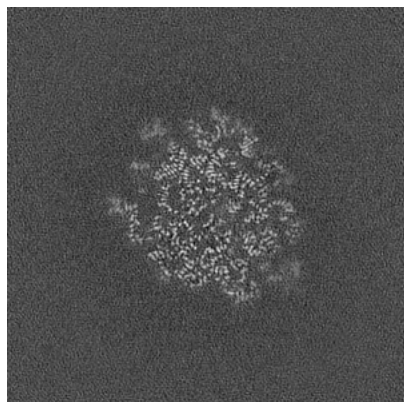


Y Index: 155

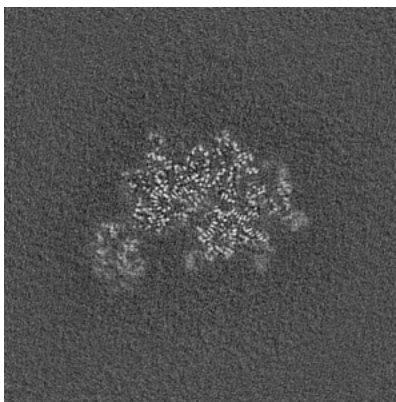


Z Index: 147

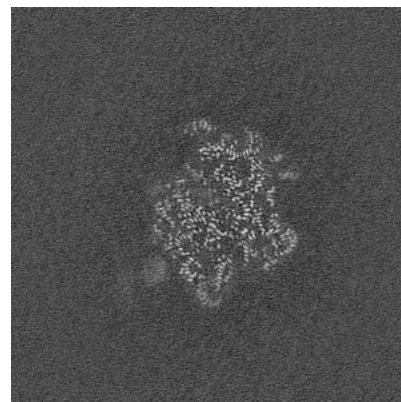
6.3.2 Raw map



X Index: 145



Y Index: 155

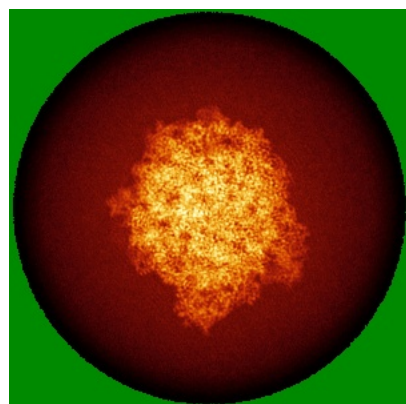


Z Index: 147

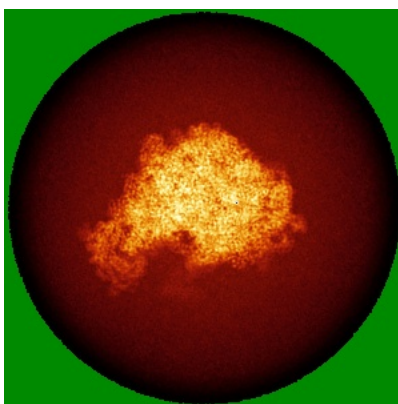
The images above show the largest variance slices of the map in three orthogonal directions.

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

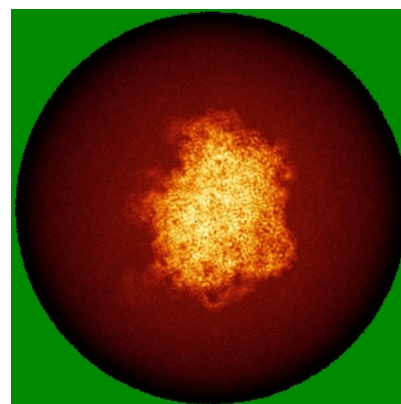
6.4.1 Primary map



X

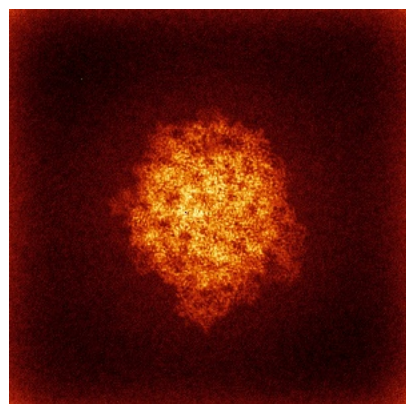


Y

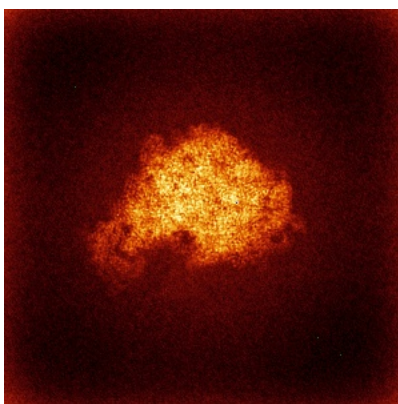


Z

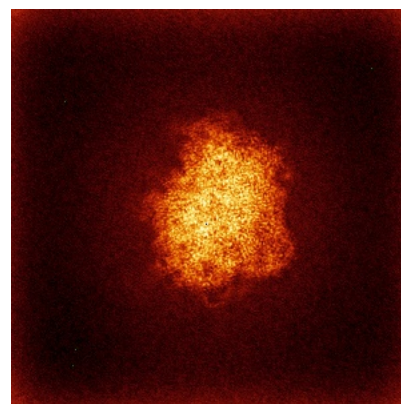
6.4.2 Raw map



X



Y



Z

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

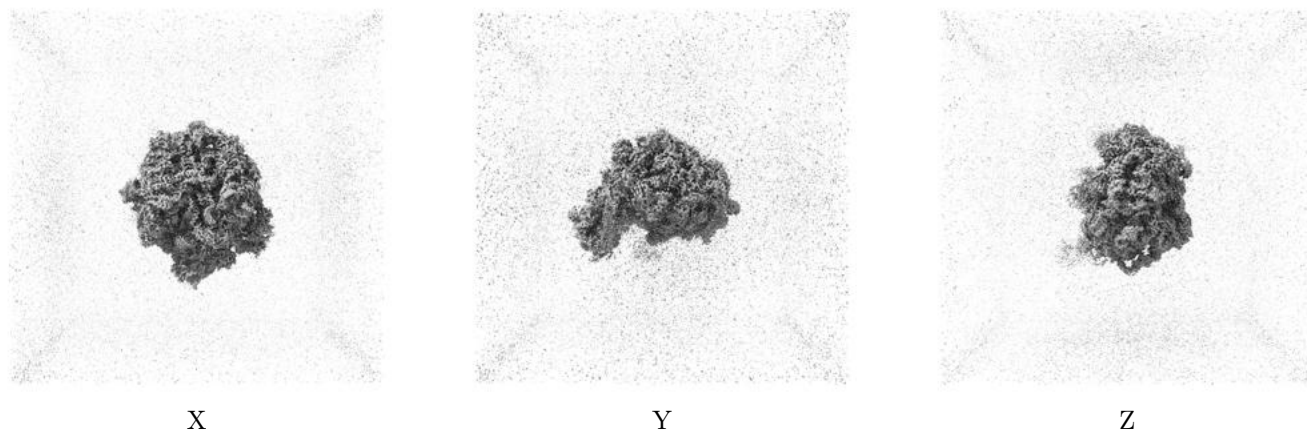
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

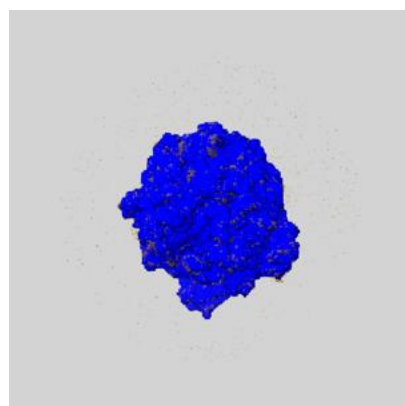
6.6 Mask visualisation [i](#)

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

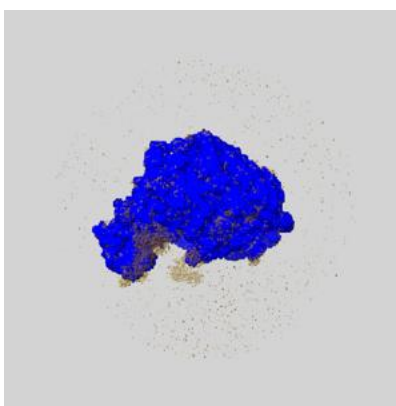
A mask typically either:

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

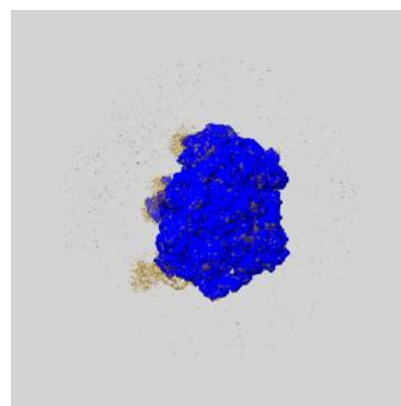
6.6.1 emd_51978_msk_1.map [i](#)



X



Y

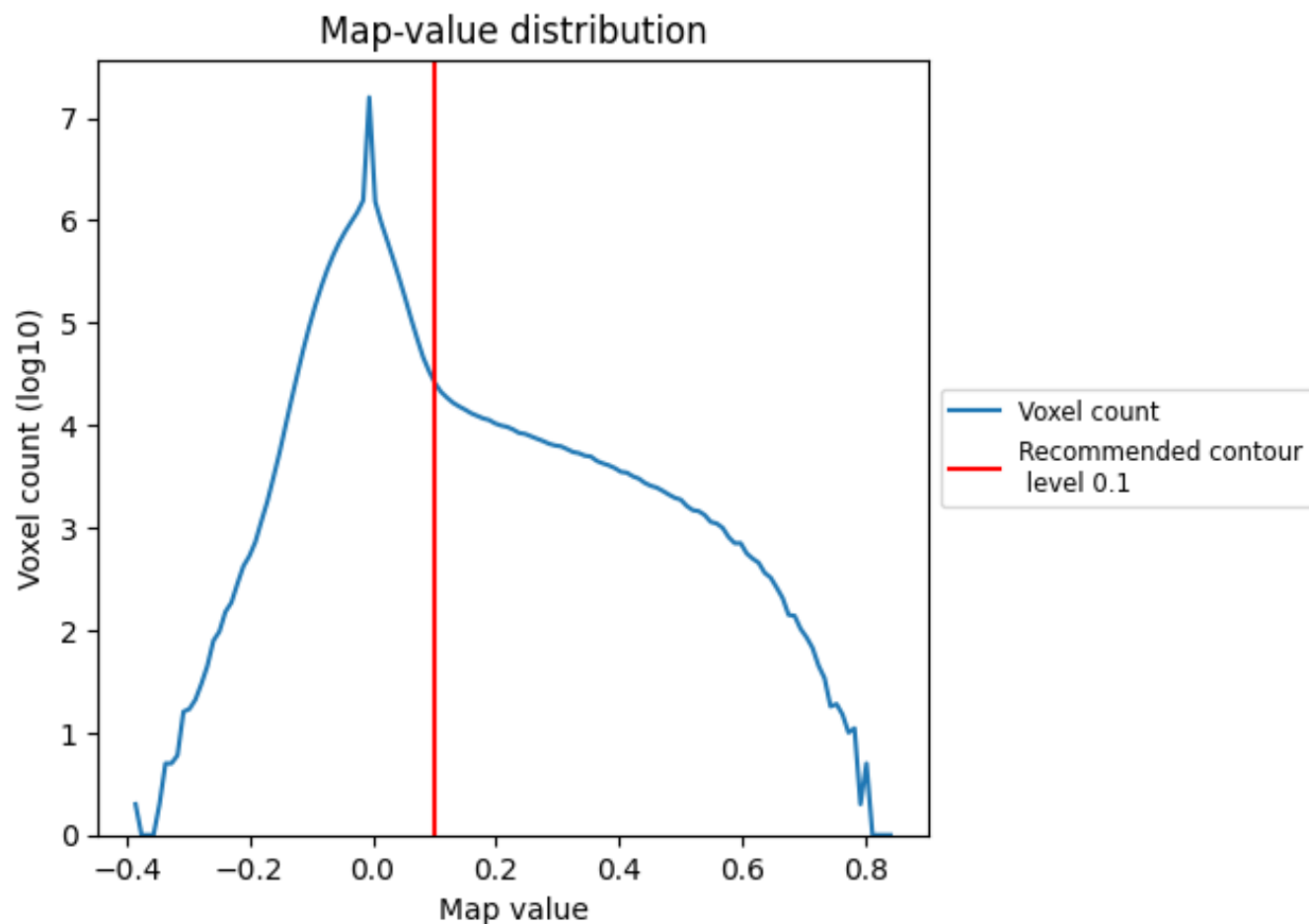


Z

7 Map analysis [i](#)

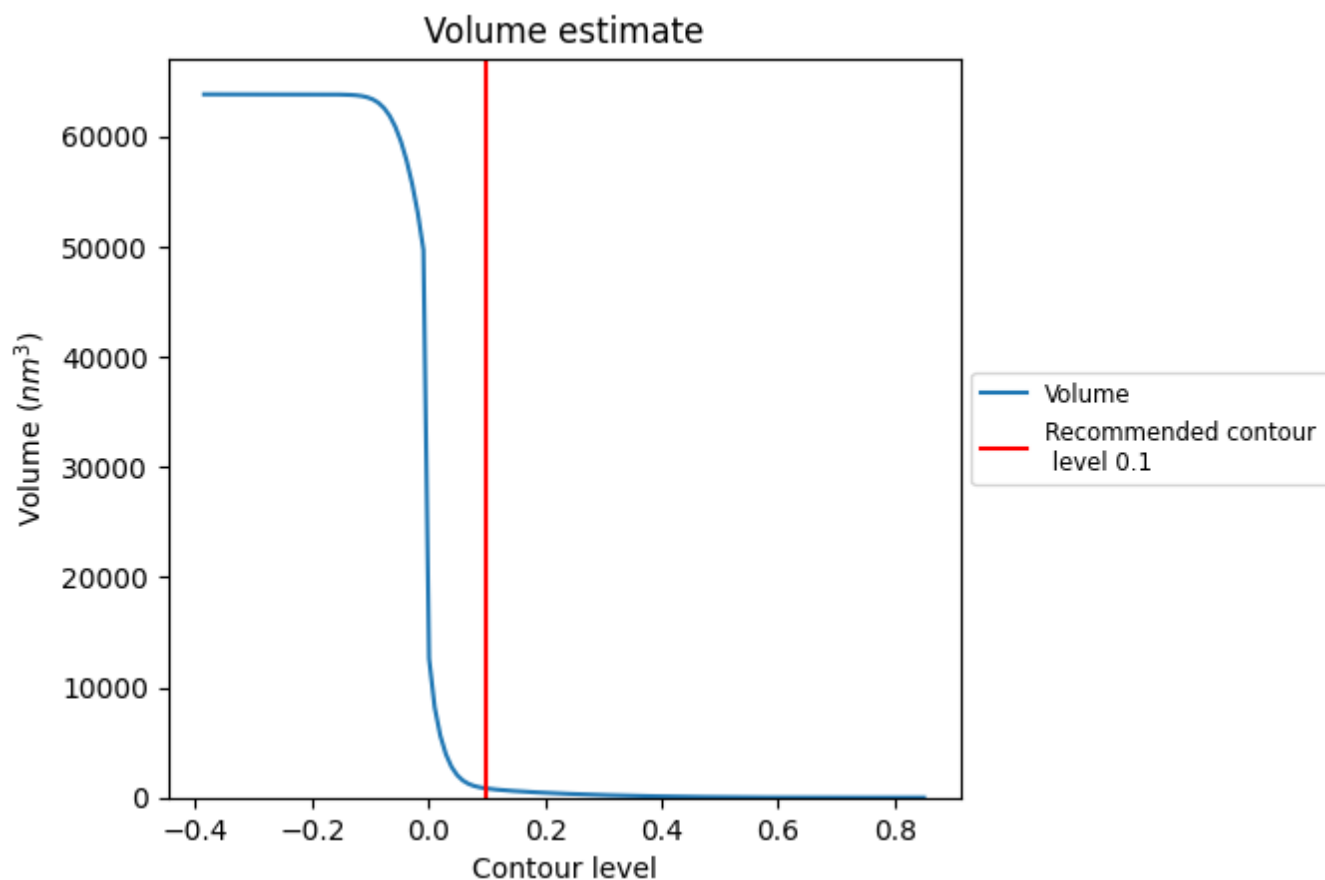
This section contains the results of statistical analysis of the map.

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.

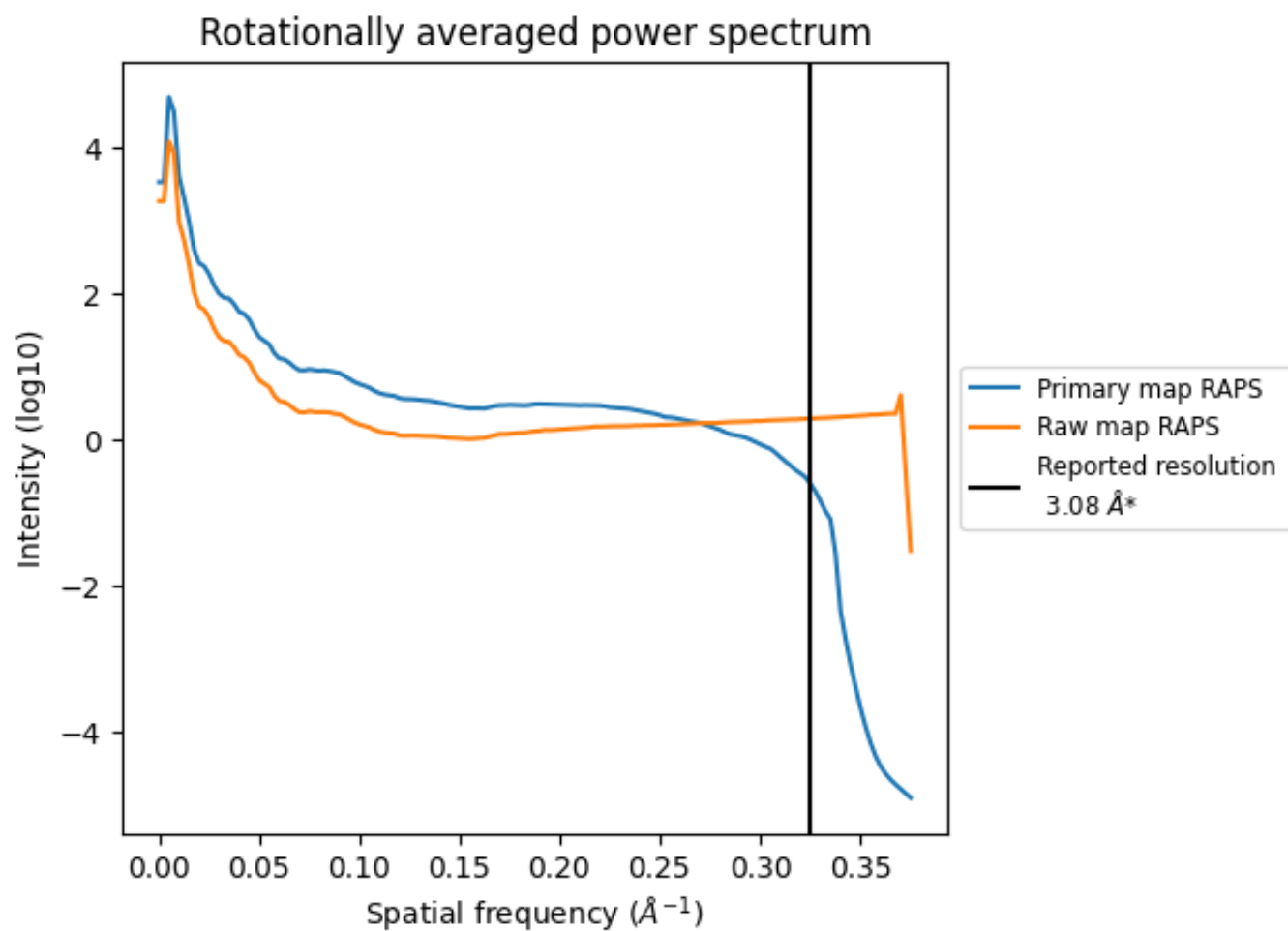
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm^3 ; this corresponds to an approximate mass of 744 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 ⓘ

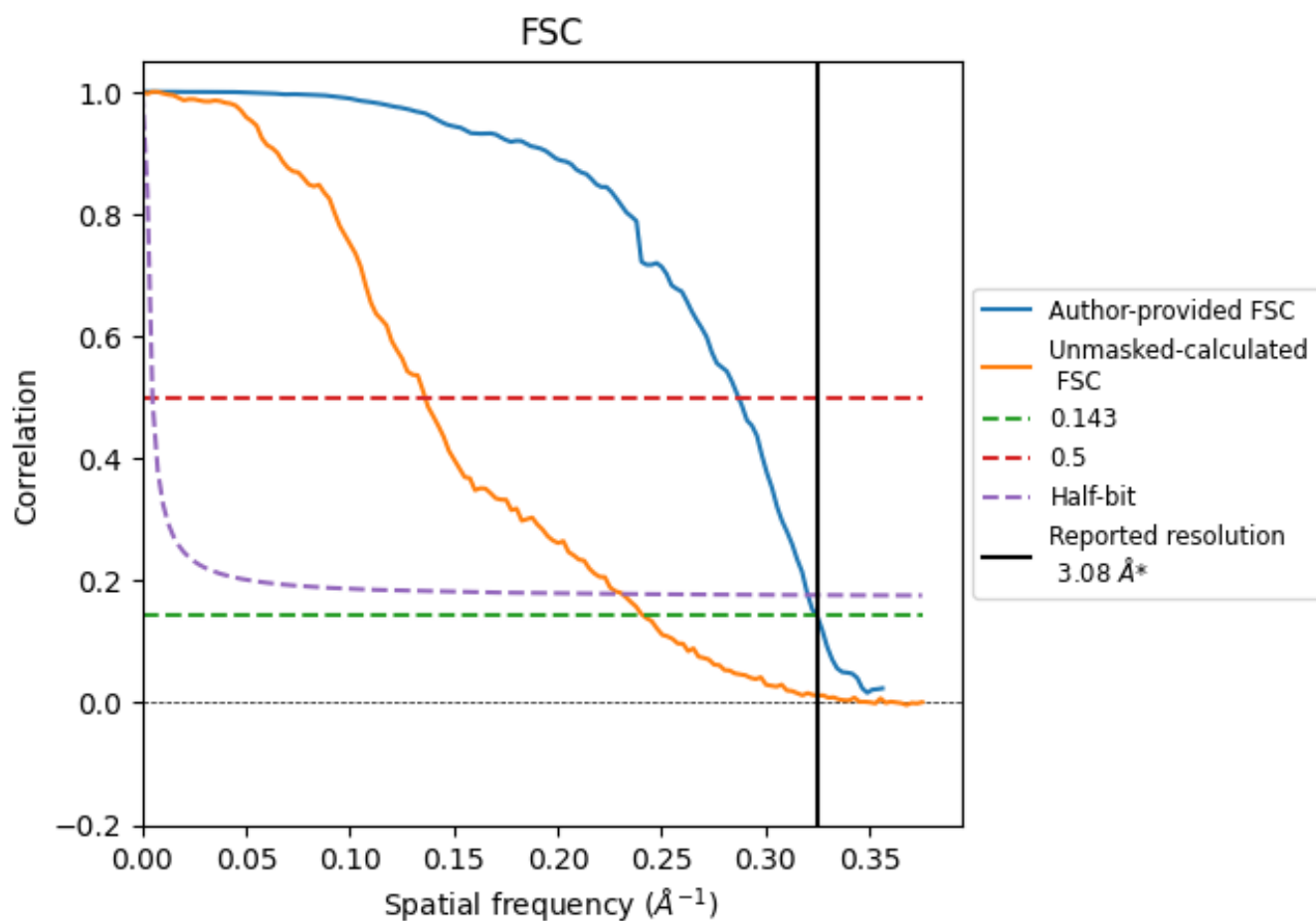


*Reported resolution corresponds to spatial frequency of 0.325 \AA^{-1}

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 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

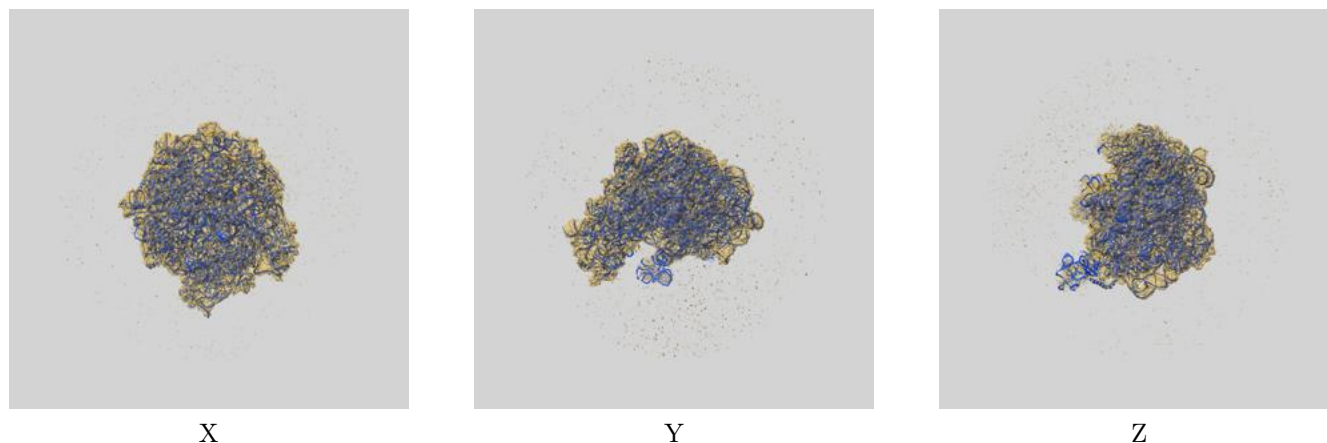
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.48	3.12
Unmasked-calculated*	4.15	7.34	4.33

*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 4.15 differs from the reported value 3.08 by more than 10 %

9 Map-model fit [i](#)

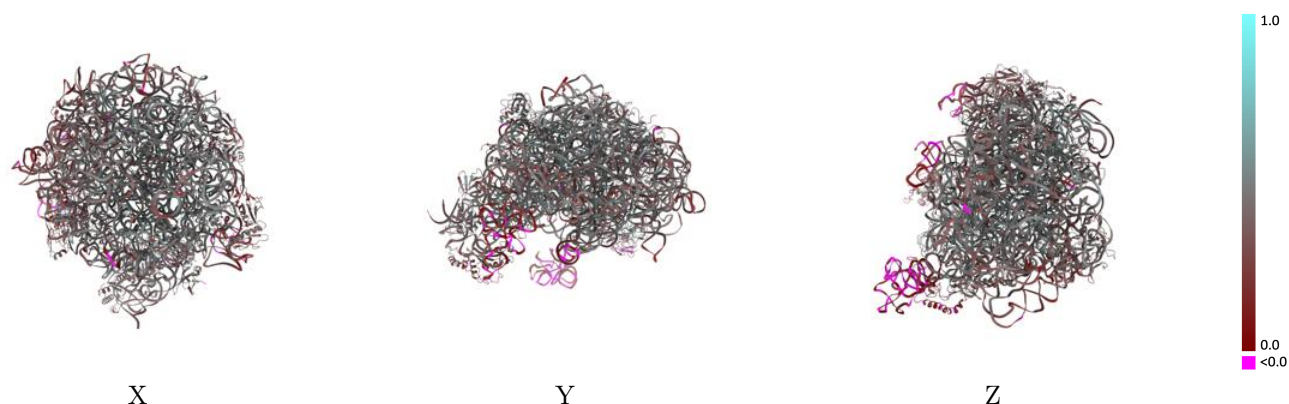
This section contains information regarding the fit between EMDB map EMD-51978 and PDB model 9HA6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



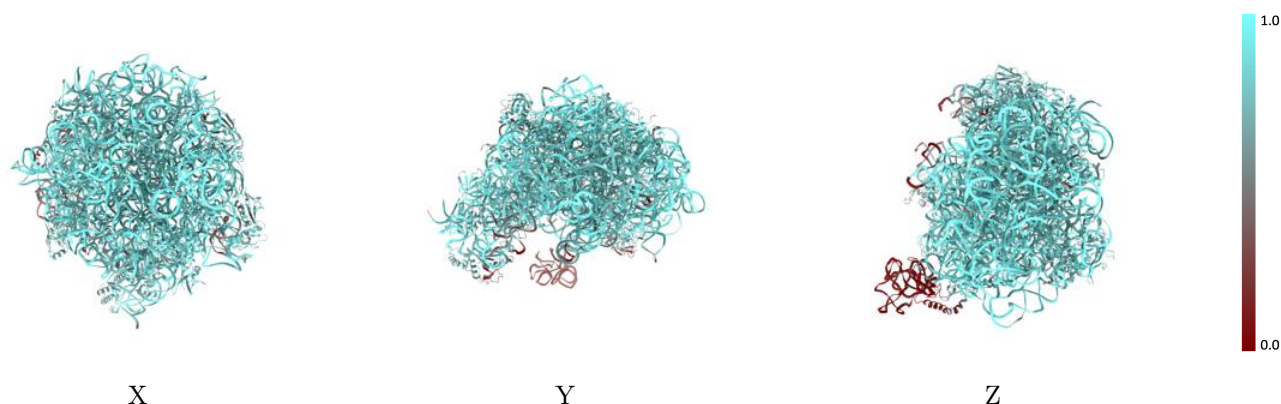
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



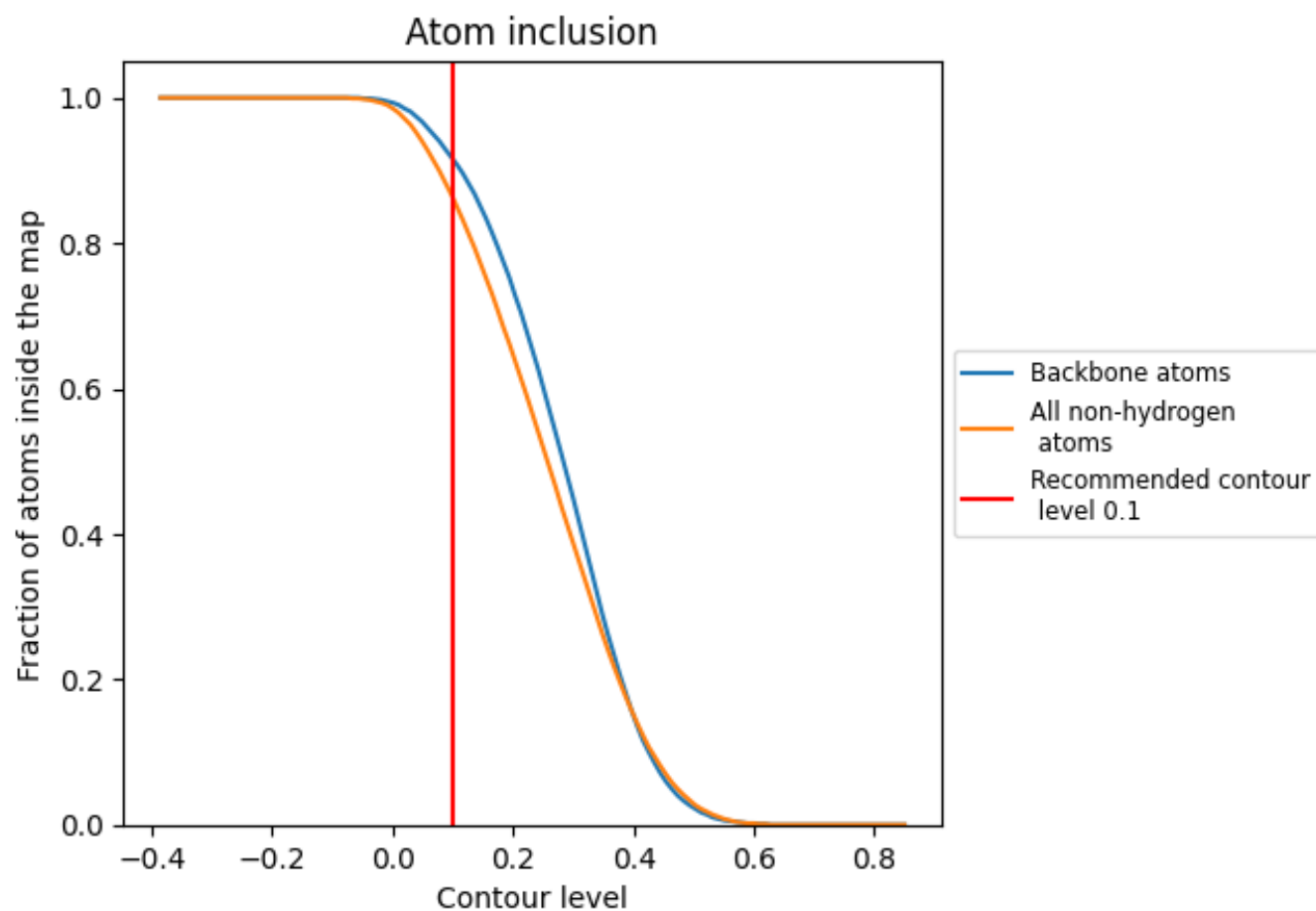
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.4120
0	 0.8670	 0.4750
1	 0.6680	 0.4040
2	 0.8900	 0.4910
3	 0.8530	 0.4570
4	 0.7840	 0.4130
A	 0.8950	 0.4150
B	 0.9310	 0.4110
C	 0.8560	 0.4680
D	 0.8220	 0.4430
E	 0.7800	 0.3860
F	 0.6700	 0.2910
G	 0.7310	 0.3400
H	 0.2230	 0.1780
J	 0.8640	 0.4700
K	 0.7340	 0.3650
L	 0.8030	 0.4030
M	 0.8370	 0.4500
N	 0.8620	 0.4520
O	 0.7970	 0.3850
P	 0.7340	 0.3880
Q	 0.8810	 0.4770
R	 0.8180	 0.4260
S	 0.8460	 0.4630
T	 0.8100	 0.4360
U	 0.7900	 0.3910
V	 0.8280	 0.4170
W	 0.8610	 0.4820
X	 0.8550	 0.4540
Y	 0.7470	 0.3460
Z	 0.8120	 0.4540
y	 0.4100	 0.2240
z	 0.4460	 0.3410

