



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:37 PM UTC

PDB ID : 7AS8 / pdb_00007as8
EMDB ID : EMD-11889
Title : Bacillus subtilis ribosome quality control complex state B. Ribosomal 50S subunit with P-tRNA, RqcH, and RqcP/YabO
Authors : Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on : 2020-10-27
Resolution : 2.90 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:

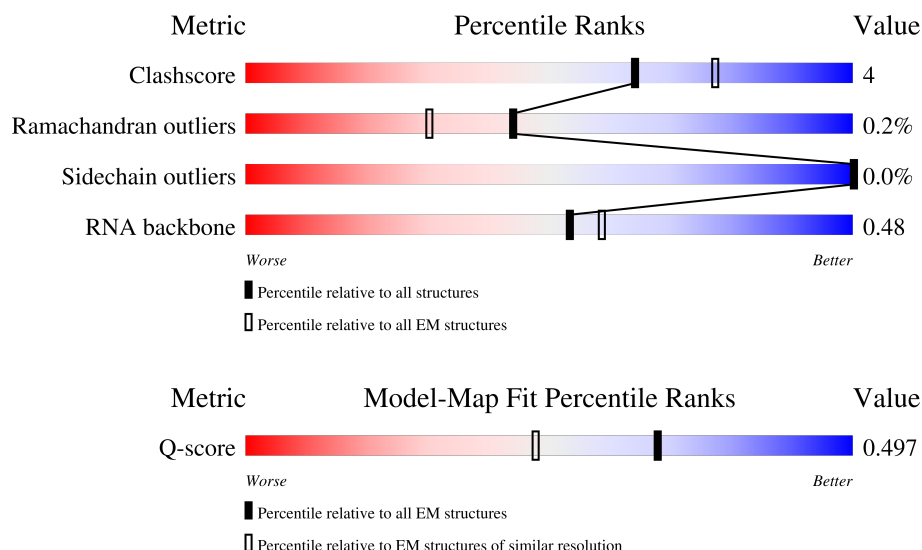
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	13054 (2.40 - 3.40)

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	597	27% 80% 10% 10%
2	1	86	8% 67% 29% .
3	2	76	. 55% 24% 17% .

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Mol	Chain	Length	Quality of chain
4	A	2926	
5	B	119	
6	E	277	
7	F	209	
8	G	207	
9	H	179	
10	I	179	
11	K	141	
12	L	166	
13	N	145	
14	O	122	
15	P	146	
16	Q	144	
17	R	120	
18	S	120	
19	T	115	
20	U	119	
21	V	102	
22	W	113	
23	X	95	
24	Y	103	
25	a	94	
26	b	62	
27	c	66	
28	d	59	

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Mol	Chain	Length	Quality of chain
29	f	59	71% 19% 10%
30	g	49	86% 12%
31	h	44	84% 16%
32	i	66	82% 15%
33	j	37	89% 11%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 93801 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 Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	536	Total	C	N	O	S	0	0
			3993	2520	713	750	10		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	571	GLY	-	expression tag	UNP O34693
0	572	SER	-	expression tag	UNP O34693
0	573	GLY	-	expression tag	UNP O34693
0	574	GLY	-	expression tag	UNP O34693
0	575	ASP	-	expression tag	UNP O34693
0	576	TYR	-	expression tag	UNP O34693
0	577	LYS	-	expression tag	UNP O34693
0	578	ASP	-	expression tag	UNP O34693
0	579	HIS	-	expression tag	UNP O34693
0	580	ASP	-	expression tag	UNP O34693
0	581	GLY	-	expression tag	UNP O34693
0	582	ASP	-	expression tag	UNP O34693
0	583	TYR	-	expression tag	UNP O34693
0	584	LYS	-	expression tag	UNP O34693
0	585	ASP	-	expression tag	UNP O34693
0	586	HIS	-	expression tag	UNP O34693
0	587	ASP	-	expression tag	UNP O34693
0	588	ILE	-	expression tag	UNP O34693
0	589	ASP	-	expression tag	UNP O34693
0	590	TYR	-	expression tag	UNP O34693
0	591	LYS	-	expression tag	UNP O34693
0	592	ASP	-	expression tag	UNP O34693
0	593	ASP	-	expression tag	UNP O34693
0	594	ASP	-	expression tag	UNP O34693
0	595	ASP	-	expression tag	UNP O34693
0	596	LYS	-	expression tag	UNP O34693
0	597	GLY	-	expression tag	UNP O34693

- Molecule 2 is a protein called Uncharacterized protein YabO.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	83	Total	C	N	O	S	0	0
			659	410	121	126	2		

- Molecule 3 is a RNA chain called tRNA-Ala-1-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	73	Total	C	N	O	P	0	0
			1563	695	283	512	73		

- Molecule 4 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2812	Total	C	N	O	P	0	0
			60389	26942	11160	19477	2810		

- Molecule 5 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	164	Total	C	N	O	S	0	0
			1284	813	228	236	7		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	132	Total	C	N	O	S	0	0
			974	612	172	184	6		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	113	Total	C	N	O	S	0	0
			886	559	152	174	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	115	Total	C	N	O	S	0	0
			944	600	185	158	1		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	100	Total	C	N	O	0	0
			781	498	138	145		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	a	81	Total	C	N	O	0	0
			624	387	122	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 30 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 31 is a protein called 50S ribosomal protein L34.

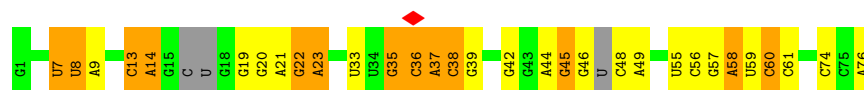
Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 32 is a protein called 50S ribosomal protein L35.

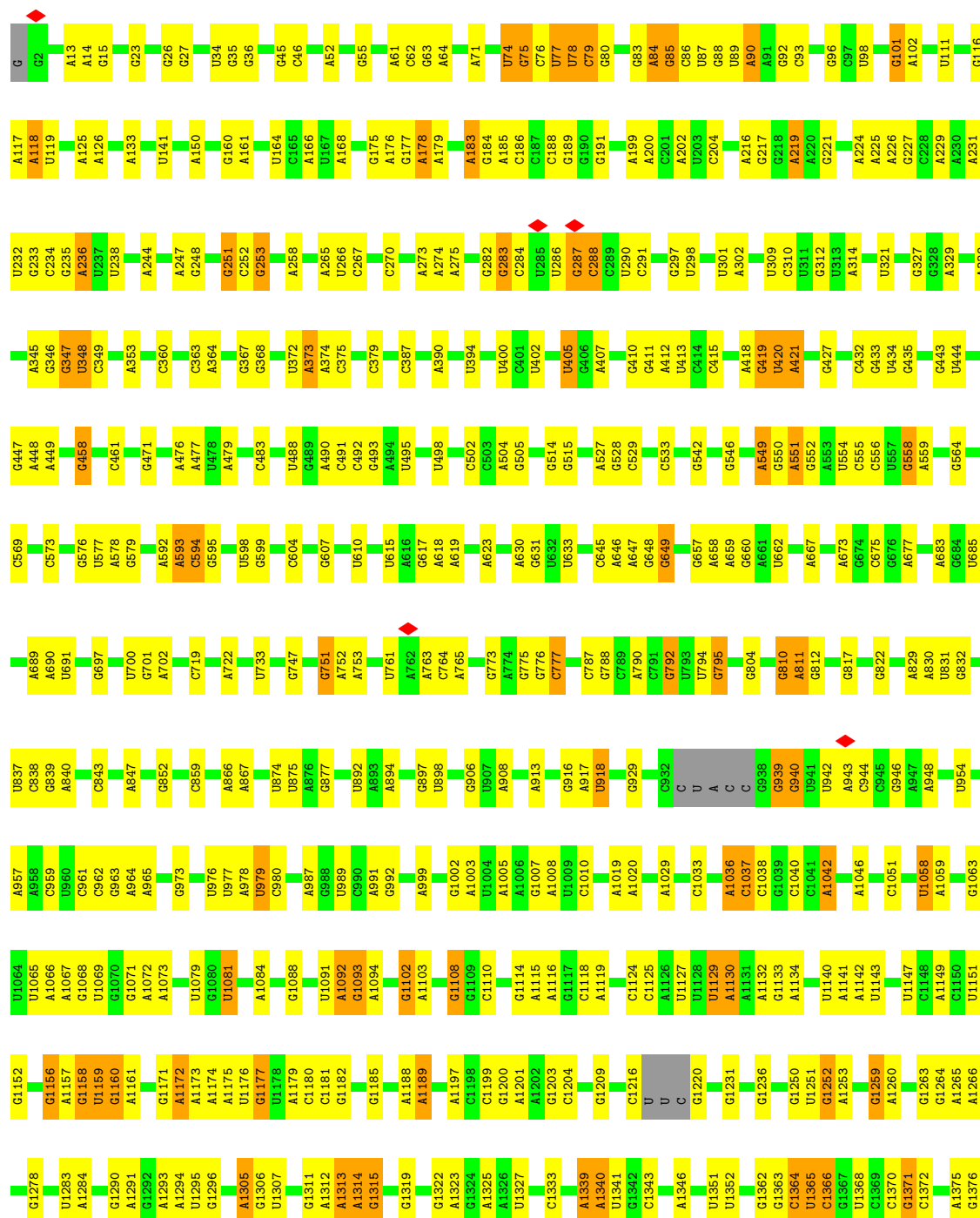
Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	37	Total	C	N	O	S	0	0
			296	186	60	45	5		



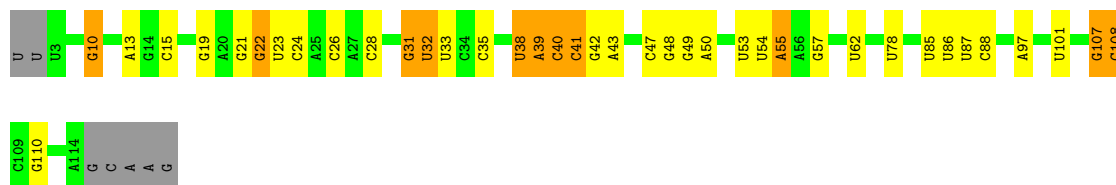
• Molecule 4: 23S rRNA



G2864	G2731	G2605	A2488	C2379	A2302	G	A	A2026	G1935	C1811	A1699	A	A1498	U1379
G2868	G2743	A2606	C2496	C2384	G2305	G	G	A2027	G1936	A1812	A1700	A	A1499	U1380
U2872	U2755	C2608	A2497	C2385	G2306	U	C	C2035	U1940	A1813	U1704	U	U1500	U1501
A2875	A2762	G2611	A2498	U2386	A2307	G	U	G2038	A	A1814	C1705	A	G1502	C1384
G2882	G2763	G2612	U2502	A2390	G2308	A	U	G2041	C	A1820	U1708	U	G1385	A
A2885	G2764	U2613	A2505	G2401	C2312	U	C	U2048	U	G1828	U1709	G	A1506	A1388
C2886	G2765	A2629	C2506	A2402	G2313	A	A	U2049	A	A1829	A1710	A	U1507	C1389
U2890	U2772	C2630	A2403	G2403	A2314	C	G	U2050	U	G1830	G1711	G	C1508	U1390
G2891	G2773	A2631	U2508	C2404	A2315	A	G	U2051	A	A1831	A1712	U	C1509	U1391
G2892	G2774	C2632	C2509	G2404	A2316	C	A	C2052	C	A1839	A1713	U	A1516	A1403
A2779	A2779	G2637	A2510	A2407	A2317	C	U	A2053	G	U1839	G1719	U	G1404	A1404
C2784	C2784	U2638	C2512	G2412	U2320	C	A	C2054	C	G1840	U1733	U	A1405	A1406
U2785	U2785	G2639	G2513	G2413	C2323	G	U	A2055	A1956	U1841	A1734	U	A1527	A1528
A2643	A2643	U2642	U2520	C2414	C2324	G	U	U2060	A1957	A1844	U1738	U	G1530	A1417
U2644	U2644	U2643	U2521	U2415	C2325	C	A	G2061	G1958	A1845	U1743	U	G1531	U1418
G2652	G2652	A2417	G2523	U2416	C2326	U	G	A2062	G1959	G1846	A1745	U	A1532	A1424
G2659	G2659	A2420	A2327	A2417	A2327	G	A	G2064	U1960	U1849	A1745	U	A1533	C1425
C2525	C2525	G2420	A2328	A2421	G2328	A	C	C2072	A1965	G1853	G1748	U	A1536	A1426
C2527	C2527	A2421	G2332	U2218	G2332	U	C	A2078	A1966	U1857	G1757	U	C1539	G1427
G2531	G2531	G2425	G2333	G2219	G2333	U	U	C2079	U1967	U1856	C1765	U	A1540	G1428
U2532	U2532	U2430	G2334	U2226	U2334	G	C	G2081	U1969	G1857	U1758	U	A1541	G1431
G2533	G2533	U2431	G2336	A2227	G2336	G	G	U2080	U1970	G1864	U1759	U	A1542	A1434
G2534	G2534	U2432	G2337	A2228	G2337	A	G	U2081	U1971	C1865	A1760	U	U1543	A1435
A2542	A2542	C2435	A2338	G2232	A2338	A	A	G2084	U1972	C1866	G1761	U	C1544	U1436
C2451	C2451	U2341	A2340	C2233	A2340	C	C	G2085	A1981	C1872	G1765	U	C1545	A1442
A2452	A2452	G2342	U2341	U2240	G2342	C	C	A2089	G1982	A1876	C1766	U	C1550	U1448
C2453	C2453	U2343	A2343	G2245	A2343	G	G	U2090	U1984	A1877	A1767	U	C1551	C1449
A2455	A2455	U2344	U2344	G2246	U2344	A	A	G2098	U1985	A1877	A1768	U	C1552	C1450
C2456	C2456	U2345	G2346	G2249	U2345	C	C	G2099	A1989	A1882	C1771	U	A1553	U1459
G2457	G2457	G2347	G2347	G2249	G2347	G	G	U2100	G1990	A1883	G1774	U	A1555	G1460
C2458	C2458	U2348	C2348	A2252	C2348	C	C	U2104	C1991	G1884	A1774	U	A1556	G1461
A2459	A2459	A2349	A2349	G2253	A2349	C	C	U2105	G1992	A1885	G1775	U	G1557	A1462
U2460	U2460	G2350	G2350	A2254	G2350	G	G	C2107	G1993	G1886	A1776	U	G1558	C1463
A2461	A2461	A2351	A2351	C2255	A2351	C	C	U2108	C1994	G1887	G1777	U	U1560	A1464
A2464	A2464	G2354	G2354	G2267	G2354	U	U	G2109	A1995	G1891	A1778	U	A1465	A1465
A2468	A2468	A2355	A2355	G2267	G2355	U	U	U2112	C1996	C1892	G1779	U	U1466	U1466
C2469	C2469	A2356	A2356	G2268	A2356	C	C	U2121	A1999	U1893	G1782	U	U1565	G1472
C2470	C2470	G2361	G2361	G2278	G2361	G	G	A2122	A2000	U1894	C1783	U	G1566	A1473
C2471	C2471	A2362	A2362	G2279	A2362	U	U	A2123	G2001	A1895	A1784	U	U1567	C1474
C2472	C2472	C2363	C2363	G2280	C2363	G	G	U2125	G2009	G1898	G1785	U	G1475	A1475
G2473	G2473	A2364	A2364	G2281	A2364	G	G	G2126	A2010	U1899	U1790	U	A1569	C1476
G2474	G2474	A2365	A2365	G2282	A2365	A	A	U2127	U2011	A1999	A1791	U	G1571	U1570
G2475	G2475	U2372	U2372	C2287	U2372	C	C	U2128	G1904	G1792	U1692	U	G1481	G1481
G2476	G2476	G2373	G2373	C2287	U2373	C	C	G2129	U2020	G1793	C1693	U	A1485	A1485
A2477	A2477	G2374	G2374	U2294	G2374	C	C	G2130	G2021	A1928	G1694	U	A1575	A1575
G2484	G2484	A2375	A2375	A2295	A2375	U	U	U2131	U2022	A1929	A1802	U	C1577	U1489
		C2376	C2376	A2296	C2376	C	C	C2025	C2025	A1930	C1803	U	A	A1490

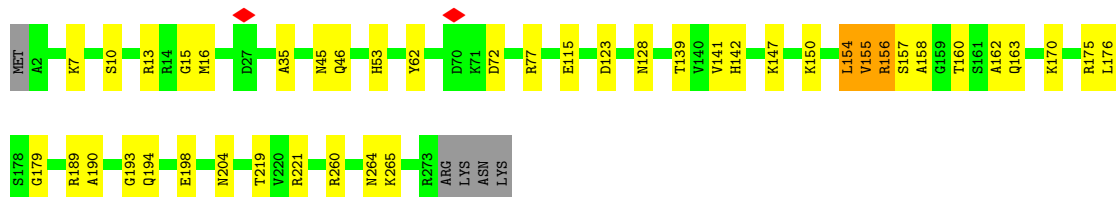
• Molecule 5: 5s rRNA

Chain B: 



- Molecule 6: 50S ribosomal protein L2

Chain E: 



- Molecule 7: 50S ribosomal protein L3

Chain F: 



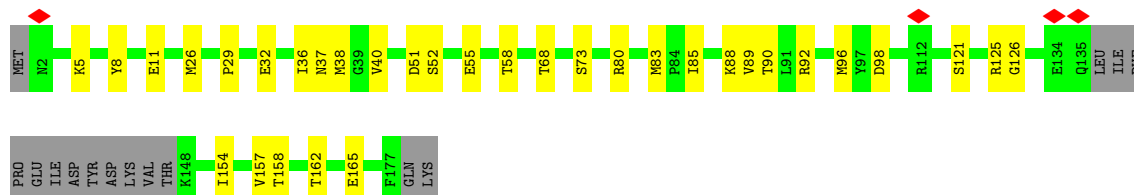
- Molecule 8: 50S ribosomal protein L4

Chain G: 



- Molecule 9: 50S ribosomal protein L5

Chain H: 



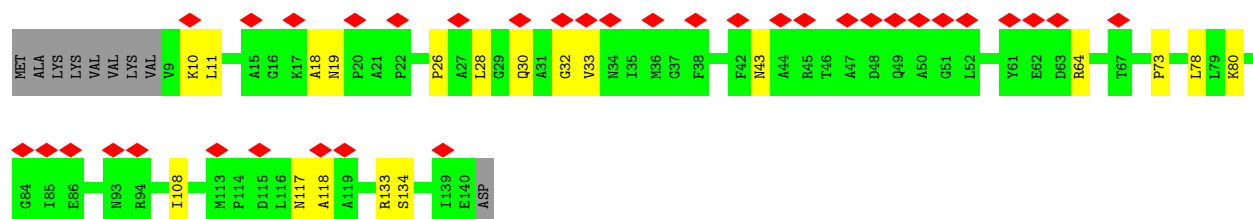
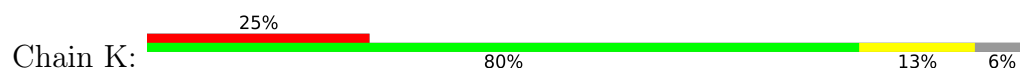
- Molecule 10: 50S ribosomal protein L6

Chain I: 

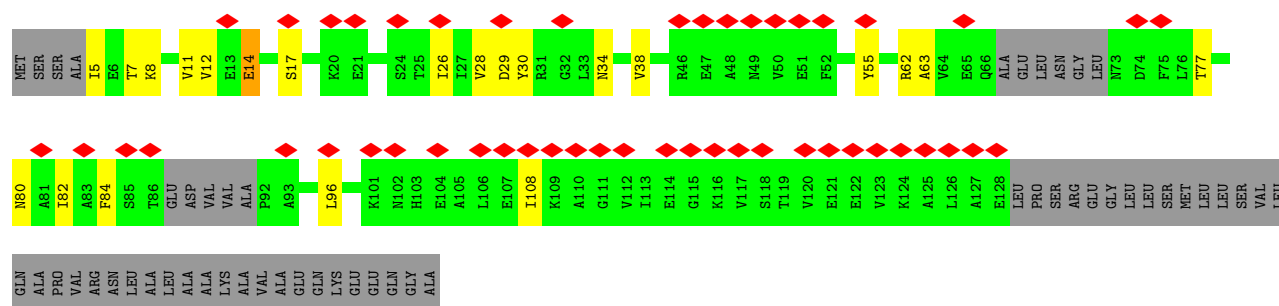




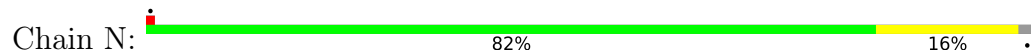
- Molecule 11: 50S ribosomal protein L11



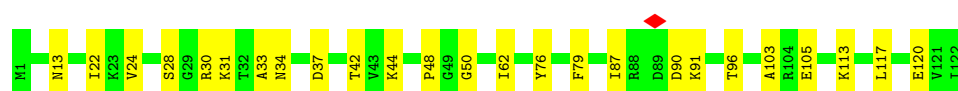
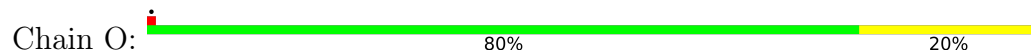
- Molecule 12: 50S ribosomal protein L10



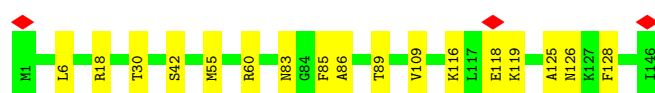
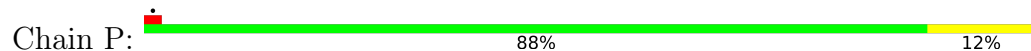
- Molecule 13: 50S ribosomal protein L13



- Molecule 14: 50S ribosomal protein L14



- Molecule 15: 50S ribosomal protein L15



- Molecule 16: 50S ribosomal protein L16

Chain Q:  78% 16% 6%



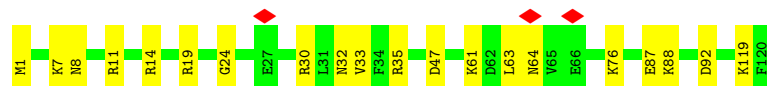
- Molecule 17: 50S ribosomal protein L17

Chain R:  78% 21% .



- Molecule 18: 50S ribosomal protein L18

Chain S:  83% 17%



- Molecule 19: 50S ribosomal protein L19

Chain T:  7% 87% 13%



- Molecule 20: 50S ribosomal protein L20

Chain U:  85% 13% ..



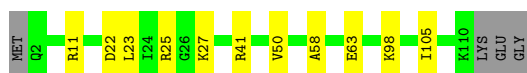
- Molecule 21: 50S ribosomal protein L21

Chain V:  88% 10% .

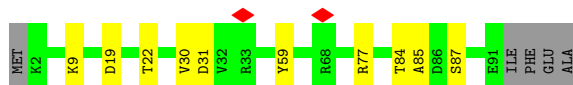
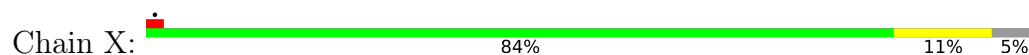


- Molecule 22: 50S ribosomal protein L22

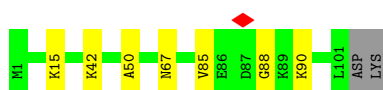
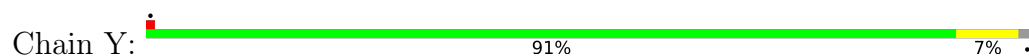
Chain W:  87% 10% .



- Molecule 23: 50S ribosomal protein L23



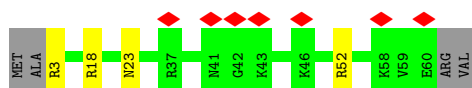
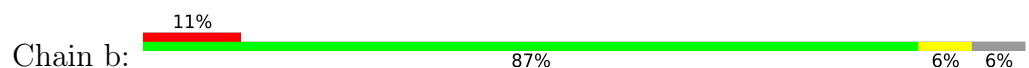
- Molecule 24: 50S ribosomal protein L24



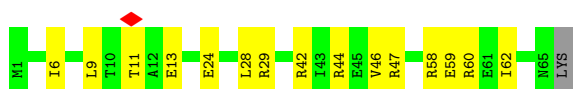
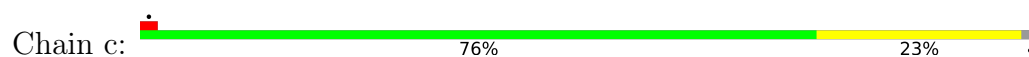
- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28



- Molecule 27: 50S ribosomal protein L29



- Molecule 28: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L32

Chain f:  71% 19% 10%



- Molecule 30: 50S ribosomal protein L33 1

Chain g:  86% 12% .



- Molecule 31: 50S ribosomal protein L34

Chain h:  84% 16%



- Molecule 32: 50S ribosomal protein L35

Chain i:  82% 15% .



- Molecule 33: 50S ribosomal protein L36

Chain j:  89% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74210	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size ($\text{\AA}$)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	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	0.30	0/4058	0.56	7/5485 (0.1%)
2	1	0.39	0/662	0.48	0/882
3	2	0.36	0/1744	0.47	0/2712
4	A	0.55	0/67639	0.47	0/105512
5	B	0.43	0/2675	0.43	0/4170
6	E	0.69	0/2120	0.55	0/2845
7	F	0.70	0/1591	0.54	0/2132
8	G	0.67	0/1580	0.53	0/2132
9	H	0.42	0/1299	0.53	0/1740
10	I	0.49	0/1360	0.48	0/1832
11	K	0.26	0/988	0.47	0/1336
12	L	0.26	0/892	0.49	0/1196
13	N	0.70	0/1146	0.50	0/1542
14	O	0.64	0/927	0.57	0/1245
15	P	0.64	0/1093	0.52	0/1457
16	Q	0.67	0/1099	0.53	0/1468
17	R	0.69	1/960 (0.1%)	0.58	0/1284
18	S	0.54	0/921	0.56	0/1236
19	T	0.63	0/957	0.57	0/1279
20	U	0.74	0/952	0.58	0/1266
21	V	0.69	0/792	0.53	0/1063
22	W	0.68	0/851	0.55	0/1146
23	X	0.62	0/731	0.51	0/974
24	Y	0.58	0/772	0.61	2/1032 (0.2%)
25	a	0.70	0/632	0.57	0/839
26	b	0.45	0/448	0.54	0/596
27	c	0.54	0/531	0.59	0/707
28	d	0.64	0/457	0.55	0/613
29	f	0.64	0/425	0.52	0/563
30	g	0.59	0/406	0.54	0/540
31	h	0.74	0/370	0.51	0/483
32	i	0.67	0/519	0.50	0/680
33	j	0.70	0/299	0.50	0/393
All	All	0.55	1/101896 (0.0%)	0.48	9/152380 (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
6	E	0	1
11	K	0	1
16	Q	0	1
21	V	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	119	LEU	CA-CB	-5.10	1.44	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	544	PRO	N-CA-CB	8.14	110.44	103.35
1	0	448	PRO	N-CA-CB	7.99	110.28	103.17
1	0	491	PRO	N-CA-CB	7.38	111.00	103.25
1	0	527	PRO	N-CA-CB	7.20	110.52	102.67
1	0	559	PRO	N-CA-CB	6.58	110.16	103.25
1	0	539	PRO	N-CA-CB	6.57	110.23	103.00
1	0	502	PRO	N-CA-CB	6.36	109.93	103.25
24	Y	50	ALA	CA-C-N	5.73	135.77	121.80
24	Y	50	ALA	C-N-CA	5.73	135.77	121.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	E	154	LEU	Peptide
11	K	19	ASN	Peptide
16	Q	60	ARG	Peptide
21	V	50	ASN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	3993	0	3689	28	0
2	1	659	0	705	15	0
3	2	1563	0	794	14	0
4	A	60389	0	30398	319	0
5	B	2392	0	1213	12	0
6	E	2083	0	2168	28	0
7	F	1569	0	1637	17	0
8	G	1561	0	1647	14	0
9	H	1284	0	1344	24	0
10	I	1342	0	1388	17	0
11	K	974	0	1011	14	0
12	L	886	0	920	15	0
13	N	1123	0	1162	16	0
14	O	920	0	977	21	0
15	P	1081	0	1132	12	0
16	Q	1076	0	1145	16	0
17	R	953	0	983	16	0
18	S	912	0	947	13	0
19	T	944	0	1020	11	0
20	U	940	0	1005	14	0
21	V	781	0	821	9	0
22	W	842	0	899	7	0
23	X	725	0	770	7	0
24	Y	762	0	821	5	0
25	a	624	0	639	9	0
26	b	444	0	487	4	0
27	c	530	0	568	10	0
28	d	455	0	491	14	0
29	f	418	0	435	8	0
30	g	401	0	413	4	0
31	h	367	0	410	5	0
32	i	512	0	564	8	0
33	j	296	0	342	3	0
All	All	93801	0	62945	597	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 4.

All (597) 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)
4:A:312:G:N2	4:A:405:U:C5	2.33	0.95
3:2:36:C:H2'	3:2:36:C:O2	1.70	0.92
4:A:327:G:H1	4:A:400:U:H3	1.18	0.86
4:A:810:G:O2'	4:A:811:A:O5'	1.95	0.84
4:A:1216:C:O2	4:A:1220:G:N2	2.12	0.82
4:A:1790:U:O2'	4:A:1791:A:O4'	1.98	0.80
4:A:2496:C:OP1	33:j:8:LYS:NZ	2.17	0.78
4:A:2009:G:O2'	4:A:2011:U:OP2	2.02	0.78
9:H:68:THR:OG1	9:H:85:ILE:O	2.00	0.77
4:A:84:A:N6	4:A:101:G:O2'	2.18	0.77
4:A:1263:G:OP2	21:V:89:ARG:NH1	2.17	0.77
4:A:917:A:OP1	16:Q:6:ARG:NH2	2.17	0.77
4:A:1159:U:OP1	10:I:2:SER:OG	2.03	0.77
4:A:2806:G:OP2	4:A:2810:A:O2'	2.02	0.77
4:A:840:A:OP2	4:A:2100:A:O2'	2.04	0.76
4:A:363:C:OP2	8:G:137:LYS:NZ	2.18	0.76
32:i:32:LEU:O	32:i:36:LYS:NZ	2.17	0.76
17:R:94:ARG:NH1	17:R:120:VAL:O	2.19	0.76
29:f:32:SER:OG	29:f:46:CYS:SG	2.43	0.76
4:A:364:A:N3	8:G:169:ASN:ND2	2.34	0.75
13:N:88:ARG:NH1	13:N:97:TYR:OH	2.19	0.75
3:2:36:C:O2	3:2:38:C:N4	2.19	0.75
4:A:1259:G:OP2	20:U:19:LYS:NZ	2.18	0.75
21:V:68:ALA:O	21:V:89:ARG:NE	2.17	0.75
4:A:1886:G:O2'	4:A:1887:G:O4'	2.03	0.75
4:A:898:U:OP1	28:d:49:LYS:NZ	2.20	0.75
16:Q:25:THR:OG1	16:Q:26:GLU:OE1	2.05	0.75
17:R:46:LYS:O	17:R:49:THR:OG1	2.05	0.75
4:A:817:G:OP1	31:h:8:ASN:ND2	2.20	0.74
4:A:458:G:OP2	4:A:2435:C:O2'	2.06	0.74
3:2:58:A:O2'	3:2:60:C:OP2	2.05	0.74
4:A:2532:A:O2'	4:A:2534:G:OP2	2.06	0.73
23:X:9:LYS:O	27:c:29:ARG:NH1	2.20	0.73
5:B:38:U:O2'	5:B:43:A:N6	2.21	0.73
7:F:26:THR:OG1	7:F:190:GLY:O	2.06	0.73
4:A:2127:U:O2'	4:A:2128:U:OP1	2.06	0.73
1:0:25:THR:OG1	1:0:38:HIS:O	2.05	0.73
4:A:697:G:OP1	32:i:19:SER:OG	2.03	0.73
4:A:1114:G:N2	4:A:1141:A:O2'	2.21	0.73
4:A:79:C:O2'	4:A:390:A:N3	2.18	0.72
4:A:2341:U:O2	9:H:37:ASN:ND2	2.22	0.72
4:A:274:A:HO2'	4:A:415:C:HO2'	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:84:THR:OG1	23:X:87:SER:OG	2.05	0.72
1:0:53:HIS:O	1:0:57:SER:N	2.22	0.72
9:H:126:GLY:O	9:H:158:THR:OG1	2.07	0.72
13:N:15:LYS:N	13:N:53:ASP:OD1	2.21	0.72
4:A:1315:G:OP2	4:A:1690:G:O2'	2.04	0.72
4:A:1036:A:O2'	4:A:1037:C:OP1	2.07	0.72
4:A:2498:A:O2'	16:Q:56:ARG:NH1	2.22	0.72
7:F:9:LYS:NZ	7:F:194:GLY:O	2.20	0.72
4:A:1784:A:O2'	4:A:1785:G:OP1	2.06	0.72
4:A:1542:A:O2'	4:A:1544:C:N4	2.23	0.72
23:X:19:ASP:O	23:X:22:THR:OG1	2.07	0.72
4:A:918:U:OP1	16:Q:5:LYS:N	2.22	0.71
4:A:2025:C:OP1	14:O:31:LYS:NZ	2.22	0.71
4:A:2332:G:O2'	9:H:121:SER:O	2.09	0.71
4:A:282:G:O2'	4:A:283:G:O4'	2.09	0.71
4:A:419:G:N2	4:A:448:A:OP2	2.16	0.71
7:F:95:GLN:NE2	7:F:96:GLU:O	2.23	0.71
9:H:8:TYR:OH	9:H:29:PRO:O	2.09	0.71
4:A:2595:A:N1	14:O:28:SER:OG	2.24	0.71
4:A:1811:C:O2	4:A:2637:G:O2'	2.04	0.71
10:I:57:SER:OG	10:I:59:GLN:OE1	2.04	0.71
2:1:21:GLU:OE2	2:1:25:GLN:NE2	2.24	0.70
17:R:19:ASP:OD1	17:R:67:ARG:NH1	2.24	0.70
15:P:85:PHE:O	15:P:119:LYS:NZ	2.17	0.70
4:A:1088:G:H1	4:A:1159:U:H3	1.36	0.70
4:A:2772:U:OP2	4:A:2784:C:N4	2.25	0.70
4:A:1362:G:OP1	22:W:98:LYS:NZ	2.24	0.70
4:A:1876:A:O2'	4:A:1877:A:N7	2.23	0.70
4:A:2343:A:OP1	9:H:88:LYS:NZ	2.20	0.70
1:0:27:ILE:O	1:0:80:ARG:NH2	2.25	0.70
18:S:92:ASP:OD1	18:S:119:LYS:NZ	2.25	0.70
4:A:1694:G:O2'	17:R:110:ASP:OD1	2.07	0.69
3:2:36:C:O2	3:2:36:C:C2'	2.39	0.69
4:A:1291:A:OP1	20:U:10:THR:OG1	2.10	0.69
4:A:2922:U:O2'	13:N:137:LYS:NZ	2.25	0.69
1:0:480:ARG:O	1:0:534:ARG:N	2.25	0.69
4:A:177:G:O2'	4:A:178:A:O5'	2.10	0.69
4:A:1265:A:OP1	21:V:70:LYS:NZ	2.25	0.69
4:A:1828:G:OP1	6:E:260:ARG:NH1	2.26	0.69
4:A:2314:C:OP2	30:g:2:ARG:NH2	2.26	0.69
4:A:1231:G:OP1	15:P:30:THR:OG1	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:341:LYS:NZ	4:A:2689:A:OP1	2.23	0.68
4:A:2287:C:O2'	4:A:2456:C:OP2	2.11	0.68
4:A:2294:U:OP2	4:A:2295:A:O2'	2.10	0.68
17:R:52:LYS:NZ	17:R:94:ARG:O	2.27	0.68
4:A:312:G:N2	4:A:405:U:C4	2.62	0.68
4:A:1365:U:O2'	4:A:1366:C:O4'	2.12	0.68
3:2:13:C:O2'	3:2:14:A:OP1	2.10	0.67
4:A:204:C:OP1	26:b:18:ARG:NH2	2.27	0.67
4:A:160:G:N2	4:A:168:A:OP2	2.27	0.67
5:B:28:C:OP1	18:S:7:LYS:NZ	2.26	0.67
4:A:515:G:N7	31:h:39:ARG:NH2	2.42	0.67
4:A:719:C:OP2	15:P:42:SER:OG	2.12	0.67
4:A:1983:G:O2'	4:A:1985:U:O4	2.08	0.67
4:A:52:A:OP2	4:A:118:A:N6	2.28	0.67
4:A:790:A:O2'	4:A:1704:U:OP1	2.12	0.66
19:T:88:ARG:NH1	19:T:112:GLU:OE1	2.29	0.66
4:A:1695:A:O2'	4:A:1696:G:O5'	2.13	0.66
6:E:72:ASP:OD2	6:E:189:ARG:NH2	2.28	0.66
4:A:1171:G:OP2	4:A:1172:A:O2'	2.09	0.66
4:A:251:G:O2'	4:A:2461:A:OP1	2.12	0.65
4:A:161:A:OP2	4:A:166:A:N6	2.30	0.65
4:A:2121:U:N3	4:A:2255:C:OP2	2.29	0.65
6:E:13:ARG:NH1	6:E:16:MET:SD	2.70	0.65
4:A:1325:A:O2'	4:A:1327:U:OP2	2.13	0.65
4:A:312:G:C2	4:A:405:U:C4	2.85	0.65
18:S:61:LYS:O	18:S:64:ASN:ND2	2.29	0.65
20:U:90:VAL:O	21:V:11:GLN:NE2	2.30	0.65
4:A:1403:G:N2	4:A:1406:A:OP2	2.25	0.65
4:A:1216:C:N3	4:A:1220:G:N1	2.44	0.64
4:A:1364:C:OP1	4:A:1692:U:O2'	2.15	0.64
4:A:1991:C:O2'	4:A:1993:G:OP2	2.14	0.64
5:B:47:C:OP2	18:S:35:ARG:NH2	2.29	0.64
11:K:26:PRO:O	11:K:30:GLN:NE2	2.28	0.64
4:A:77:U:O2'	4:A:78:U:O5'	2.16	0.64
4:A:1130:A:N3	4:A:1151:U:O2'	2.21	0.64
4:A:2364:A:O2'	4:A:2365:A:O5'	2.14	0.64
4:A:2513:G:OP1	16:Q:45:ARG:NH1	2.30	0.64
4:A:2872:U:OP1	19:T:96:LYS:NZ	2.28	0.64
29:f:35:GLU:OE2	29:f:45:ALA:HB3	1.98	0.64
4:A:1072:A:OP2	4:A:1180:C:O2'	2.14	0.64
4:A:2307:A:OP2	25:a:20:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:867:A:N3	4:A:989:U:O2'	2.31	0.64
1:O:121:GLU:OE2	1:O:162:TYR:OH	2.15	0.63
4:A:633:U:O3'	8:G:95:ARG:NH1	2.31	0.63
4:A:1108:G:N3	11:K:134:SER:OG	2.31	0.63
4:A:604:C:O2	20:U:48:ARG:NH2	2.31	0.63
4:A:2497:A:O2'	4:A:2498:A:O4'	2.17	0.63
6:E:194:GLN:NE2	6:E:198:GLU:OE1	2.31	0.63
4:A:186:C:O2'	4:A:479:A:N3	2.25	0.63
4:A:2060:A:N3	4:A:2484:G:O2'	2.28	0.63
2:1:42:LYS:N	2:1:45:ASP:OD2	2.32	0.63
4:A:2027:A:OP2	7:F:141:ARG:NH1	2.32	0.62
20:U:39:VAL:O	20:U:42:SER:OG	2.11	0.62
4:A:1313:A:O2'	4:A:1314:A:OP1	2.17	0.62
4:A:1065:U:OP1	4:A:1081:U:O2'	2.17	0.62
4:A:2130:G:N2	4:A:2218:U:O2	2.30	0.62
13:N:59:ASN:N	13:N:128:GLY:O	2.32	0.62
13:N:78:HIS:ND1	13:N:79:THR:O	2.29	0.62
4:A:2372:U:HO2'	4:A:2402:A:HO2'	1.46	0.62
4:A:2468:A:O2'	4:A:2629:A:OP1	2.13	0.62
4:A:1856:U:OP2	6:E:221:ARG:NH1	2.32	0.62
5:B:26:C:O2	5:B:57:G:N2	2.33	0.62
15:P:55:MET:O	15:P:60:ARG:NH2	2.33	0.62
30:g:9:CYS:SG	30:g:10:THR:N	2.71	0.62
4:A:1094:A:OP2	4:A:1156:G:N2	2.25	0.62
4:A:1379:U:OP2	23:X:59:TYR:OH	2.17	0.62
4:A:1124:C:OP1	11:K:133:ARG:NH2	2.32	0.61
4:A:1695:A:HO2'	4:A:1696:G:P	2.22	0.61
4:A:1757:G:O2'	4:A:1758:U:O3'	2.16	0.61
14:O:13:ASN:ND2	14:O:96:THR:OG1	2.32	0.61
4:A:372:U:O2'	24:Y:67:ASN:ND2	2.33	0.61
4:A:1264:G:OP2	21:V:67:ARG:NH2	2.33	0.61
9:H:36:ILE:HG22	9:H:154:ILE:HG22	1.82	0.61
4:A:1530:G:O2'	4:A:1531:G:OP1	2.14	0.61
4:A:2026:A:O5'	7:F:130:ARG:NH1	2.33	0.61
10:I:8:LEU:HD22	10:I:52:THR:HG22	1.83	0.61
2:1:80:LYS:NZ	2:1:81:GLU:O	2.34	0.61
4:A:353:A:N3	4:A:373:A:O2'	2.31	0.61
4:A:2882:G:N2	4:A:2885:A:OP2	2.29	0.61
9:H:162:THR:OG1	9:H:165:GLU:OE1	2.11	0.61
4:A:274:A:O2'	4:A:415:C:O2'	2.15	0.61
4:A:2548:U:O4'	4:A:2571:A:N6	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2080:A:O2'	4:A:2643:A:N6	2.34	0.61
4:A:2856:G:N2	4:A:2909:U:OP2	2.34	0.61
1:O:60:HIS:NE2	1:O:271:SER:O	2.34	0.60
4:A:2605:G:O2'	4:A:2608:C:OP2	2.16	0.60
8:G:109:ALA:O	8:G:112:SER:OG	2.17	0.60
4:A:347:G:O2'	4:A:348:U:OP1	2.19	0.60
9:H:55:GLU:O	9:H:58:THR:OG1	2.16	0.60
3:2:56:C:O4'	9:H:73:SER:OG	2.09	0.60
9:H:96:MET:SD	9:H:96:MET:N	2.74	0.60
4:A:1036:A:O2'	4:A:1038:C:OP2	2.20	0.60
4:A:2404:G:N2	4:A:2407:A:OP2	2.31	0.60
4:A:448:A:O2'	4:A:449:A:O4'	2.11	0.59
4:A:2054:C:OP1	7:F:153:ARG:NH2	2.35	0.59
4:A:753:A:OP1	6:E:7:LYS:NZ	2.36	0.59
4:A:1125:C:O4'	11:K:133:ARG:NH1	2.36	0.59
4:A:2864:G:O2'	17:R:45:GLU:OE1	2.14	0.59
4:A:1204:C:OP1	28:d:30:LYS:NZ	2.36	0.59
17:R:52:LYS:NZ	17:R:98:TYR:OH	2.25	0.59
8:G:101:LEU:O	8:G:106:ARG:NH2	2.35	0.59
28:d:18:ASP:OD1	28:d:19:GLN:N	2.35	0.59
4:A:2361:C:OP1	25:a:84:ARG:NH1	2.35	0.59
4:A:1199:C:OP1	20:U:92:ARG:NH2	2.35	0.59
14:O:13:ASN:OD1	14:O:96:THR:N	2.35	0.59
4:A:2104:U:OP2	4:A:2267:G:O2'	2.16	0.58
28:d:8:LEU:HD21	28:d:28:LEU:HD13	1.85	0.58
4:A:2688:G:N2	4:A:2691:A:OP2	2.35	0.58
4:A:2841:C:O2	4:A:2908:A:O2'	2.15	0.58
4:A:1102:G:O2'	4:A:1149:A:N6	2.36	0.58
16:Q:77:LYS:NZ	16:Q:84:GLY:O	2.32	0.58
1:O:392:GLU:OE1	1:O:395:ARG:NH2	2.37	0.58
3:2:56:C:N4	3:2:57:G:O6	2.36	0.58
14:O:87:ILE:HD13	14:O:90:ASP:O	2.04	0.58
4:A:546:G:N1	4:A:549:A:OP2	2.35	0.57
4:A:1501:U:O2'	4:A:1502:G:N7	2.37	0.57
4:A:2106:A:OP1	4:A:2267:G:N2	2.33	0.57
4:A:1830:G:OP2	6:E:150:LYS:NZ	2.38	0.57
4:A:2890:U:OP2	4:A:2891:G:O2'	2.13	0.57
6:E:77:ARG:NH2	6:E:115:GLU:OE2	2.38	0.57
4:A:1509:C:HO2'	4:A:2731:G:HO2'	1.49	0.57
4:A:420:U:O2'	4:A:421:A:O5'	2.22	0.57
28:d:39:ASP:OD1	28:d:44:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:41:GLY:N	25:a:72:ASP:OD1	2.37	0.57
4:A:843:C:O3'	8:G:62:ARG:NH2	2.37	0.57
13:N:14:ARG:NH2	13:N:50:ASP:O	2.36	0.56
4:A:1993:G:O2'	4:A:1996:C:OP2	2.18	0.56
4:A:2054:C:OP2	7:F:153:ARG:NE	2.38	0.56
6:E:45:ASN:OD1	6:E:46:GLN:N	2.38	0.56
12:L:29:ASP:OD1	12:L:30:TYR:N	2.38	0.56
31:h:20:SER:O	31:h:23:SER:OG	2.20	0.56
19:T:28:VAL:HG12	19:T:84:ILE:HG22	1.87	0.56
4:A:2522:U:O2'	16:Q:80:GLU:OE2	2.19	0.56
4:A:1757:G:O2'	4:A:1758:U:O5'	2.23	0.56
4:A:1008:A:HO2'	4:A:2525:C:HO2'	1.54	0.56
4:A:1058:U:O4	13:N:31:SER:OG	2.24	0.56
4:A:1782:G:OP1	19:T:93:ARG:NH1	2.38	0.56
4:A:2324:C:OP2	18:S:14:ARG:NE	2.37	0.56
4:A:2226:U:O2'	4:A:2227:A:O5'	2.21	0.56
4:A:675:C:O2	4:A:685:U:O2'	2.24	0.56
6:E:155:VAL:O	6:E:160:THR:OG1	2.19	0.56
10:I:158:TYR:O	10:I:172:ARG:NH1	2.39	0.56
4:A:75:G:OP1	27:c:44:ARG:NH2	2.39	0.56
4:A:1127:U:O2	11:K:117:ASN:ND2	2.37	0.56
4:A:2038:G:OP1	22:W:41:ARG:NH1	2.40	0.55
4:A:2859:G:O2'	4:A:2860:A:O5'	2.24	0.55
2:1:10:SER:OG	2:1:75:MET:SD	2.63	0.55
4:A:792:G:O2'	4:A:795:G:O2'	2.16	0.55
4:A:1820:A:N6	4:A:1857:G:O2'	2.35	0.55
4:A:1883:A:O2'	4:A:1884:G:OP1	2.23	0.55
14:O:22:ILE:HD11	14:O:42:THR:HG23	1.89	0.55
4:A:623:A:O2'	4:A:2048:U:OP1	2.24	0.55
4:A:897:G:O2'	28:d:22:THR:HG22	2.07	0.55
4:A:2108:U:O2'	26:b:23:ASN:OD1	2.23	0.55
27:c:13:GLU:N	27:c:13:GLU:OE1	2.39	0.55
4:A:2684:G:O2'	4:A:2693:G:O6	2.20	0.55
6:E:142:HIS:ND1	6:E:193:GLY:O	2.40	0.55
10:I:89:GLU:OE1	10:I:89:GLU:N	2.40	0.55
4:A:761:U:O2'	4:A:763:A:N7	2.38	0.55
14:O:33:ALA:HB1	14:O:37:ASP:CB	2.36	0.54
4:A:2390:A:OP2	32:i:24:ARG:NH2	2.38	0.54
4:A:116:G:OP2	4:A:118:A:O2'	2.26	0.54
16:Q:30:GLY:O	16:Q:134:ARG:NH2	2.41	0.54
29:f:30:CYS:N	29:f:35:GLU:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:21:G:O2'	5:B:22:G:O5'	2.15	0.54
4:A:339:A:O3'	24:Y:90:LYS:NZ	2.41	0.54
4:A:373:A:N1	24:Y:15:LYS:NZ	2.56	0.54
12:L:5:ILE:N	12:L:8:LYS:HZ3	2.06	0.54
4:A:2386:U:OP1	25:a:28:ARG:NH1	2.41	0.54
15:P:116:LYS:NZ	15:P:118:GLU:OE2	2.40	0.54
1:0:126:HIS:NE2	3:2:35:G:O2'	2.33	0.53
4:A:1110:C:OP1	11:K:80:LYS:NZ	2.41	0.53
9:H:37:ASN:OD1	9:H:38:MET:N	2.40	0.53
9:H:80:ARG:O	9:H:83:MET:HE2	2.08	0.53
28:d:15:ARG:O	28:d:20:ARG:NH2	2.41	0.53
4:A:593:A:O2'	4:A:594:C:O5'	2.26	0.53
4:A:1972:U:O2'	4:A:1973:U:OP2	2.26	0.53
27:c:6:ILE:O	27:c:60:ARG:NH2	2.41	0.53
3:2:9:A:N3	3:2:45:G:O2'	2.34	0.53
4:A:253:G:OP1	32:i:13:ARG:NH2	2.36	0.53
4:A:1417:A:O2'	4:A:1418:U:OP2	2.25	0.53
1:0:185:LEU:HD11	1:0:192:LEU:HD13	1.91	0.53
4:A:1713:A:O2'	4:A:1719:G:N7	2.29	0.53
4:A:1263:G:N2	4:A:1266:A:OP2	2.38	0.53
13:N:30:SER:HA	13:N:33:VAL:HG22	1.91	0.53
1:0:9:TYR:O	1:0:12:THR:OG1	2.27	0.53
6:E:154:LEU:O	6:E:156:ARG:N	2.41	0.53
11:K:10:LYS:C	11:K:11:LEU:HD12	2.34	0.53
4:A:83:G:N2	4:A:102:A:OP2	2.22	0.53
4:A:236:A:H61	4:A:476:A:H61	1.57	0.53
18:S:24:GLY:O	18:S:47:ASP:N	2.42	0.53
4:A:2712:C:O2	14:O:76:TYR:OH	2.24	0.53
33:j:14:CYS:SG	33:j:32:HIS:ND1	2.81	0.53
13:N:50:ASP:OD1	13:N:122:LYS:NZ	2.42	0.53
7:F:43:ASN:OD1	7:F:44:ASP:N	2.41	0.52
8:G:80:SER:HG	8:G:83:TRP:CD1	2.27	0.52
11:K:117:ASN:OD1	11:K:118:ALA:N	2.42	0.52
18:S:87:GLU:OE2	18:S:88:LYS:NZ	2.43	0.52
2:1:16:ARG:NH1	4:A:1954:C:OP2	2.42	0.52
4:A:111:U:OP1	27:c:58:ARG:NH2	2.42	0.52
4:A:2233:C:OP1	6:E:147:LYS:NZ	2.42	0.52
4:A:287:G:N3	4:A:288:C:N4	2.58	0.52
4:A:488:U:O2	8:G:46:GLN:NE2	2.41	0.52
4:A:1010:C:O2'	4:A:2302:A:N3	2.37	0.52
4:A:1033:C:O2'	4:A:1046:A:N3	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:42:ILE:HD12	16:Q:97:VAL:HG21	1.91	0.52
5:B:41:C:N3	9:H:90:THR:OG1	2.41	0.52
18:S:30:ARG:NH2	18:S:47:ASP:OD1	2.43	0.52
4:A:898:U:O2	28:d:42:ALA:HB1	2.09	0.52
4:A:1129:U:N3	4:A:1132:A:OP2	2.41	0.52
4:A:419:G:O2'	4:A:447:G:O6	2.24	0.51
4:A:2278:U:N3	4:A:2282:G:OP2	2.41	0.51
4:A:1498:U:O2'	4:A:1499:A:N7	2.42	0.51
17:R:8:ARG:O	17:R:13:ARG:NH2	2.43	0.51
4:A:2551:U:O2'	4:A:2676:U:OP1	2.29	0.51
4:A:2850:G:O6	7:F:163:ARG:NH1	2.44	0.51
14:O:120:GLU:OE1	19:T:65:SER:OG	2.25	0.51
4:A:2048:U:OP2	29:f:6:ARG:NH2	2.44	0.51
4:A:2384:C:O4'	25:a:44:ILE:HD11	2.11	0.51
5:B:31:G:O2'	5:B:32:U:OP1	2.27	0.51
4:A:273:A:OP2	4:A:297:G:N2	2.42	0.51
8:G:112:SER:O	8:G:115:SER:OG	2.23	0.51
32:i:40:GLN:O	32:i:44:LEU:HD13	2.11	0.51
2:1:4:ASP:OD1	2:1:5:LYS:N	2.44	0.50
10:I:108:VAL:HG13	10:I:109:GLY:H	1.76	0.50
4:A:2830:A:O2'	4:A:2831:A:OP2	2.22	0.50
12:L:7:THR:O	12:L:11:VAL:HG23	2.12	0.50
20:U:102:ASP:OD2	21:V:2:TYR:OH	2.28	0.50
28:d:18:ASP:O	28:d:22:THR:HG23	2.12	0.50
2:1:58:VAL:HG12	2:1:78:ILE:HD12	1.93	0.50
4:A:52:A:OP2	4:A:116:G:N1	2.44	0.50
4:A:1460:G:O2'	4:A:1631:A:N6	2.44	0.50
4:A:1970:C:N4	4:A:1994:C:O4'	2.45	0.50
18:S:63:LEU:O	18:S:76:LYS:NZ	2.37	0.50
4:A:265:A:N3	4:A:477:A:O2'	2.39	0.50
6:E:123:ASP:OD1	6:E:128:ASN:ND2	2.45	0.50
14:O:48:PRO:O	14:O:50:GLY:N	2.43	0.50
11:K:33:VAL:HG12	11:K:64:ARG:HG2	1.94	0.49
4:A:1981:A:OP1	14:O:44:LYS:NZ	2.31	0.49
6:E:176:LEU:O	6:E:179:GLY:N	2.40	0.49
4:A:1140:U:O2'	4:A:1142:A:N7	2.35	0.49
6:E:53:HIS:CE1	6:E:219:THR:HG23	2.47	0.49
25:a:23:ASP:OD1	25:a:24:SER:N	2.45	0.49
4:A:1189:A:OP1	13:N:28:ARG:NH1	2.43	0.49
4:A:1462:G:HO2'	4:A:1633:G:HO2'	1.57	0.49
18:S:8:ASN:OD1	18:S:11:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:490:A:OP1	8:G:46:GLN:N	2.42	0.49
4:A:1040:C:O2'	4:A:1042:A:OP1	2.24	0.49
4:A:2252:A:OP1	6:E:170:LYS:NZ	2.45	0.49
10:I:59:GLN:OE1	10:I:62:HIS:ND1	2.44	0.49
1:O:94:ALA:HB2	1:O:101:ILE:HD11	1.95	0.49
4:A:630:A:H5'	8:G:89:VAL:HG21	1.93	0.49
4:A:1177:G:O2'	4:A:2054:C:O2'	2.15	0.49
20:U:90:VAL:HG12	21:V:39:LEU:HD13	1.94	0.49
4:A:747:G:O2'	4:A:1677:A:N3	2.39	0.49
4:A:777:C:OP1	4:A:1804:U:O2'	2.20	0.49
27:c:59:GLU:HA	27:c:62:ILE:HG22	1.94	0.49
10:I:8:LEU:CD2	10:I:52:THR:HG22	2.42	0.48
4:A:1158:G:O2'	4:A:1159:U:O5'	2.31	0.48
4:A:1759:U:H3	4:A:1774:A:H62	1.61	0.48
4:A:2922:U:O3'	13:N:137:LYS:NZ	2.46	0.48
4:A:45:G:H21	4:A:183:A:H61	1.61	0.48
6:E:15:GLY:O	6:E:204:ASN:ND2	2.46	0.48
4:A:85:G:N1	4:A:98:U:C2	2.82	0.48
4:A:1339:A:H4'	4:A:1340:A:H5'	1.95	0.48
13:N:63:ILE:O	13:N:94:ARG:NH2	2.46	0.48
4:A:2320:U:O2'	4:A:2403:C:O2	2.30	0.48
4:A:1853:G:OP2	6:E:53:HIS:ND1	2.46	0.48
4:A:514:G:OP2	31:h:34:ARG:NH2	2.46	0.48
4:A:2817:C:O2'	4:A:2834:A:N3	2.45	0.48
15:P:83:ASN:O	15:P:119:LYS:NZ	2.24	0.48
1:O:21:GLY:N	1:O:88:ILE:O	2.44	0.48
4:A:965:A:N3	5:B:78:U:O2'	2.46	0.48
15:P:125:ALA:HB3	15:P:128:PHE:HE1	1.79	0.48
25:a:80:PHE:N	25:a:84:ARG:O	2.46	0.48
2:1:30:ILE:HG22	2:1:35:ALA:HB2	1.96	0.48
5:B:10:G:OP2	25:a:79:ARG:NH1	2.47	0.48
11:K:18:ALA:HB3	11:K:43:ASN:ND2	2.28	0.48
22:W:23:LEU:O	22:W:27:LYS:NZ	2.45	0.48
4:A:1159:U:O2'	4:A:1160:G:OP2	2.30	0.48
1:O:133:ASP:OD1	1:O:134:ALA:N	2.47	0.47
4:A:64:A:H61	4:A:90:A:H61	1.62	0.47
20:U:90:VAL:HG23	20:U:91:ASN:H	1.79	0.47
4:A:776:G:OP1	6:E:10:SER:OG	2.32	0.47
4:A:1831:A:H2	4:A:1844:A:H62	1.61	0.47
6:E:141:VAL:CG1	6:E:190:ALA:HB1	2.44	0.47
10:I:64:ALA:O	10:I:68:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:108:GLY:O	13:N:112:LYS:NZ	2.48	0.47
1:0:128:ASN:OD1	1:0:129:ILE:N	2.45	0.47
5:B:39:A:O2'	5:B:40:C:OP1	2.33	0.47
32:i:4:MET:HE1	32:i:60:GLN:HE21	1.80	0.47
1:0:286:ARG:NH2	3:2:42:G:OP1	2.48	0.47
4:A:27:G:N2	4:A:558:G:O2'	2.47	0.47
4:A:527:A:O2'	24:Y:42:LYS:O	2.32	0.47
18:S:19:ARG:NH1	18:S:47:ASP:OD2	2.43	0.47
4:A:593:A:O2'	4:A:593:A:N3	2.43	0.47
13:N:96:ASN:O	13:N:127:ARG:NH2	2.47	0.47
20:U:88:ILE:HG22	20:U:88:ILE:O	2.15	0.47
3:2:7:U:O2'	3:2:8:U:OP1	2.31	0.47
4:A:312:G:C2	4:A:405:U:O4	2.68	0.47
4:A:1305:A:O3'	29:f:16:ARG:NH2	2.48	0.47
9:H:51:ASP:OD1	9:H:52:SER:N	2.48	0.47
19:T:34:GLU:OE2	19:T:39:ARG:NH2	2.48	0.47
22:W:58:ALA:O	22:W:63:GLU:N	2.48	0.47
28:d:44:ARG:HD3	28:d:47:ILE:HD11	1.96	0.47
4:A:1403:G:OP1	26:b:3:ARG:NH1	2.48	0.47
4:A:1516:A:N7	4:A:1569:A:N1	2.62	0.47
28:d:8:LEU:CD2	28:d:28:LEU:HD13	2.45	0.47
4:A:248:G:N7	32:i:8:ARG:NH2	2.63	0.46
4:A:1371:G:N7	4:A:1654:A:O2'	2.45	0.46
4:A:1645:C:OP1	23:X:77:ARG:NH1	2.48	0.46
17:R:17:LEU:O	17:R:21:THR:HG23	2.15	0.46
4:A:1699:A:N6	4:A:2035:C:O4'	2.48	0.46
4:A:1867:C:N4	4:A:1928:A:O4'	2.48	0.46
12:L:77:THR:O	12:L:80:ASN:ND2	2.44	0.46
20:U:69:ALA:O	20:U:74:LEU:N	2.48	0.46
1:0:246:VAL:O	1:0:246:VAL:HG13	2.16	0.46
4:A:810:G:HO2'	4:A:811:A:P	2.31	0.46
4:A:1252:G:O2'	4:A:1253:A:OP2	2.33	0.46
4:A:1574:G:N1	4:A:1592:A:OP2	2.43	0.46
7:F:15:VAL:O	7:F:23:ILE:N	2.49	0.46
10:I:166:GLU:OE1	10:I:166:GLU:N	2.42	0.46
30:g:36:CYS:O	30:g:40:LYS:N	2.46	0.46
2:1:25:GLN:OE1	2:1:27:ARG:NE	2.48	0.46
4:A:1542:A:N3	4:A:1625:C:O2'	2.49	0.46
4:A:2279:G:N2	4:A:2305:G:OP1	2.45	0.46
4:A:1092:A:N3	12:L:62:ARG:NH1	2.63	0.46
17:R:18:ARG:O	17:R:21:THR:OG1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:50:VAL:HG13	22:W:105:ILE:HD12	1.98	0.46
27:c:9:LEU:HD23	27:c:11:THR:H	1.81	0.46
4:A:2664:U:O2'	7:F:82:GLU:OE1	2.27	0.46
7:F:206:VAL:O	7:F:206:VAL:HG13	2.16	0.46
4:A:363:C:P	8:G:137:LYS:HZ2	2.39	0.46
4:A:1955:U:O2'	4:A:1957:A:N7	2.34	0.46
11:K:73:PRO:CG	11:K:78:LEU:HD21	2.46	0.46
4:A:287:G:H21	4:A:288:C:H42	1.63	0.46
4:A:2898:A:O2'	4:A:2899:C:OP1	2.28	0.46
9:H:125:ARG:HD2	18:S:1:MET:HE3	1.98	0.46
20:U:97:ASP:OD1	20:U:101:ASN:ND2	2.49	0.46
24:Y:85:VAL:HG13	24:Y:88:GLY:O	2.15	0.46
4:A:447:G:O6	26:b:52:ARG:NH1	2.49	0.46
12:L:34:ASN:O	12:L:38:VAL:HG23	2.16	0.46
4:A:64:A:H61	4:A:90:A:N6	2.14	0.45
14:O:87:ILE:HD13	14:O:90:ASP:H	1.81	0.45
1:O:240:ILE:HG23	1:O:240:ILE:O	2.16	0.45
4:A:1462:G:O2'	4:A:1633:G:O2'	2.28	0.45
4:A:2875:A:OP2	4:A:2891:G:N1	2.49	0.45
9:H:5:LYS:NZ	9:H:98:ASP:OD1	2.49	0.45
25:a:77:PHE:CD1	25:a:87:VAL:HG12	2.51	0.45
4:A:1158:G:HO2'	4:A:1159:U:P	2.39	0.45
14:O:113:LYS:O	14:O:117:LEU:HD23	2.16	0.45
17:R:102:MET:HE2	17:R:116:ILE:HD11	1.98	0.45
29:f:33:CYS:N	29:f:46:CYS:SG	2.86	0.45
9:H:89:VAL:HG12	9:H:90:THR:O	2.17	0.45
30:g:11:GLU:OE1	30:g:11:GLU:N	2.48	0.45
4:A:2053:C:O2'	4:A:2054:C:O5'	2.34	0.45
7:F:28:ILE:HD12	7:F:188:ILE:HD12	1.99	0.45
4:A:2041:G:OP1	22:W:11:ARG:NH2	2.45	0.45
12:L:28:VAL:HG12	12:L:108:ILE:HA	1.98	0.45
16:Q:72:LYS:O	16:Q:94:VAL:N	2.48	0.45
6:E:162:ALA:HB1	6:E:175:ARG:O	2.17	0.45
12:L:82:ILE:HD12	12:L:84:PHE:CE2	2.51	0.45
3:2:57:G:O2'	3:2:58:A:O4'	2.34	0.45
4:A:2334:U:O2'	4:A:2335:U:O5'	2.35	0.45
4:A:2593:A:OP1	4:A:2677:G:O2'	2.29	0.45
4:A:2823:C:O2'	4:A:2824:G:O4'	2.25	0.45
15:P:86:ALA:O	15:P:89:THR:HG22	2.16	0.45
4:A:1283:U:O2'	15:P:6:LEU:O	2.35	0.45
2:1:61:ASN:HD21	2:1:77:THR:HG23	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1698:G:O6	17:R:7:GLY:N	2.44	0.44
4:A:1734:A:OP2	4:A:1743:A:N6	2.32	0.44
7:F:111:THR:OG1	7:F:170:THR:HG22	2.16	0.44
16:Q:44:ASN:OD1	16:Q:45:ARG:N	2.50	0.44
28:d:19:GLN:O	28:d:22:THR:OG1	2.30	0.44
1:O:171:ILE:N	1:O:199:HIS:O	2.50	0.44
11:K:78:LEU:HD13	11:K:108:ILE:HG23	1.98	0.44
4:A:569:C:O2	4:A:598:U:O2'	2.34	0.44
4:A:2703:G:H4'	14:O:30:ARG:HE	1.81	0.44
10:I:108:VAL:HG13	10:I:109:GLY:N	2.32	0.44
11:K:73:PRO:HG2	11:K:78:LEU:HD21	1.99	0.44
2:1:9:VAL:HB	2:1:67:THR:HG21	1.99	0.44
4:A:2719:A:N6	17:R:39:GLU:OE1	2.44	0.44
29:f:30:CYS:O	29:f:34:GLY:N	2.44	0.44
20:U:88:ILE:O	20:U:90:VAL:N	2.51	0.44
28:d:40:ASN:OD1	28:d:41:ALA:N	2.50	0.44
4:A:347:G:HO2'	4:A:348:U:P	2.40	0.44
4:A:461:C:O2	4:A:1893:U:O2'	2.30	0.44
14:O:24:VAL:HG11	14:O:33:ALA:HB2	1.99	0.44
27:c:42:ARG:O	27:c:46:VAL:HG23	2.18	0.44
4:A:610:U:OP1	21:V:81:ASN:ND2	2.47	0.44
4:A:1895:A:N6	4:A:1904:G:O2'	2.49	0.44
7:F:48:ALA:HB1	7:F:83:LEU:O	2.17	0.44
4:A:1485:A:H2	4:A:1600:G:H21	1.65	0.44
4:A:1691:A:O2'	4:A:1692:U:OP2	2.24	0.44
3:2:22:G:O2'	3:2:23:A:O5'	2.35	0.43
4:A:492:C:H2'	4:A:493:G:O4'	2.18	0.43
4:A:2063:U:HO2'	4:A:2064:G:P	2.40	0.43
4:A:2688:G:P	10:I:159:LYS:HZ1	2.40	0.43
4:A:2080:A:N6	4:A:2643:A:O2'	2.45	0.43
17:R:26:ILE:O	17:R:82:LYS:NZ	2.51	0.43
19:T:71:GLU:OE1	19:T:101:ARG:NH1	2.51	0.43
1:O:362:PRO:C	1:O:363:LEU:HD12	2.44	0.43
4:A:74:U:OP1	27:c:47:ARG:NH2	2.47	0.43
4:A:1366:C:O2'	17:R:108:ARG:NH1	2.45	0.43
4:A:1849:U:OP1	6:E:177:ASN:ND2	2.50	0.43
9:H:11:GLU:N	9:H:11:GLU:OE1	2.51	0.43
12:L:108:ILE:HG22	12:L:108:ILE:O	2.18	0.43
14:O:105:GLU:OE1	14:O:105:GLU:N	2.52	0.43
4:A:1783:C:OP1	19:T:94:ARG:NE	2.51	0.43
9:H:92:ARG:C	9:H:96:MET:HE3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:85:G:C6	4:A:98:U:N3	2.86	0.43
4:A:1965:A:OP2	4:A:1991:C:N4	2.47	0.43
7:F:134:SER:OG	7:F:135:HIS:N	2.50	0.43
15:P:125:ALA:HB3	15:P:128:PHE:CE1	2.54	0.43
2:1:12:LEU:HD21	2:1:76:TYR:CZ	2.53	0.43
5:B:107:G:HO2'	5:B:108:C:H6	1.64	0.43
21:V:36:GLU:OE1	21:V:36:GLU:N	2.51	0.43
2:1:46:GLU:C	2:1:47:LEU:HD22	2.44	0.43
4:A:2327:A:H62	4:A:2347:G:H21	1.66	0.43
6:E:157:SER:OG	6:E:158:ALA:N	2.52	0.43
4:A:1758:U:O2'	4:A:1759:U:OP1	2.35	0.43
4:A:2667:G:HO2'	4:A:2668:A:H8	1.67	0.43
8:G:53:ASN:OD1	8:G:54:ARG:N	2.52	0.43
1:0:149:SER:O	3:2:37:A:N6	2.52	0.42
1:0:242:ASN:HB3	1:0:266:ARG:HG2	2.00	0.42
4:A:751:G:H2'	4:A:773:G:H22	1.83	0.42
4:A:2420:G:O2'	4:A:2421:A:O5'	2.30	0.42
7:F:40:THR:OG1	7:F:43:ASN:OD1	2.31	0.42
27:c:24:GLU:O	27:c:28:LEU:HD23	2.18	0.42
4:A:722:A:N3	4:A:2472:C:O2'	2.43	0.42
4:A:894:A:H62	4:A:979:U:H3	1.66	0.42
9:H:36:ILE:HG22	9:H:154:ILE:CG2	2.46	0.42
1:0:7:PHE:HA	1:0:254:LEU:HD11	1.99	0.42
4:A:1846:G:OP2	6:E:156:ARG:NH2	2.44	0.42
9:H:32:GLU:N	9:H:157:VAL:O	2.50	0.42
14:O:34:ASN:O	14:O:62:ILE:HG21	2.20	0.42
4:A:2695:C:N4	10:I:109:GLY:O	2.50	0.42
14:O:24:VAL:CG1	14:O:33:ALA:HB2	2.49	0.42
23:X:84:THR:OG1	23:X:85:ALA:O	2.38	0.42
4:A:1058:U:O2	13:N:28:ARG:NH1	2.52	0.42
4:A:1365:U:HO2'	4:A:1366:C:H6	1.67	0.42
2:1:9:VAL:CB	2:1:67:THR:HG21	2.50	0.42
4:A:2060:A:O2'	4:A:2061:G:OP1	2.34	0.42
5:B:55:A:N6	9:H:26:MET:HE2	2.34	0.42
12:L:14:GLU:O	12:L:17:SER:OG	2.21	0.42
13:N:6:MET:SD	13:N:6:MET:N	2.93	0.42
17:R:85:SER:OG	17:R:86:ASP:N	2.52	0.42
1:0:97:ASP:OD1	1:0:98:ARG:N	2.50	0.42
2:1:22:VAL:HG23	2:1:27:ARG:HD2	2.02	0.42
4:A:939:G:O2'	4:A:940:G:O5'	2.38	0.42
4:A:1464:A:H2	4:A:1627:A:H62	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1765:G:N2	4:A:1768:A:OP2	2.52	0.42
4:A:1784:A:HO2'	4:A:1785:G:P	2.37	0.42
9:H:40:VAL:HG23	9:H:40:VAL:O	2.20	0.42
4:A:283:G:O6	4:A:287:G:N2	2.53	0.42
4:A:514:G:O2'	4:A:843:C:O2'	2.23	0.42
4:A:1733:U:O2'	4:A:1745:A:N7	2.43	0.42
10:I:38:PHE:CE2	10:I:73:LEU:HD21	2.55	0.42
10:I:55:ARG:NH2	10:I:58:ASP:OD1	2.51	0.42
14:O:103:ALA:HB1	14:O:105:GLU:OE1	2.20	0.42
4:A:906:G:O2'	4:A:963:G:O6	2.30	0.42
4:A:2785:U:OP2	33:j:19:ARG:NH2	2.45	0.42
20:U:26:GLY:O	20:U:29:HIS:ND1	2.53	0.42
28:d:38:GLU:OE1	28:d:38:GLU:N	2.53	0.42
22:W:22:ASP:OD1	22:W:25:ARG:NH1	2.46	0.41
4:A:1290:G:O6	15:P:18:ARG:NH2	2.50	0.41
16:Q:12:GLU:O	16:Q:87:LYS:NZ	2.54	0.41
12:L:14:GLU:C	12:L:17:SER:HG	2.17	0.41
14:O:90:ASP:OD1	14:O:91:LYS:N	2.52	0.41
1:O:139:ILE:HD13	1:O:156:VAL:O	2.20	0.41
4:A:2089:A:O2'	4:A:2090:G:OP2	2.37	0.41
12:L:26:ILE:HG21	12:L:96:LEU:HD13	2.03	0.41
1:O:46:GLN:OE1	1:O:46:GLN:N	2.53	0.41
1:O:335:ASN:ND2	1:O:348:VAL:HG13	2.35	0.41
4:A:217:G:N2	4:A:219:A:N3	2.63	0.41
4:A:551:A:O2'	4:A:552:G:O5'	2.38	0.41
4:A:657:G:O2'	4:A:660:G:O6	2.37	0.41
4:A:1093:G:N2	4:A:1156:G:O2'	2.54	0.41
4:A:1929:A:O2'	4:A:1930:A:OP1	2.35	0.41
6:E:139:THR:N	6:E:163:GLN:OE1	2.54	0.41
12:L:12:VAL:HG23	12:L:63:ALA:HB2	2.03	0.41
15:P:109:VAL:N	15:P:126:ASN:OD1	2.54	0.41
16:Q:28:HIS:O	16:Q:134:ARG:NH2	2.53	0.41
11:K:28:LEU:O	11:K:32:GLY:N	2.48	0.41
4:A:1046:A:OP2	4:A:1200:G:N1	2.44	0.41
4:A:2868:G:H21	19:T:2:GLN:HE22	1.68	0.41
4:A:247:A:OP2	32:i:8:ARG:NH2	2.46	0.41
4:A:775:G:H3'	4:A:776:G:H5'	2.03	0.41
4:A:1152:G:O2'	12:L:30:TYR:OH	2.03	0.41
4:A:1464:A:O2'	4:A:1465:A:O5'	2.36	0.41
4:A:2713:U:OP2	19:T:51:ARG:NH1	2.54	0.41
4:A:2774:C:H42	4:A:2788:G:H1	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:35:ALA:O	6:E:62:TYR:N	2.51	0.41
6:E:264:ASN:OD1	6:E:265:LYS:N	2.51	0.41
10:I:21:ASP:OD1	10:I:24:THR:OG1	2.31	0.41
31:h:35:ARG:O	31:h:38:GLY:N	2.54	0.41
8:G:167:ALA:HA	8:G:170:ILE:HD13	2.02	0.41
29:f:28:THR:O	29:f:37:LYS:N	2.54	0.41
4:A:2502:U:OP1	4:A:2558:G:N2	2.48	0.40
12:L:55:TYR:CE2	12:L:82:ILE:HD11	2.56	0.40
1:O:350:ASN:OD1	1:O:351:TYR:N	2.54	0.40
4:A:221:G:H22	4:A:238:U:H4'	1.86	0.40
4:A:1322:G:N1	4:A:1325:A:OP2	2.54	0.40
10:I:163:ILE:HD12	10:I:163:ILE:H	1.86	0.40
16:Q:50:ALA:HB1	16:Q:121:ALA:HB1	2.04	0.40
23:X:30:VAL:HG12	23:X:31:ASP:N	2.35	0.40
4:A:645:C:O2'	4:A:649:G:OP1	2.31	0.40
4:A:1002:G:OP2	16:Q:14:ARG:NH2	2.54	0.40
4:A:1759:U:O2'	4:A:1760:A:O5'	2.40	0.40
18:S:32:ASN:OD1	18:S:33:VAL:N	2.50	0.40
4:A:1866:C:O2'	4:A:1956:A:N3	2.43	0.40
4:A:2063:U:O2'	4:A:2064:G:O5'	2.34	0.40
14:O:79:PHE:CE1	19:T:70:VAL:HG13	2.55	0.40
16:Q:26:GLU:OE1	16:Q:26:GLU:N	2.55	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	524/597 (88%)	480 (92%)	41 (8%)	3 (1%)	21	51
2	1	81/86 (94%)	76 (94%)	5 (6%)	0	100	100
6	E	270/277 (98%)	257 (95%)	11 (4%)	2 (1%)	18	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F	204/209 (98%)	187 (92%)	17 (8%)	0	100	100
8	G	203/207 (98%)	184 (91%)	19 (9%)	0	100	100
9	H	160/179 (89%)	141 (88%)	19 (12%)	0	100	100
10	I	173/179 (97%)	153 (88%)	20 (12%)	0	100	100
11	K	130/141 (92%)	115 (88%)	15 (12%)	0	100	100
12	L	107/166 (64%)	106 (99%)	1 (1%)	0	100	100
13	N	140/145 (97%)	127 (91%)	13 (9%)	0	100	100
14	O	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
15	P	144/146 (99%)	136 (94%)	8 (6%)	0	100	100
16	Q	133/144 (92%)	117 (88%)	16 (12%)	0	100	100
17	R	117/120 (98%)	106 (91%)	11 (9%)	0	100	100
18	S	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
19	T	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
20	U	115/119 (97%)	106 (92%)	8 (7%)	1 (1%)	14	41
21	V	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
22	W	107/113 (95%)	94 (88%)	13 (12%)	0	100	100
23	X	88/95 (93%)	83 (94%)	5 (6%)	0	100	100
24	Y	99/103 (96%)	84 (85%)	15 (15%)	0	100	100
25	a	79/94 (84%)	71 (90%)	8 (10%)	0	100	100
26	b	56/62 (90%)	50 (89%)	6 (11%)	0	100	100
27	c	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
28	d	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
29	f	51/59 (86%)	47 (92%)	4 (8%)	0	100	100
30	g	46/49 (94%)	41 (89%)	5 (11%)	0	100	100
31	h	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
32	i	62/66 (94%)	59 (95%)	3 (5%)	0	100	100
33	j	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	3734/4021 (93%)	3404 (91%)	324 (9%)	6 (0%)	44	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	491	PRO

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Mol	Chain	Res	Type
6	E	156	ARG
6	E	155	VAL
1	0	447	ASN
1	0	538	LYS
20	U	90	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	372/527 (71%)	372 (100%)	0	100	100
2	1	73/75 (97%)	73 (100%)	0	100	100
6	E	220/225 (98%)	220 (100%)	0	100	100
7	F	167/170 (98%)	167 (100%)	0	100	100
8	G	169/170 (99%)	169 (100%)	0	100	100
9	H	139/154 (90%)	139 (100%)	0	100	100
10	I	148/151 (98%)	148 (100%)	0	100	100
11	K	102/110 (93%)	102 (100%)	0	100	100
12	L	98/138 (71%)	97 (99%)	1 (1%)	68	89
13	N	120/123 (98%)	120 (100%)	0	100	100
14	O	101/101 (100%)	101 (100%)	0	100	100
15	P	110/110 (100%)	110 (100%)	0	100	100
16	Q	109/116 (94%)	109 (100%)	0	100	100
17	R	99/100 (99%)	99 (100%)	0	100	100
18	S	93/93 (100%)	93 (100%)	0	100	100
19	T	100/100 (100%)	100 (100%)	0	100	100
20	U	96/98 (98%)	96 (100%)	0	100	100
21	V	83/84 (99%)	83 (100%)	0	100	100
22	W	90/93 (97%)	90 (100%)	0	100	100
23	X	81/85 (95%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y	85/87 (98%)	85 (100%)	0	100	100
25	a	63/74 (85%)	63 (100%)	0	100	100
26	b	47/50 (94%)	47 (100%)	0	100	100
27	c	56/57 (98%)	56 (100%)	0	100	100
28	d	52/53 (98%)	52 (100%)	0	100	100
29	f	47/53 (89%)	47 (100%)	0	100	100
30	g	46/47 (98%)	46 (100%)	0	100	100
31	h	39/39 (100%)	39 (100%)	0	100	100
32	i	54/56 (96%)	54 (100%)	0	100	100
33	j	35/35 (100%)	35 (100%)	0	100	100
All	All	3094/3374 (92%)	3093 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
12	L	14	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	259	HIS
1	0	393	GLN
16	Q	13	HIS
20	U	38	GLN
20	U	101	ASN
22	W	37	ASN
22	W	97	ASN
24	Y	2	HIS
24	Y	53	GLN
24	Y	67	ASN
27	c	16	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	71/76 (93%)	22 (30%)	5 (7%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	2805/2926 (95%)	665 (23%)	59 (2%)
5	B	111/119 (93%)	31 (27%)	3 (2%)
All	All	2987/3121 (95%)	718 (24%)	67 (2%)

All (718) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	8	U
3	2	14	A
3	2	19	G
3	2	21	A
3	2	23	A
3	2	33	U
3	2	35	G
3	2	36	C
3	2	37	A
3	2	38	C
3	2	39	G
3	2	44	A
3	2	45	G
3	2	46	G
3	2	49	A
3	2	55	U
3	2	58	A
3	2	59	U
3	2	60	C
3	2	61	C
3	2	74	C
3	2	76	A
4	A	13	A
4	A	14	A
4	A	15	G
4	A	23	G
4	A	26	G
4	A	34	U
4	A	35	G
4	A	36	G
4	A	46	C
4	A	55	G
4	A	61	A
4	A	62	C
4	A	63	G

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Mol	Chain	Res	Type
4	A	71	A
4	A	74	U
4	A	75	G
4	A	76	C
4	A	77	U
4	A	78	U
4	A	79	C
4	A	80	G
4	A	84	A
4	A	85	G
4	A	86	C
4	A	87	U
4	A	89	U
4	A	90	A
4	A	92	G
4	A	93	C
4	A	96	G
4	A	101	G
4	A	117	A
4	A	118	A
4	A	119	U
4	A	125	A
4	A	126	A
4	A	133	A
4	A	141	U
4	A	150	A
4	A	164	U
4	A	175	G
4	A	176	A
4	A	178	A
4	A	179	A
4	A	183	A
4	A	184	G
4	A	185	A
4	A	188	C
4	A	189	G
4	A	191	G
4	A	199	A
4	A	200	A
4	A	202	A
4	A	216	A
4	A	219	A

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Mol	Chain	Res	Type
4	A	224	A
4	A	225	A
4	A	226	A
4	A	227	G
4	A	229	A
4	A	231	A
4	A	232	U
4	A	233	G
4	A	234	C
4	A	235	G
4	A	236	A
4	A	244	A
4	A	251	G
4	A	252	C
4	A	253	G
4	A	258	A
4	A	266	U
4	A	267	C
4	A	270	C
4	A	275	A
4	A	283	G
4	A	284	C
4	A	286	U
4	A	287	G
4	A	288	C
4	A	290	U
4	A	291	C
4	A	298	U
4	A	301	U
4	A	302	A
4	A	309	U
4	A	310	C
4	A	314	A
4	A	321	U
4	A	329	A
4	A	345	A
4	A	346	G
4	A	348	U
4	A	349	C
4	A	360	C
4	A	367	G
4	A	368	G

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Mol	Chain	Res	Type
4	A	373	A
4	A	374	A
4	A	375	C
4	A	379	C
4	A	387	C
4	A	394	U
4	A	402	U
4	A	405	U
4	A	407	A
4	A	410	G
4	A	411	G
4	A	412	A
4	A	413	U
4	A	418	A
4	A	419	G
4	A	420	U
4	A	421	A
4	A	427	G
4	A	432	C
4	A	433	G
4	A	434	U
4	A	435	G
4	A	444	U
4	A	458	G
4	A	471	G
4	A	483	C
4	A	491	C
4	A	495	U
4	A	498	U
4	A	502	C
4	A	504	A
4	A	505	G
4	A	528	G
4	A	529	C
4	A	533	C
4	A	542	G
4	A	550	G
4	A	551	A
4	A	554	U
4	A	555	C
4	A	556	C
4	A	559	A

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Mol	Chain	Res	Type
4	A	564	G
4	A	573	C
4	A	576	G
4	A	577	U
4	A	578	A
4	A	579	G
4	A	592	A
4	A	593	A
4	A	594	C
4	A	595	G
4	A	599	G
4	A	607	G
4	A	615	U
4	A	617	G
4	A	618	A
4	A	619	A
4	A	631	G
4	A	646	A
4	A	647	A
4	A	648	G
4	A	649	G
4	A	658	A
4	A	659	A
4	A	662	U
4	A	667	A
4	A	673	A
4	A	677	A
4	A	683	A
4	A	690	A
4	A	691	U
4	A	700	U
4	A	701	G
4	A	702	A
4	A	733	U
4	A	752	A
4	A	764	C
4	A	765	A
4	A	777	C
4	A	787	C
4	A	788	G
4	A	792	G
4	A	794	U

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Mol	Chain	Res	Type
4	A	795	G
4	A	804	G
4	A	810	G
4	A	811	A
4	A	812	G
4	A	822	G
4	A	829	A
4	A	830	A
4	A	831	U
4	A	832	G
4	A	837	U
4	A	838	C
4	A	839	G
4	A	847	A
4	A	852	G
4	A	859	C
4	A	866	A
4	A	874	U
4	A	875	U
4	A	877	G
4	A	892	U
4	A	908	A
4	A	913	A
4	A	916	G
4	A	918	U
4	A	929	G
4	A	939	G
4	A	940	G
4	A	942	U
4	A	943	A
4	A	944	C
4	A	946	G
4	A	948	A
4	A	954	U
4	A	957	A
4	A	959	C
4	A	961	C
4	A	962	C
4	A	964	A
4	A	973	G
4	A	977	U
4	A	978	A

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Mol	Chain	Res	Type
4	A	979	U
4	A	980	C
4	A	987	A
4	A	991	A
4	A	992	G
4	A	999	A
4	A	1003	A
4	A	1005	A
4	A	1007	G
4	A	1019	A
4	A	1020	A
4	A	1029	A
4	A	1036	A
4	A	1037	C
4	A	1042	A
4	A	1051	C
4	A	1058	U
4	A	1059	A
4	A	1063	G
4	A	1067	A
4	A	1068	G
4	A	1069	U
4	A	1071	G
4	A	1073	A
4	A	1079	U
4	A	1081	U
4	A	1084	A
4	A	1091	U
4	A	1092	A
4	A	1093	G
4	A	1102	G
4	A	1103	A
4	A	1108	G
4	A	1115	A
4	A	1116	A
4	A	1118	C
4	A	1119	A
4	A	1129	U
4	A	1130	A
4	A	1133	G
4	A	1134	A
4	A	1143	U

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Mol	Chain	Res	Type
4	A	1147	U
4	A	1156	G
4	A	1157	A
4	A	1158	G
4	A	1159	U
4	A	1160	G
4	A	1161	A
4	A	1173	A
4	A	1174	A
4	A	1175	A
4	A	1176	U
4	A	1177	G
4	A	1179	A
4	A	1181	C
4	A	1182	G
4	A	1185	G
4	A	1188	A
4	A	1189	A
4	A	1197	A
4	A	1201	A
4	A	1203	G
4	A	1209	G
4	A	1236	G
4	A	1251	U
4	A	1252	G
4	A	1259	G
4	A	1260	A
4	A	1278	G
4	A	1284	A
4	A	1293	A
4	A	1295	U
4	A	1296	G
4	A	1305	A
4	A	1306	G
4	A	1307	U
4	A	1311	G
4	A	1312	A
4	A	1313	A
4	A	1314	A
4	A	1315	G
4	A	1319	G
4	A	1323	A

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Mol	Chain	Res	Type
4	A	1333	C
4	A	1339	A
4	A	1340	A
4	A	1341	U
4	A	1343	C
4	A	1346	A
4	A	1351	U
4	A	1352	U
4	A	1363	G
4	A	1364	C
4	A	1365	U
4	A	1366	C
4	A	1368	U
4	A	1370	C
4	A	1371	G
4	A	1372	C
4	A	1375	A
4	A	1376	G
4	A	1380	U
4	A	1384	C
4	A	1385	G
4	A	1388	A
4	A	1389	C
4	A	1391	U
4	A	1404	A
4	A	1417	A
4	A	1418	U
4	A	1424	A
4	A	1425	C
4	A	1426	A
4	A	1427	G
4	A	1428	G
4	A	1431	G
4	A	1434	A
4	A	1435	U
4	A	1436	U
4	A	1442	A
4	A	1448	U
4	A	1449	C
4	A	1450	C
4	A	1459	U
4	A	1460	G

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Mol	Chain	Res	Type
4	A	1465	A
4	A	1466	U
4	A	1472	G
4	A	1473	A
4	A	1474	C
4	A	1476	C
4	A	1481	G
4	A	1489	U
4	A	1490	A
4	A	1499	A
4	A	1500	U
4	A	1501	U
4	A	1502	G
4	A	1506	A
4	A	1507	U
4	A	1508	C
4	A	1516	A
4	A	1525	G
4	A	1526	G
4	A	1527	C
4	A	1528	U
4	A	1529	G
4	A	1530	G
4	A	1531	G
4	A	1532	A
4	A	1533	A
4	A	1536	A
4	A	1539	C
4	A	1540	A
4	A	1542	A
4	A	1543	U
4	A	1545	C
4	A	1550	C
4	A	1551	C
4	A	1553	A
4	A	1556	A
4	A	1558	G
4	A	1559	C
4	A	1560	U
4	A	1561	G
4	A	1566	G
4	A	1568	G

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Mol	Chain	Res	Type
4	A	1569	A
4	A	1570	U
4	A	1571	G
4	A	1576	G
4	A	1577	C
4	A	1595	U
4	A	1602	U
4	A	1608	A
4	A	1614	A
4	A	1615	A
4	A	1617	A
4	A	1626	U
4	A	1632	G
4	A	1652	C
4	A	1653	A
4	A	1655	A
4	A	1661	A
4	A	1672	A
4	A	1684	U
4	A	1685	A
4	A	1692	U
4	A	1693	C
4	A	1696	G
4	A	1697	A
4	A	1699	A
4	A	1700	A
4	A	1705	C
4	A	1708	U
4	A	1710	A
4	A	1712	G
4	A	1713	A
4	A	1719	G
4	A	1738	U
4	A	1743	A
4	A	1745	A
4	A	1748	G
4	A	1757	G
4	A	1758	U
4	A	1759	U
4	A	1760	A
4	A	1761	G
4	A	1762	G

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Mol	Chain	Res	Type
4	A	1766	C
4	A	1767	A
4	A	1768	A
4	A	1771	C
4	A	1776	A
4	A	1778	A
4	A	1779	G
4	A	1782	G
4	A	1785	G
4	A	1793	G
4	A	1802	A
4	A	1811	C
4	A	1812	A
4	A	1814	A
4	A	1820	A
4	A	1829	C
4	A	1830	G
4	A	1839	A
4	A	1841	G
4	A	1845	A
4	A	1846	G
4	A	1864	G
4	A	1865	C
4	A	1872	C
4	A	1877	A
4	A	1882	A
4	A	1883	A
4	A	1884	G
4	A	1885	A
4	A	1887	G
4	A	1891	G
4	A	1898	G
4	A	1899	U
4	A	1904	G
4	A	1935	G
4	A	1936	G
4	A	1956	A
4	A	1958	G
4	A	1959	G
4	A	1960	U
4	A	1967	A
4	A	1968	U

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Mol	Chain	Res	Type
4	A	1969	U
4	A	1972	U
4	A	1973	U
4	A	1984	U
4	A	1989	A
4	A	1993	G
4	A	1996	C
4	A	1999	A
4	A	2000	A
4	A	2001	G
4	A	2020	U
4	A	2022	U
4	A	2025	C
4	A	2026	A
4	A	2049	A
4	A	2051	U
4	A	2052	A
4	A	2054	C
4	A	2060	A
4	A	2061	G
4	A	2062	A
4	A	2064	G
4	A	2072	C
4	A	2078	A
4	A	2081	G
4	A	2084	C
4	A	2085	G
4	A	2089	A
4	A	2090	G
4	A	2098	G
4	A	2109	G
4	A	2121	U
4	A	2123	A
4	A	2125	U
4	A	2128	U
4	A	2129	G
4	A	2219	G
4	A	2227	A
4	A	2228	A
4	A	2232	G
4	A	2233	C
4	A	2240	U

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Mol	Chain	Res	Type
4	A	2245	G
4	A	2246	G
4	A	2249	G
4	A	2252	A
4	A	2254	A
4	A	2255	C
4	A	2267	G
4	A	2268	G
4	A	2280	G
4	A	2296	A
4	A	2308	G
4	A	2312	C
4	A	2315	A
4	A	2316	A
4	A	2317	A
4	A	2323	C
4	A	2325	U
4	A	2328	G
4	A	2333	G
4	A	2334	U
4	A	2335	U
4	A	2336	G
4	A	2337	G
4	A	2338	A
4	A	2340	A
4	A	2341	U
4	A	2342	C
4	A	2343	A
4	A	2345	U
4	A	2347	G
4	A	2348	C
4	A	2349	A
4	A	2350	G
4	A	2351	A
4	A	2354	G
4	A	2356	A
4	A	2363	C
4	A	2364	A
4	A	2374	G
4	A	2376	C
4	A	2379	C
4	A	2390	A

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Mol	Chain	Res	Type
4	A	2401	G
4	A	2412	G
4	A	2414	C
4	A	2415	U
4	A	2417	A
4	A	2420	G
4	A	2421	A
4	A	2425	G
4	A	2430	U
4	A	2431	U
4	A	2435	C
4	A	2451	C
4	A	2452	U
4	A	2453	C
4	A	2454	A
4	A	2455	A
4	A	2458	G
4	A	2459	A
4	A	2460	U
4	A	2464	A
4	A	2468	A
4	A	2469	C
4	A	2470	C
4	A	2474	G
4	A	2476	G
4	A	2477	A
4	A	2488	A
4	A	2505	A
4	A	2507	A
4	A	2509	C
4	A	2511	A
4	A	2520	U
4	A	2523	G
4	A	2527	C
4	A	2531	G
4	A	2532	A
4	A	2533	U
4	A	2534	G
4	A	2542	A
4	A	2547	A
4	A	2548	U
4	A	2549	C

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Mol	Chain	Res	Type
4	A	2564	G
4	A	2583	U
4	A	2591	U
4	A	2595	A
4	A	2596	G
4	A	2598	G
4	A	2601	A
4	A	2602	C
4	A	2607	G
4	A	2611	G
4	A	2613	U
4	A	2631	A
4	A	2632	G
4	A	2638	U
4	A	2639	C
4	A	2642	U
4	A	2644	U
4	A	2652	G
4	A	2659	G
4	A	2665	U
4	A	2674	G
4	A	2689	A
4	A	2690	G
4	A	2696	C
4	A	2711	G
4	A	2714	G
4	A	2718	U
4	A	2720	C
4	A	2743	G
4	A	2755	U
4	A	2762	A
4	A	2764	G
4	A	2765	G
4	A	2773	G
4	A	2779	A
4	A	2785	U
4	A	2789	C
4	A	2794	A
4	A	2798	C
4	A	2806	G
4	A	2807	A
4	A	2808	U

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Mol	Chain	Res	Type
4	A	2818	C
4	A	2820	U
4	A	2823	C
4	A	2824	G
4	A	2826	A
4	A	2831	A
4	A	2843	G
4	A	2859	G
4	A	2860	A
4	A	2868	G
4	A	2886	C
4	A	2892	G
4	A	2897	G
4	A	2899	C
4	A	2900	A
4	A	2901	G
4	A	2905	C
4	A	2911	G
4	A	2916	A
4	A	2917	G
4	A	2918	G
4	A	2925	C
5	B	10	G
5	B	13	A
5	B	15	C
5	B	19	G
5	B	22	G
5	B	23	U
5	B	24	C
5	B	32	U
5	B	33	U
5	B	35	C
5	B	38	U
5	B	39	A
5	B	40	C
5	B	41	C
5	B	42	G
5	B	48	G
5	B	49	G
5	B	50	A
5	B	53	U
5	B	54	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	55	A
5	B	62	U
5	B	85	U
5	B	86	U
5	B	87	U
5	B	88	C
5	B	97	A
5	B	101	U
5	B	107	G
5	B	108	C
5	B	110	G

All (67) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	7	U
3	2	13	C
3	2	20	G
3	2	22	G
3	2	48	C
4	A	88	G
4	A	92	G
4	A	175	G
4	A	224	A
4	A	252	C
4	A	347	G
4	A	411	G
4	A	443	G
4	A	528	G
4	A	549	A
4	A	554	U
4	A	558	G
4	A	631	G
4	A	689	A
4	A	751	G
4	A	831	U
4	A	976	U
4	A	1036	A
4	A	1066	A
4	A	1172	A
4	A	1250	G
4	A	1294	A

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Mol	Chain	Res	Type
4	A	1305	A
4	A	1313	A
4	A	1339	A
4	A	1351	U
4	A	1435	U
4	A	1448	U
4	A	1449	C
4	A	1507	U
4	A	1525	G
4	A	1530	G
4	A	1565	U
4	A	1567	U
4	A	1570	U
4	A	1631	A
4	A	1671	G
4	A	1691	A
4	A	1758	U
4	A	1784	A
4	A	1813	A
4	A	1828	G
4	A	1882	A
4	A	1883	A
4	A	1886	G
4	A	2127	U
4	A	2254	A
4	A	2295	A
4	A	2316	A
4	A	2337	G
4	A	2344	U
4	A	2420	G
4	A	2452	U
4	A	2454	A
4	A	2468	A
4	A	2510	G
4	A	2631	A
4	A	2805	A
4	A	2904	A
5	B	31	G
5	B	48	G
5	B	49	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1451:U	O3'	1452:C	P	3.09

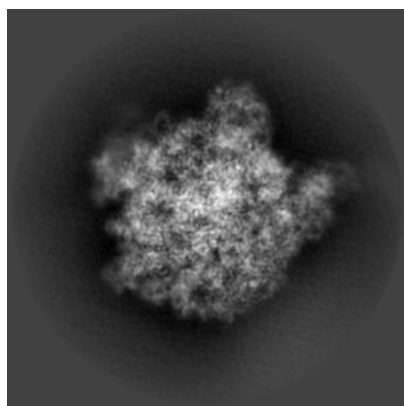
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11889. These allow visual inspection of the internal detail of the map and identification of artifacts.

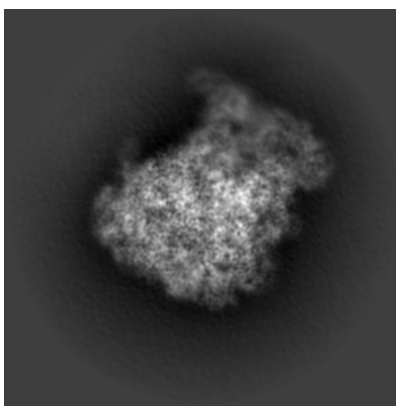
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

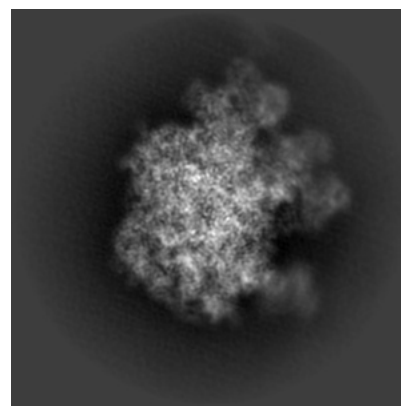
6.1.1 Primary map



X

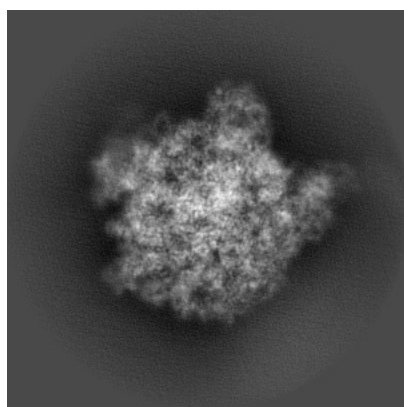


Y

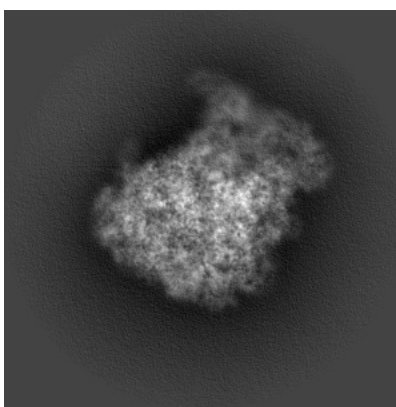


Z

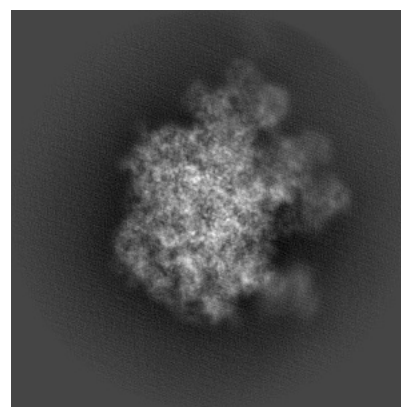
6.1.2 Raw map



X



Y

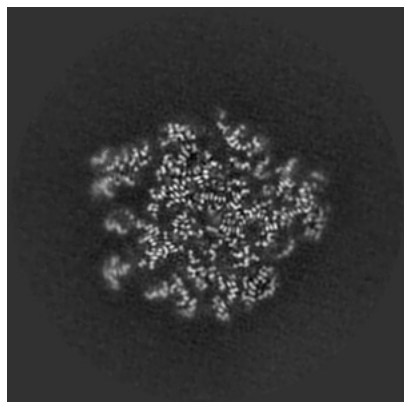


Z

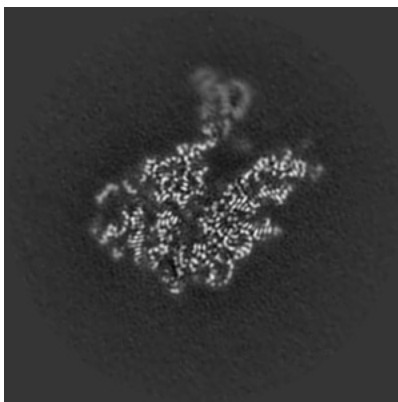
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

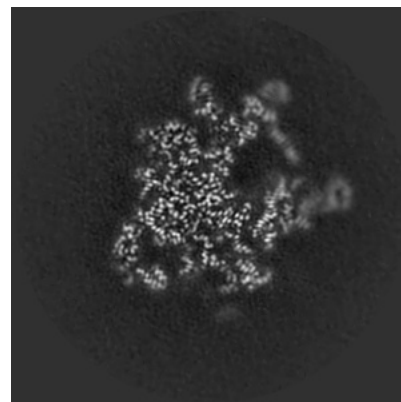
6.2.1 Primary map



X Index: 210

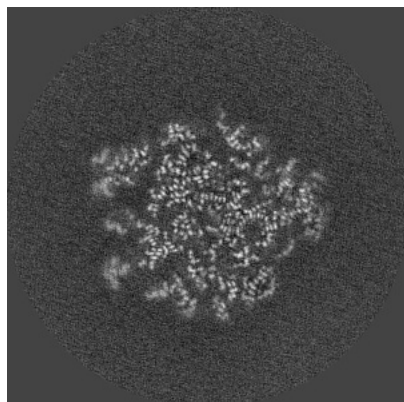


Y Index: 210

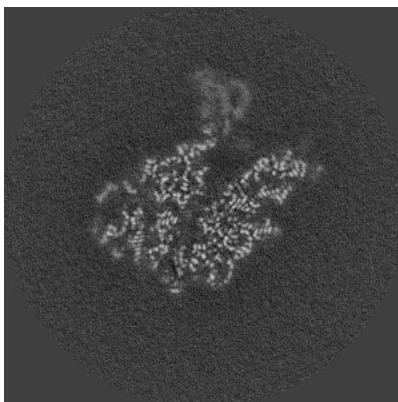


Z Index: 210

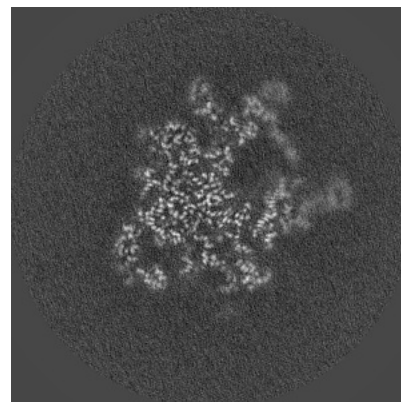
6.2.2 Raw map



X Index: 210



Y Index: 210

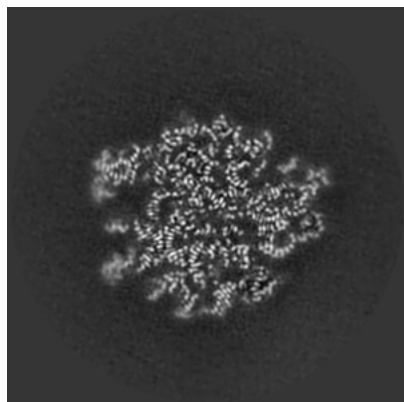


Z Index: 210

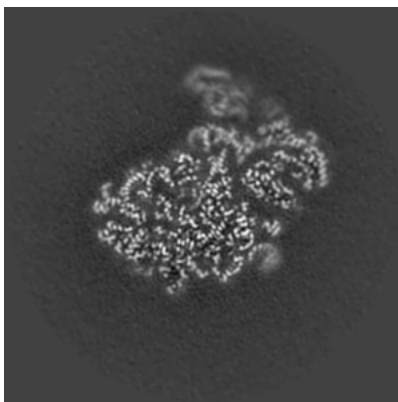
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

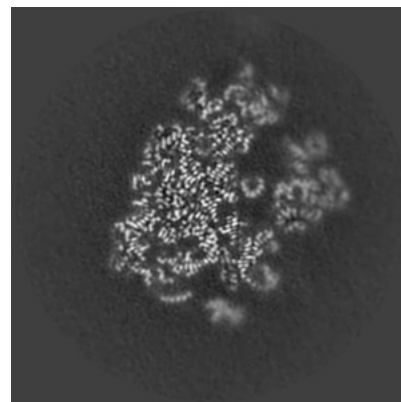
6.3.1 Primary map



X Index: 215

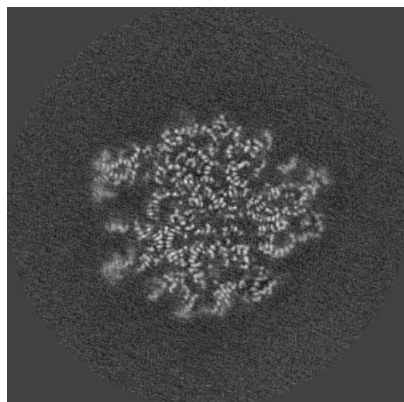


Y Index: 223

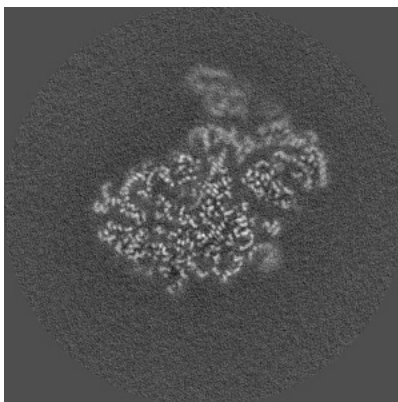


Z Index: 222

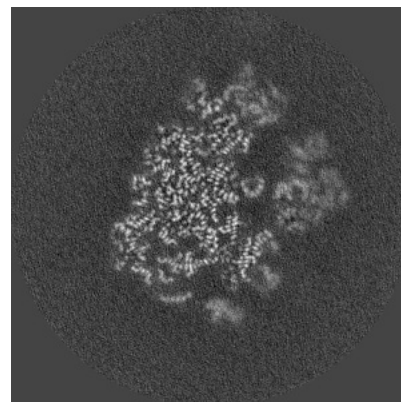
6.3.2 Raw map



X Index: 215



Y Index: 223

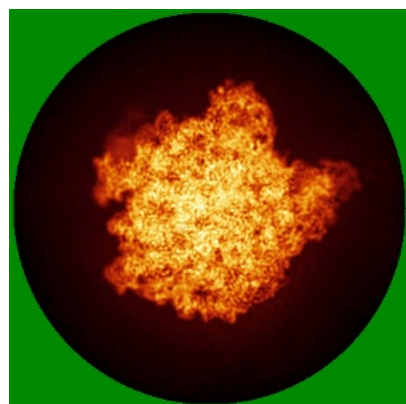


Z Index: 223

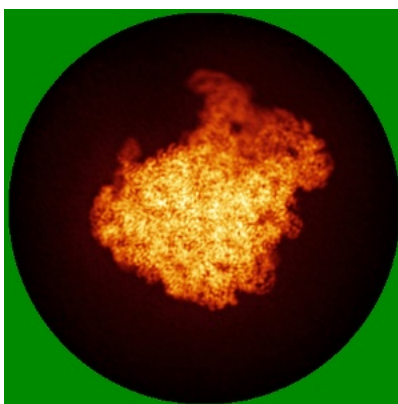
The images above show the largest variance slices of the map in three orthogonal directions.

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

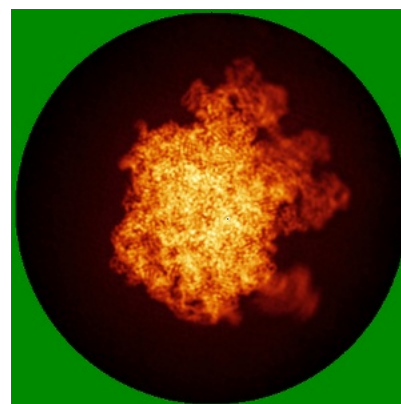
6.4.1 Primary map



X

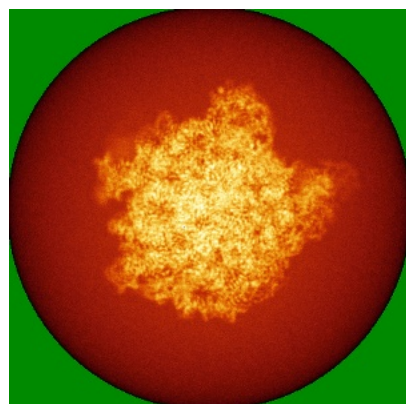


Y

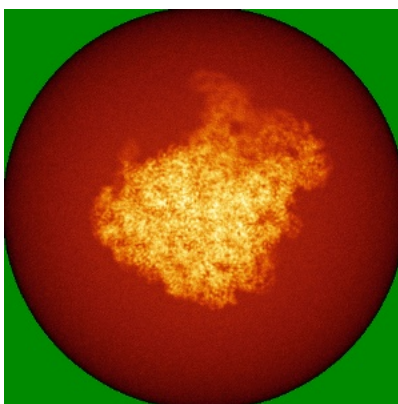


Z

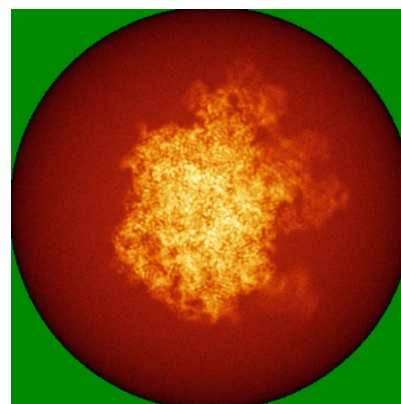
6.4.2 Raw map



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](#)

This section was not generated.

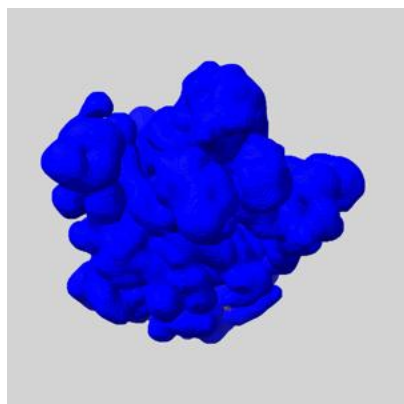
6.6 Mask visualisation [i](#)

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

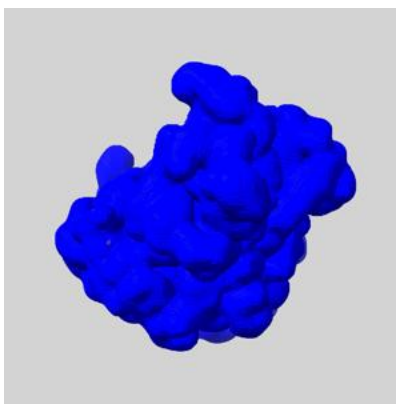
A mask typically either:

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

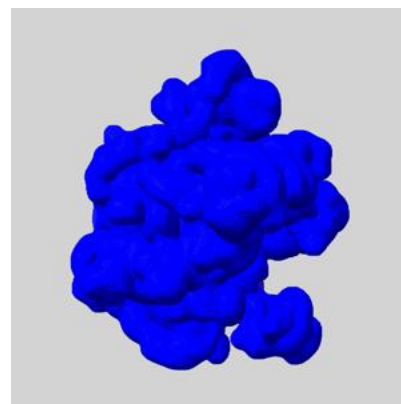
6.6.1 emd_11889_msk_1.map [i](#)



X



Y

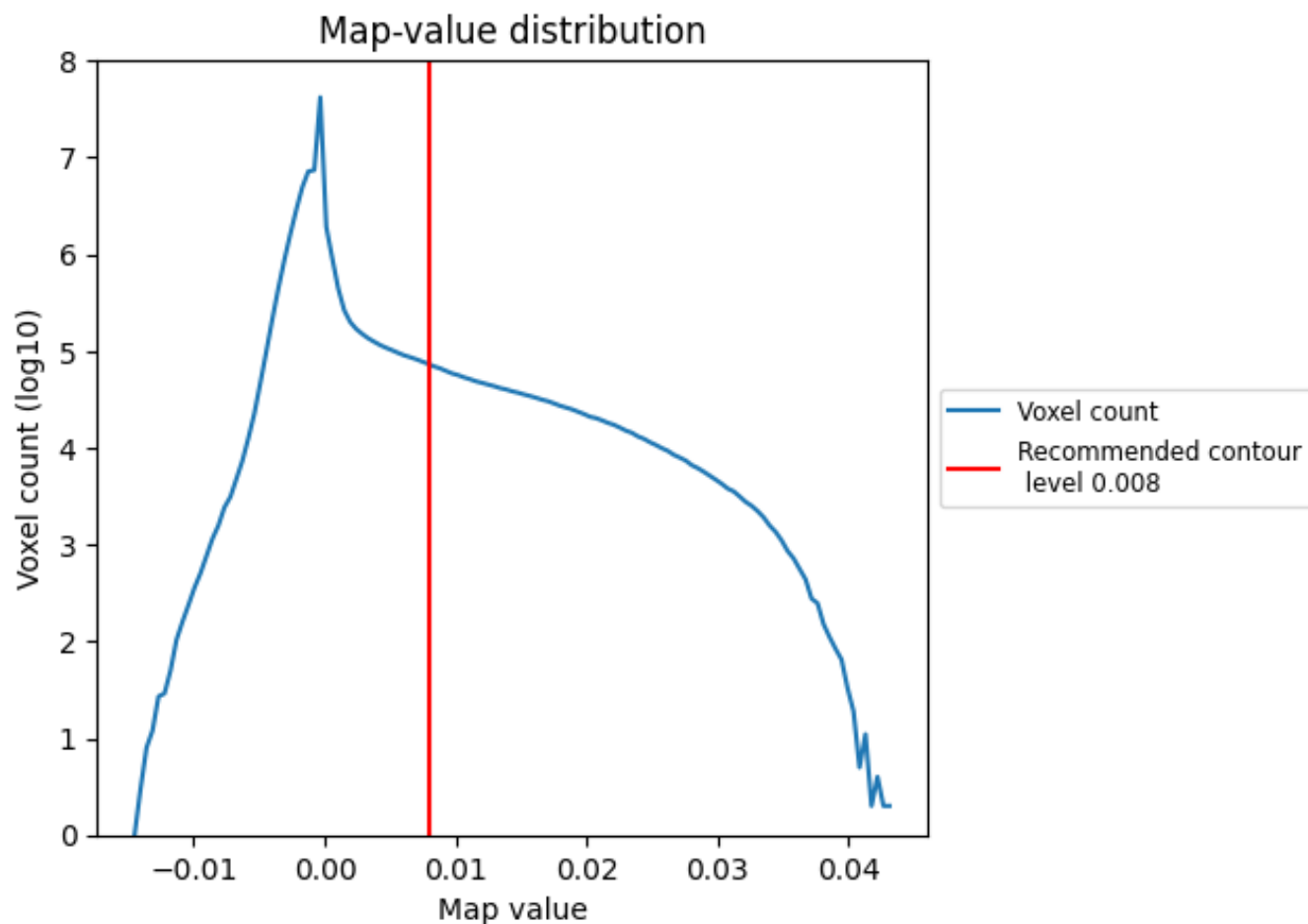


Z

7 Map analysis [i](#)

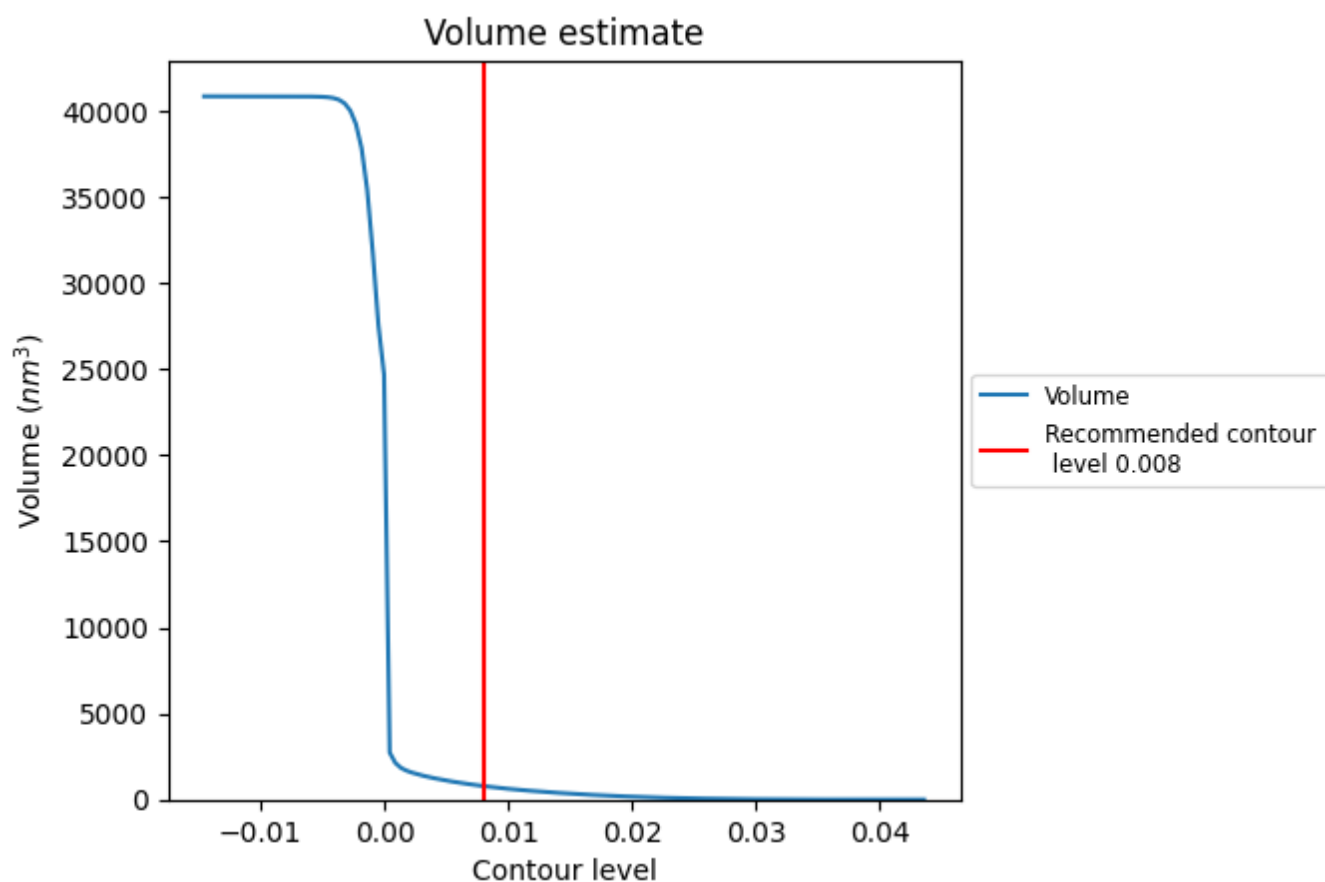
This section contains the results of statistical analysis of the map.

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.

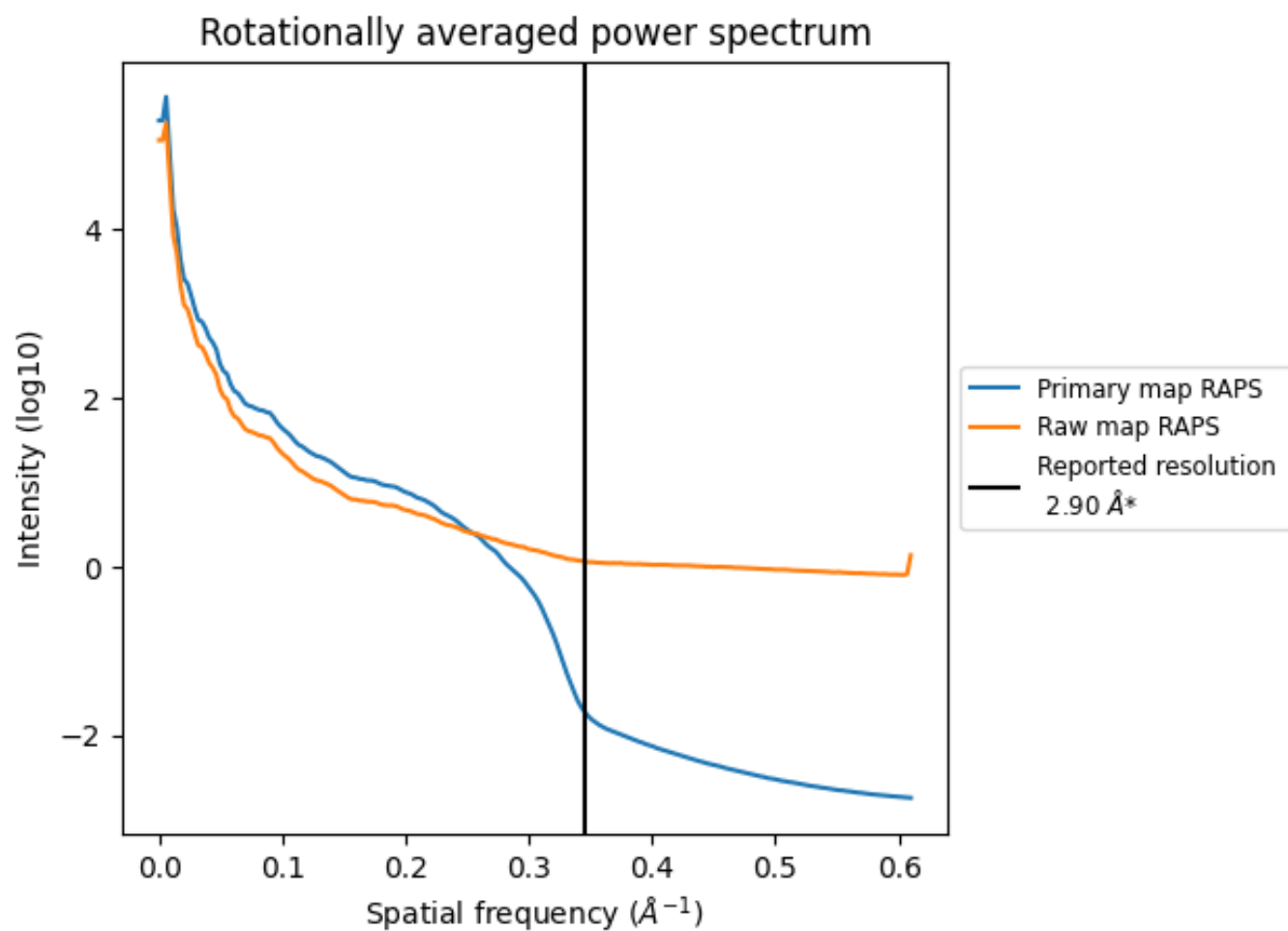
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 786 nm³; this corresponds to an approximate mass of 710 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 ⓘ

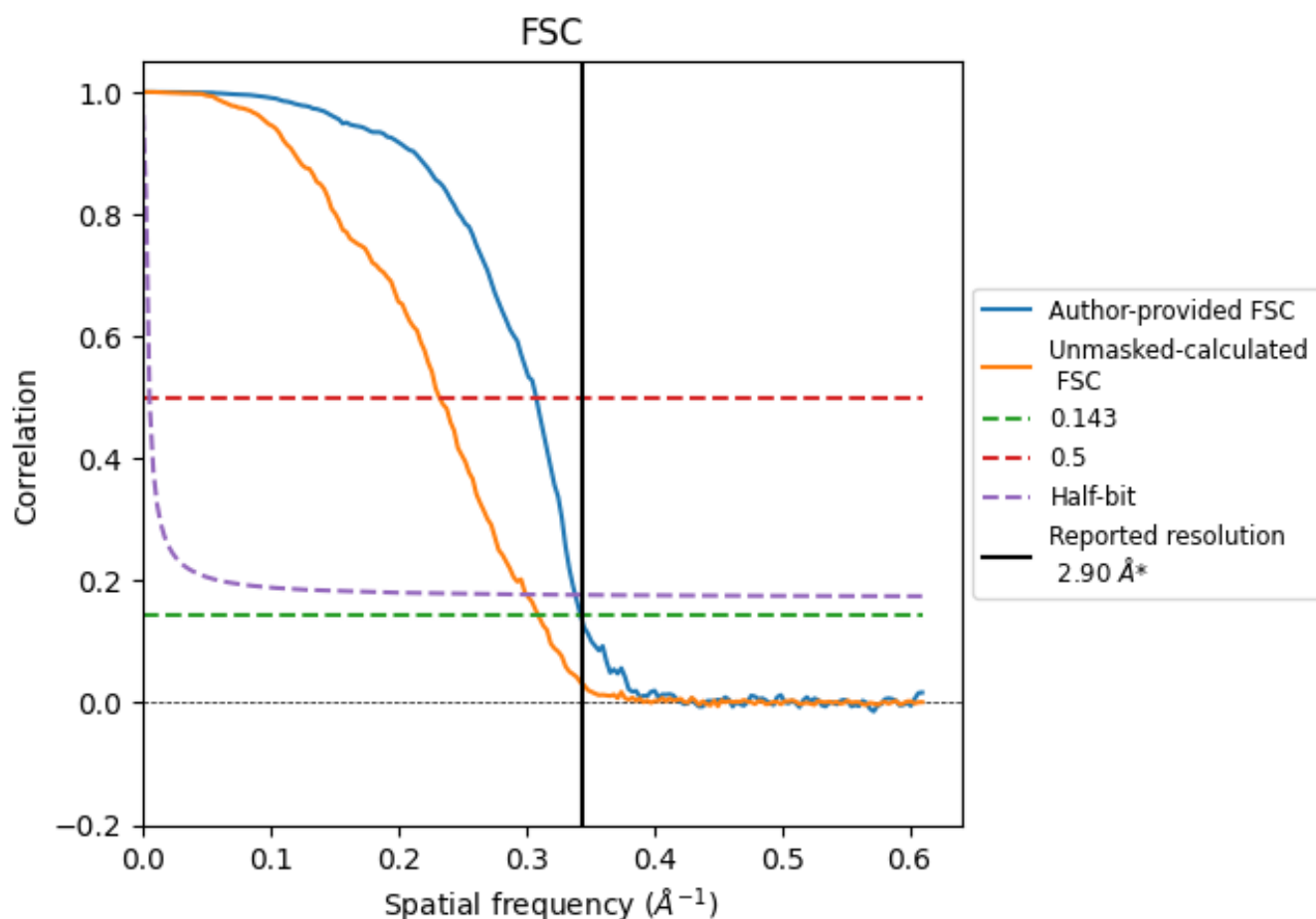


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

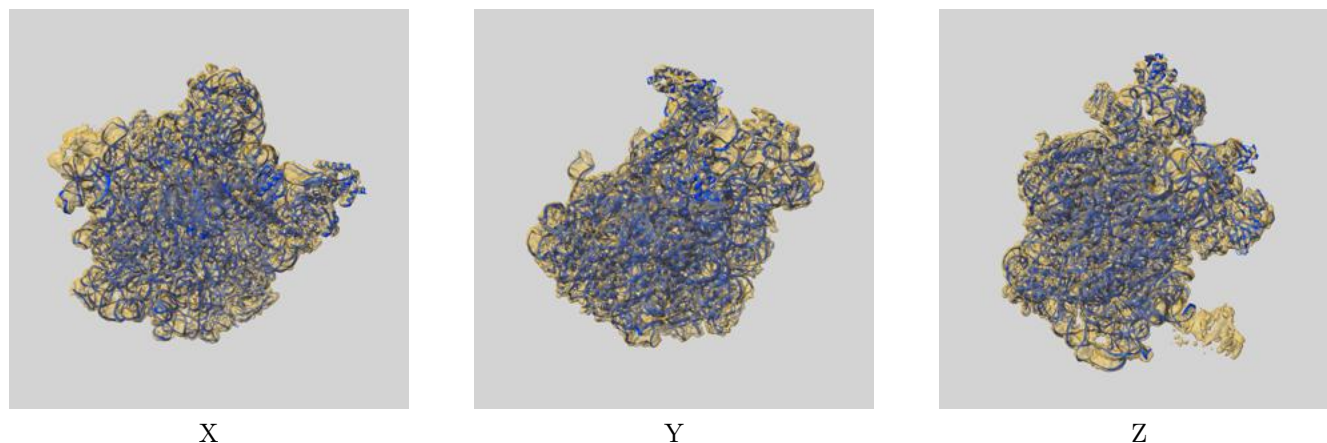
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.92	3.25	2.95
Unmasked-calculated*	3.23	4.30	3.33

*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 3.23 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

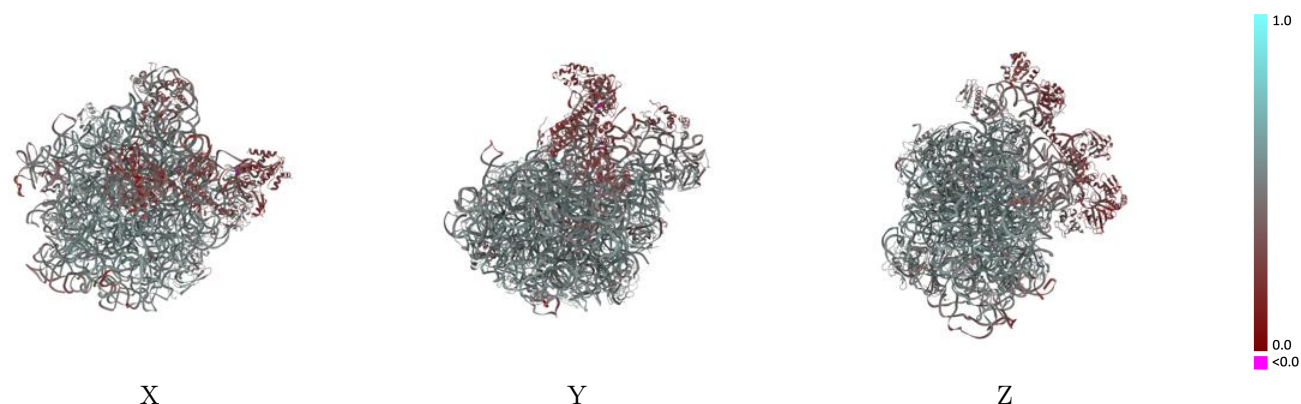
This section contains information regarding the fit between EMDB map EMD-11889 and PDB model 7AS8. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



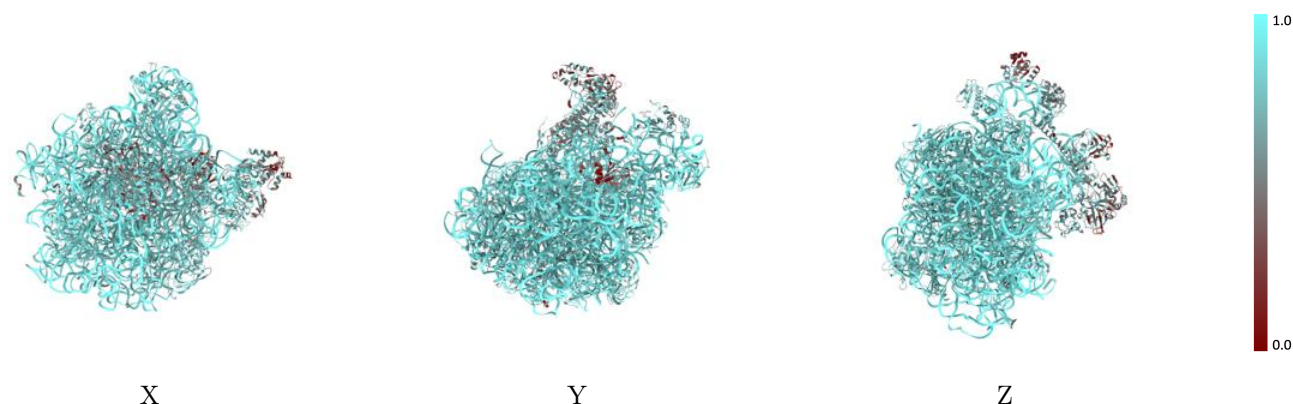
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



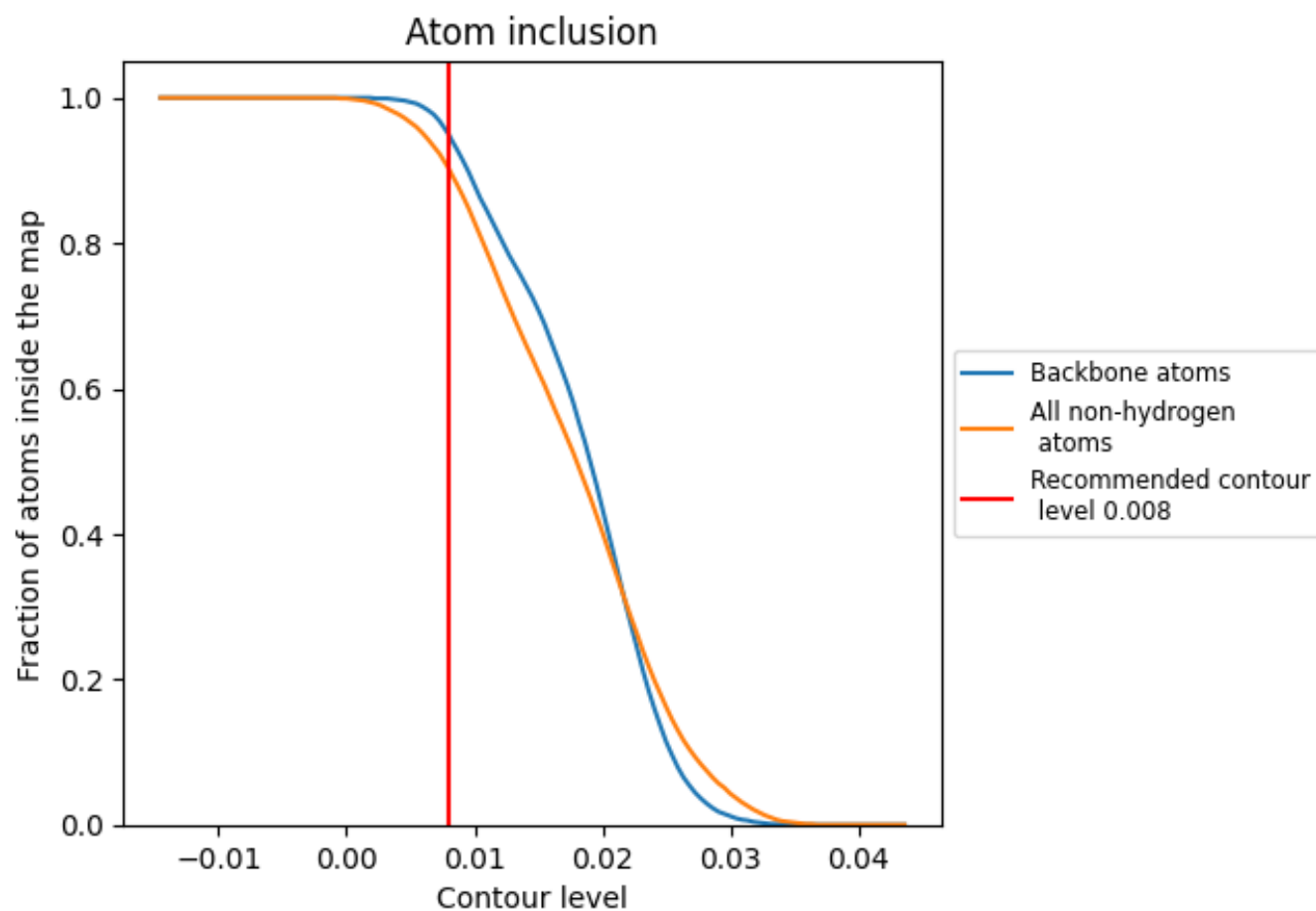
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.4970
0	 0.5310	 0.2700
1	 0.6590	 0.4060
2	 0.9200	 0.4260
A	 0.9730	 0.5250
B	 0.9700	 0.4700
E	 0.8580	 0.5290
F	 0.8240	 0.5220
G	 0.8290	 0.4960
H	 0.7260	 0.3620
I	 0.7720	 0.4410
K	 0.5310	 0.2540
L	 0.4280	 0.2840
N	 0.8320	 0.5040
O	 0.7670	 0.4930
P	 0.8280	 0.5090
Q	 0.8240	 0.5060
R	 0.8110	 0.4940
S	 0.8060	 0.4390
T	 0.7540	 0.4880
U	 0.8650	 0.5110
V	 0.8340	 0.5150
W	 0.8120	 0.5110
X	 0.7780	 0.4830
Y	 0.8030	 0.4840
a	 0.8490	 0.5240
b	 0.6090	 0.4870
c	 0.7570	 0.4190
d	 0.8180	 0.4800
f	 0.8200	 0.5190
g	 0.8170	 0.4960
h	 0.8700	 0.5390
i	 0.8500	 0.5420
j	 0.8280	 0.5240

