



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 12:49 PM EST

PDB ID : 6DZP
EMDB ID : EMD-8937
Title : Cryo-EM Structure of Mycobacterium smegmatis C(minus) 50S ribosomal subunit
Authors : Sharma, M.R.; Li, Y.; Korripella, R.; Yang, Y.; Kaushal, P.S.; Lin, Q.; Wade, J.T.; Gray, A.G.; Derbyshire, K.M.; Agrawal, R.K.; Ojha, A.
Deposited on : 2018-07-05
Resolution : 3.42 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

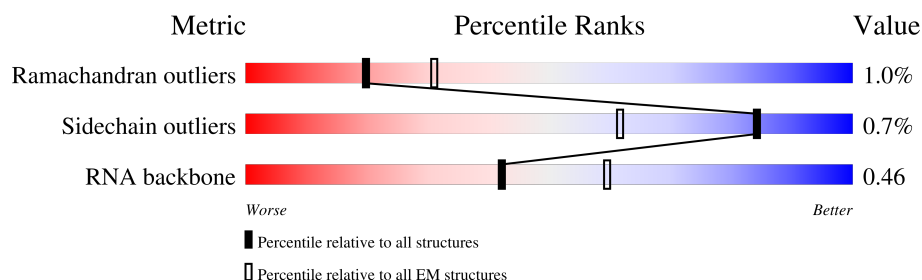
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	3119	<div> <div>5%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>
2	B	118	<div> <div>.</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
3	C	278	<div> <div>10%</div> <div>97%</div> <div>..</div> </div>
4	D	217	<div> <div>.</div> <div>96%</div> <div>..</div> </div>
5	E	214	<div> <div>.</div> <div>97%</div> <div>..</div> </div>
6	F	186	<div> <div>10%</div> <div>96%</div> <div>..</div> </div>
7	G	179	<div> <div>.</div> <div>98%</div> <div>..</div> </div>
8	H	151	<div> <div>75%</div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	175	
10	J	142	
11	K	146	
12	L	122	
13	M	147	
14	N	138	
15	O	199	
16	P	126	
17	Q	113	
18	R	129	
19	S	102	
20	T	152	
21	U	99	
22	V	105	
23	W	215	
24	X	88	
25	Z	77	
26	a	61	
27	b	57	
28	c	54	
29	d	47	
30	e	64	
31	f	37	
32	g	82	
33	y	78	

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Mol	Chain	Length	Quality of chain
34	3	23	<div><div></div><div>100%</div></div>

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 98097 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3119	Total	C	N	O	P	0	0
			66981	29854	12313	21695	3119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	151	Total	C	N	O	S	0	0
			1119	695	209	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	126	Total	C	N	O		0	0
			956	586	199	171			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	124	Total	C	N	O		0	0
			988	613	203	172			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	100	Total	C	N	O		0	0
			754	478	137	139			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	114	Total	C	N	O		0	0
			873	543	171	159			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	a	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 28 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	53	Total	C	N	O	0	0
			456	281	97	78		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	e	63	Total	C	N	O	0	0
			502	302	115	85		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 32 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	64	Total	C	N	O	S	0	0
			494	318	81	94	1		

- Molecule 33 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	y	77	Total	C	N	O	S	0	0
			617	377	132	106	2		

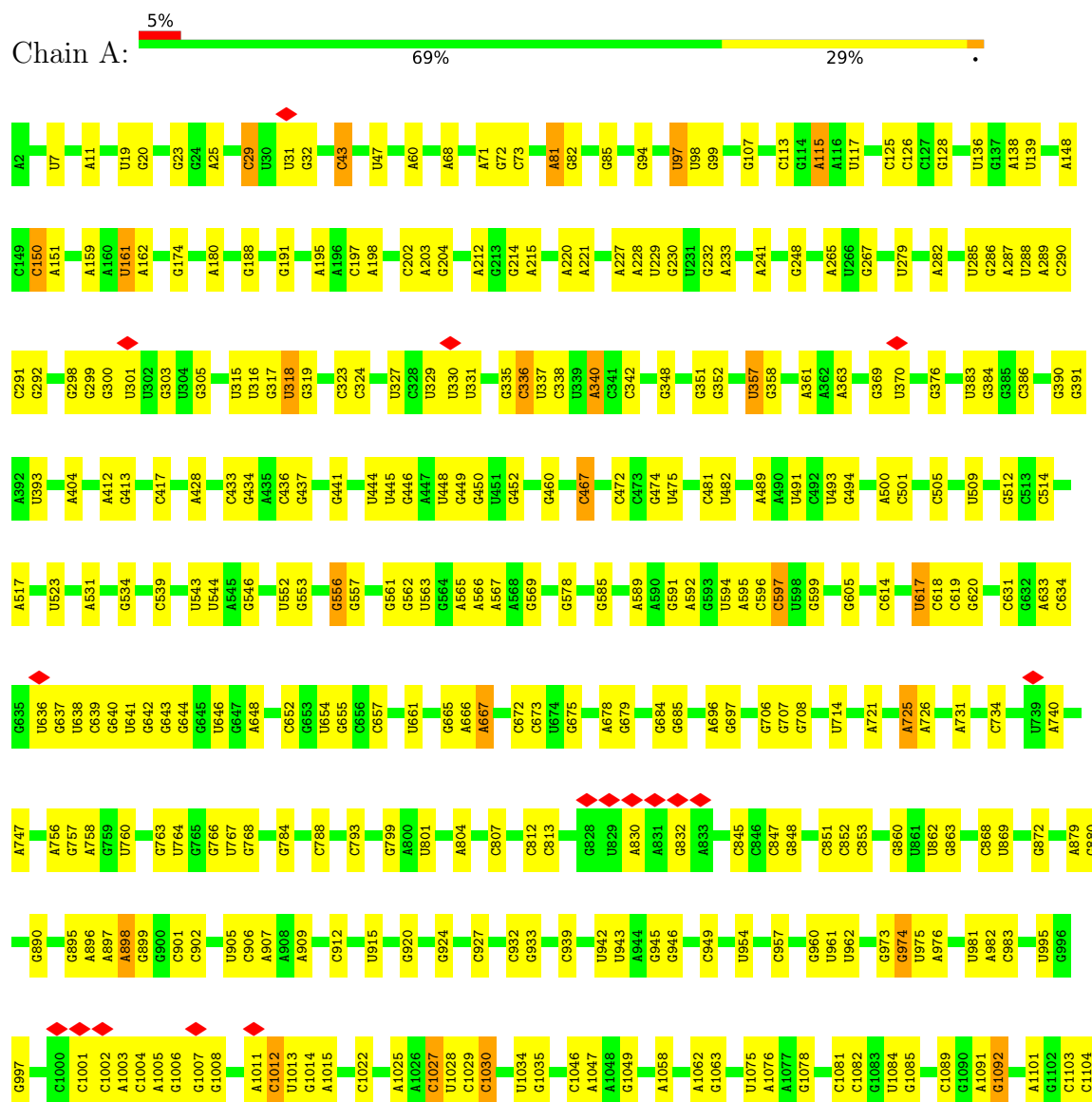
- Molecule 34 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	3	23	Total	C	N	O	0	0
			189	111	50	28		

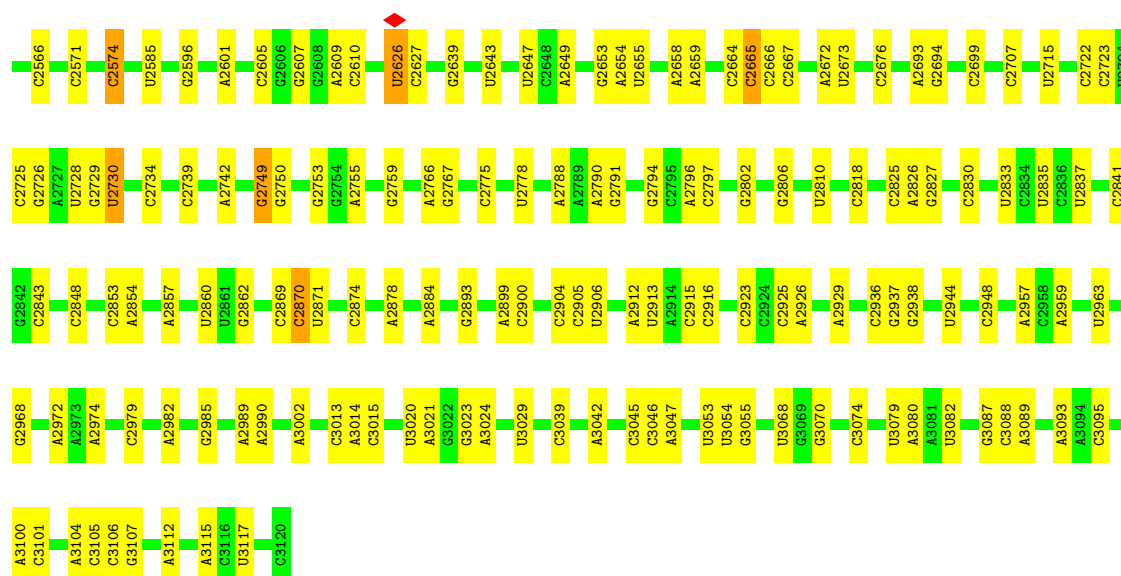
3 Residue-property plots

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

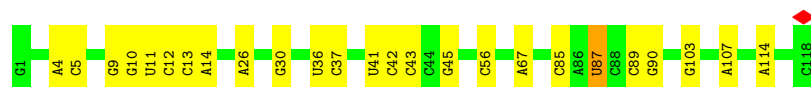
• Molecule 1: 23S rRNA



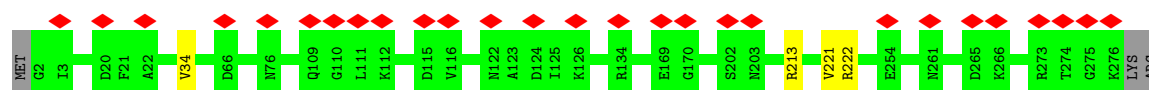
G2408	U2411	U2412	G2413	G2414	G2415	G2416	G2417	U2418	G2419	U2420	A2421	A2434	U2435	A2436	U2437	A2449	G2450	G2454	G2462	G2463	U2468	A2490	A2491	A2492	G2503	G2507	G2508	G2509	A2510	A2511	G2519	U2520	G2521	G2528	A2529	G2530	G2531	G2532	G2533	A2534	G2549	G2556	A2559	U2560	G2561														
G2346	G2347	G2348	A2349	G2350	A2351	G2352	U2353	G2354	U2355	G2356	A2357	A2358	G2359	G2360	U2361	G2362	A2363	G2366	G2367	G2368	G2369	A2370	G2373	U2374	G2375	G2376	G2377	U2378	G2379	A2381	G2382	U2383	G2384	G2385	U2386	G2387	G2388	U2389	U2390	G2391	A2392	A2393	A2394	U2395	A2396	G2397	G2398	A2399	G2400	U2401	G2402	U2403	G2404	A2405	U2406	G2407			
G2256	A2257	G2260	U2261	G2262	G2267	G2274	A2275	G2276	G2279	G2280	A2284	G2285	A2286	G2287	G2288	G2289	G2290	G2293	A2294	G2295	G2296	A2300	A2313	U2314	U2315	G2316	U2321	G2322	U2325	A2326	G2327	G2328	G2329	U2330	U2331	U2332	G2333	U2334	G2335	U2336	A2337	G2338	G2339	U2340	U2341	A2342	G2343	U2344	U2345										
A2161	A2162	U2163	U2164	G2165	G2166	U2167	U2168	G2169	G2178	U2179	U2180	G2181	A2184	G2185	U2186	U2187	G2191	A2194	U2195	G2196	G2197	G2198	G2199	G2203	U2215	U2216	U2217	U2218	U2219	G2220	A2221	G2223	G2224	G2230	G2233	G2234	G2235	U2241	G2245	U2246	A2247	G2248	G2249	A2253	A2254	A2255													
G2016	G2017	G2018	G2023	G2024	G2025	A2026	A2027	U2033	A2036	G2043	A2046	G2047	G2048	G2049	G2050	U2051	G2052	A2064	A2065	G2066	U2086	G2087	G2088	G2089	U2090	U2091	U2092	G2093	G2094	G2095	G2096	A2106	G2107	U2112	A2124	G2130	A2136	A2137	G2138	U2139	A2140	U2141	A2152	G2153	G2154	U2155													
A1873	G1874	G1878	G1888	U1889	G1890	G1891	G1892	G1893	A1894	A1895	G1901	G1902	G1909	U1910	U1911	G1912	A1916	G1917	A1918	A1919	G1921	A1925	A1931	U1946	U1947	A1948	G1949	G1950	U1968	G1973	A1974	A1975	A1979	G1980	U1981	A1990	G1991	U1992	G1998	A2003	A2004	G2005	A2008																
G1738	G1746	G1747	G1751	G1752	G1753	G1754	A1755	G1756	U1757	G1760	U1767	G1775	A1778	A1787	G1788	A1789	A1790	A1791	A1792	G1793	G1801	G1802	A1803	G1813	U1820	A1821	G1822	G1823	G1824	G1825	G1830	A1834	G1835	G1843	A1852	G1856	U1857	U1864	A1865	G1866	G1871	A1872																	
C1617	G1618	U1619	U1620	C1621	G1622	U1623	U1624	G1625	G1626	U1627	A1628	G1629	A1630	A1631	C1632	G1637	G1638	G1639	A1640	G1648	A1649	G1650	G1658	G1674	A1679	A1680	U1681	G1688	G1696	G1703	A1710	G1711	G1712	U1713	A1716	U1717	G1720	G1724	A1727	U1728	A1729	U1730	A1731	G1736	A1737														
C1557	C1558	A1559	U1560	C1561	G1562	A1563	A1564	A1565	A1566	C1567	C1568	A1569	C1570	C1571	G1572	U1573	G1574	A1575	C1576	C1577	U1578	C1579	A1580	C1581	U1582	G1583	U1584	U1585	G1586	G1587	G1588	G1589	U1590	U1591	G1592	U1593	G1594	U1595	C1596	G1597	U1598	U1599	G1600	U1601	U1602	G1603	G1604	G1605	G1606	G1607	U1608	G1609	C1610	A1611	U1612	G1613	G1614	G1615	A1616
G1458	G1462	C1463	C1465	C1466	C1472	G1473	A1480	C1481	G1486	G1492	A1499	A1500	C1501	G1507	A1508	U1509	A1510	U1511	U1512	C1513	A1518	G1522	U1523	G1524	U1525	U1529	G1530	C1531	G1534	C1535	A1536	U1537	G1538	A1539	U1540	U1544	C1545	A1546	G1547	G1550	U1551	A1552	C1553	U1554	A1555	A1556													
G1339	G1343	A1344	G1345	A1352	G1353	G1359	A1362	G1365	U1370	G1371	C1376	A1377	U1378	G1379	A1380	G1384	G1385	G1386	A1387	U1388	U1389	G1393	C1404	C1408	C1409	C1413	G1414	A1415	A1416	C1421	U1428	C1429	C1435	C1436	A1437	C1440	C1441	U1444	C1445	G1456	A1457																		
A1214	U1215	A1216	U1219	U1223	G1224	U1225	G1230	U1234	U1235	G1238	G1239	G1240	A1244	U1245	A1246	A1251	G1252	C1253	C1260	A1261	A1267	G1270	C1271	G1272	G1273	G1276	G1277	C1290	G1291	U1292	G1293	U1294	C1298	G1302	U1303	C1311	U1320	U1325	G1332																				
G1114	A1119	G1120	G1121	G1122	C1123	G1124	G1125	G1130	G1131	G1140	U1141	G1142	G1143	A1144	U1151	G1152	U1153	G1157	A1164	G1165	C1171	A1172	G1173	U1178	U1179	G1180	U1184	A1185	G1186	A1187	A1188	G1189	C1190	A1191	G1192	U1200	G1201	A1202	A1203	A1204	G1205	A1206	G1207	U1208	G1209	U1212	A1213												



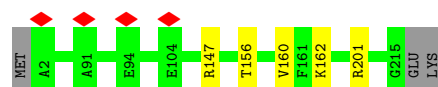
• Molecule 2: 5S rRNA



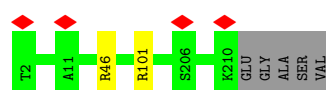
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3



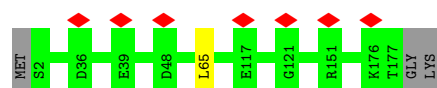
• Molecule 5: 50S ribosomal protein L4



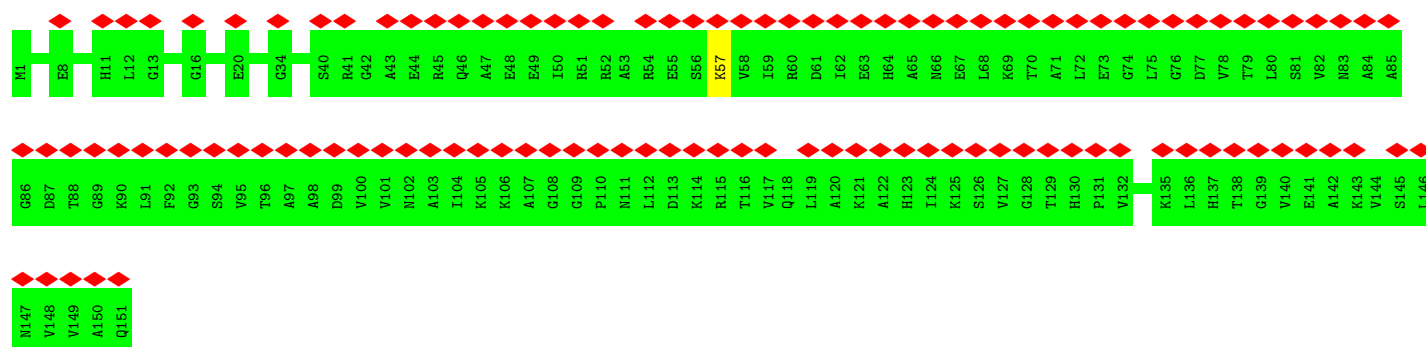
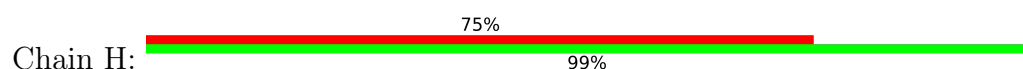
• Molecule 6: 50S ribosomal protein L5



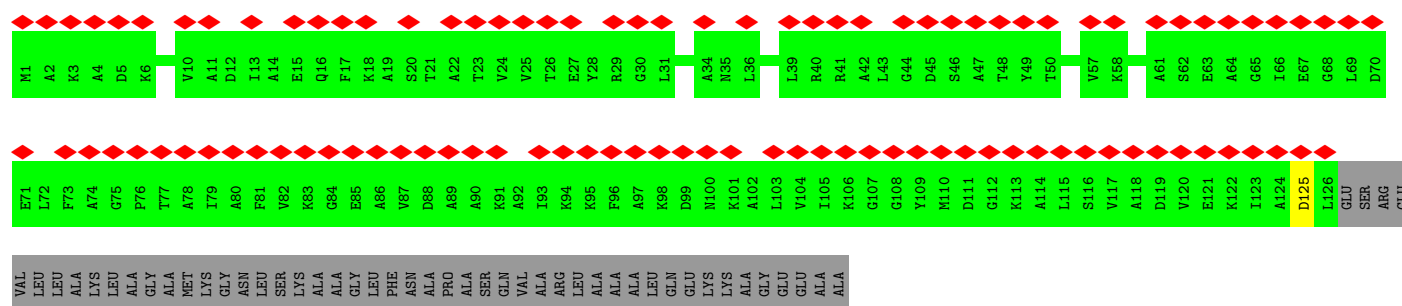
• Molecule 7: 50S ribosomal protein L6



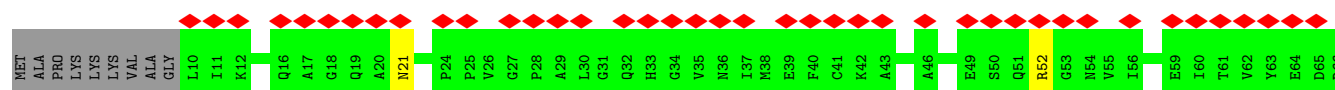
• Molecule 8: 50S ribosomal protein L9

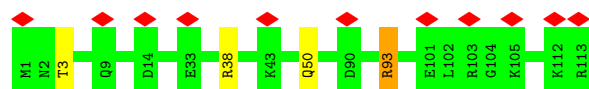


• Molecule 9: 50S ribosomal protein L10

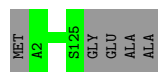


• Molecule 10: 50S ribosomal protein L11

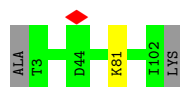




- Molecule 18: 50S ribosomal protein L20



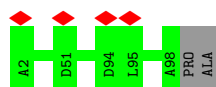
- Molecule 19: 50S ribosomal protein L21



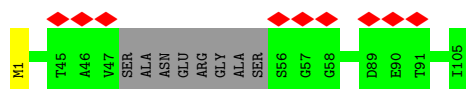
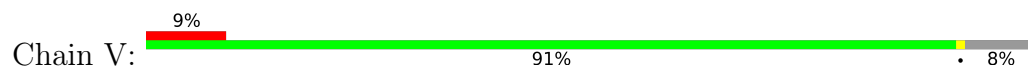
- Molecule 20: 50S ribosomal protein L22



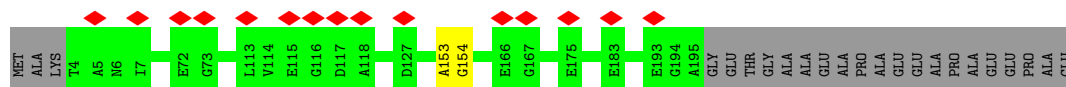
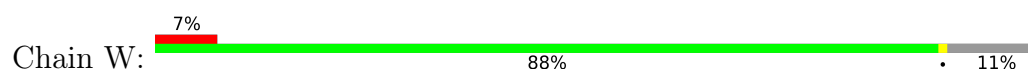
- Molecule 21: 50S ribosomal protein L23




- Molecule 22: 50S ribosomal protein L24

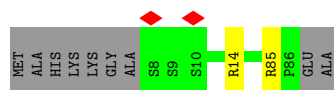


- Molecule 23: 50S ribosomal protein L25




- Molecule 24: 50S ribosomal protein L27

Chain X:  88% 10%



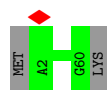
- Molecule 25: 50S ribosomal protein L29

Chain Z:  82% 17%




- Molecule 26: 50S ribosomal protein L30

Chain a:  97%




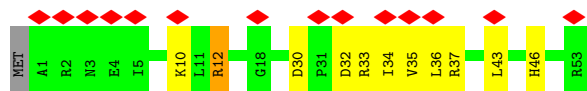
- Molecule 27: 50S ribosomal protein L32

Chain b:  89% 5% 5%



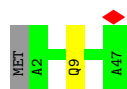
- Molecule 28: 50S ribosomal protein L33 2

Chain c:  26% 78% 19%



- Molecule 29: 50S ribosomal protein L34

Chain d:  96%



- Molecule 30: 50S ribosomal protein L35

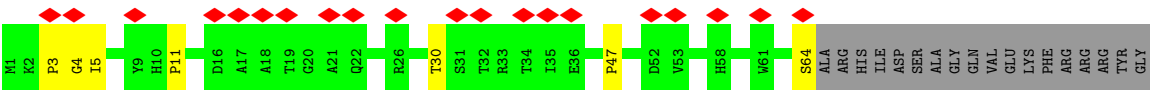
Chain e:  98%



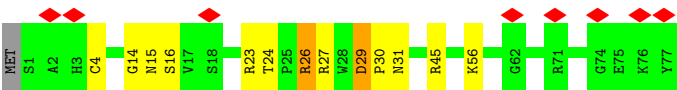
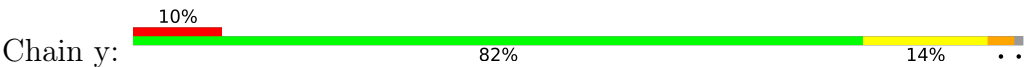
- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 50S ribosomal protein L31



- Molecule 33: 50S ribosomal protein L28



- Molecule 34: Uncharacterized protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	66840	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 ($e^-/\text{\AA}^2$)	67	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	0.300	Depositor
Minimum map value	-0.194	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	485.78003, 485.78003, 485.78003	wwPDB
Map dimensions	454, 454, 454	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	A	1.26	90/75001 (0.1%)	1.23	309/117027 (0.3%)
2	B	0.99	0/2821	1.12	5/4396 (0.1%)
3	C	0.77	1/2153 (0.0%)	0.77	3/2895 (0.1%)
4	D	0.80	0/1609	0.79	1/2165 (0.0%)
5	E	0.66	0/1592	0.67	1/2153 (0.0%)
6	F	0.49	0/1467	0.67	0/1973
7	G	0.53	0/1369	0.70	1/1848 (0.1%)
8	H	0.42	0/1129	0.75	0/1524
9	I	0.34	0/925	0.58	0/1246
10	J	0.34	0/1006	0.62	0/1364
11	K	0.71	0/1157	0.65	0/1567
12	L	0.80	0/946	0.74	0/1268
13	M	0.70	0/1091	0.76	0/1457
14	N	0.70	0/1118	0.74	1/1506 (0.1%)
15	O	0.75	0/945	0.73	0/1267
16	P	0.60	0/966	0.74	1/1298 (0.1%)
17	Q	0.80	1/921 (0.1%)	0.73	1/1236 (0.1%)
18	R	0.86	0/1000	0.75	0/1341
19	S	0.69	0/764	0.63	0/1030
20	T	0.76	0/887	0.76	0/1204
21	U	0.68	0/766	0.64	0/1030
22	V	0.55	0/738	0.63	0/987
23	W	0.52	0/1443	0.64	0/1970
24	X	0.80	0/595	0.73	0/798
25	Z	0.60	0/534	0.74	1/713 (0.1%)
26	a	0.70	0/477	0.69	0/640
27	b	0.67	0/427	0.79	1/572 (0.2%)
28	c	0.50	0/463	0.88	1/621 (0.2%)
29	d	0.84	0/380	0.99	2/500 (0.4%)
30	e	0.68	0/507	0.75	0/672
31	f	0.85	0/303	0.71	0/401
32	g	0.43	0/513	0.75	1/707 (0.1%)
33	y	0.53	0/629	0.82	1/843 (0.1%)
34	3	0.72	0/191	0.79	0/247

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.12	92/106833 (0.1%)	1.13	330/160466 (0.2%)

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
4	D	0	1
10	J	0	1
23	W	0	1
All	All	0	3

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	50	GLN	CA-CB	-8.45	1.35	1.53
1	A	1081	C	N1-C6	-6.40	1.33	1.37
1	A	2841	C	N1-C6	-6.24	1.33	1.37
1	A	901	C	N1-C6	-6.17	1.33	1.37
1	A	2008	A	N9-C4	-6.12	1.34	1.37
1	A	202	C	N1-C6	-6.07	1.33	1.37
1	A	1376	C	N1-C6	-6.00	1.33	1.37
1	A	1125	C	N1-C6	-5.95	1.33	1.37
1	A	1822	C	N1-C6	-5.93	1.33	1.37
1	A	2223	C	N1-C6	-5.92	1.33	1.37
1	A	2905	C	N1-C6	-5.89	1.33	1.37
1	A	902	C	N1-C6	-5.84	1.33	1.37
1	A	1888	C	C4-C5	-5.81	1.38	1.43
1	A	2915	C	C4-C5	-5.79	1.38	1.43
1	A	2667	C	N1-C6	-5.78	1.33	1.37
1	A	847	C	C4-C5	-5.78	1.38	1.43
1	A	1027	C	N1-C6	-5.75	1.33	1.37
1	A	799	G	N9-C4	-5.74	1.33	1.38
1	A	2248	C	C4-C5	-5.74	1.38	1.43
1	A	2005	C	C4-C5	-5.72	1.38	1.43
1	A	678	A	N7-C5	-5.72	1.35	1.39
1	A	2233	G	N9-C8	-5.67	1.33	1.37
1	A	793	C	C4-C5	-5.64	1.38	1.43
1	A	197	C	C4-C5	-5.63	1.38	1.43
1	A	2923	C	N1-C6	-5.62	1.33	1.37
1	A	2916	C	N1-C6	-5.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2830	C	N1-C6	-5.57	1.33	1.37
1	A	1413	C	C4-C5	-5.56	1.38	1.43
1	A	2224	C	N1-C6	-5.56	1.33	1.37
1	A	813	C	N1-C6	-5.54	1.33	1.37
1	A	1856	C	C4-C5	-5.52	1.38	1.43
1	A	848	G	C6-N1	-5.51	1.35	1.39
1	A	2766	A	C6-N6	-5.51	1.29	1.33
1	A	2870	C	C4-C5	-5.50	1.38	1.43
1	A	949	C	N1-C6	-5.47	1.33	1.37
1	A	1874	C	C4-C5	-5.46	1.38	1.43
1	A	1866	C	N1-C6	-5.45	1.33	1.37
1	A	906	C	C4-C5	-5.45	1.38	1.43
1	A	675	G	N9-C8	-5.42	1.34	1.37
1	A	678	A	N9-C8	-5.39	1.33	1.37
1	A	725	A	N9-C4	-5.38	1.34	1.37
1	A	847	C	N1-C6	-5.36	1.33	1.37
1	A	852	C	C4-C5	-5.36	1.38	1.43
1	A	2220	C	N1-C6	-5.33	1.33	1.37
1	A	2235	C	C4-C5	-5.33	1.38	1.43
1	A	2218	C	C4-C5	-5.30	1.38	1.43
1	A	1311	C	C4-C5	-5.29	1.38	1.43
1	A	2948	C	N1-C6	-5.28	1.33	1.37
1	A	939	C	C4-C5	-5.27	1.38	1.43
1	A	1441	C	C4-C5	-5.24	1.38	1.43
1	A	1272	C	N1-C6	-5.23	1.34	1.37
1	A	1466	C	N1-C6	-5.22	1.34	1.37
1	A	1277	C	C4-C5	-5.22	1.38	1.43
1	A	2274	C	C4-C5	-5.22	1.38	1.43
1	A	2049	C	N1-C6	-5.21	1.34	1.37
1	A	2274	C	N3-C4	-5.21	1.30	1.33
1	A	2260	C	C4-C5	-5.21	1.38	1.43
1	A	2218	C	N1-C6	-5.19	1.34	1.37
1	A	2230	C	C4-C5	-5.18	1.38	1.43
1	A	678	A	C5-C6	-5.17	1.36	1.41
3	C	34	VAL	C-N	-5.17	1.22	1.34
1	A	879	A	C6-N6	-5.16	1.29	1.33
1	A	2043	C	N1-C6	-5.15	1.34	1.37
1	A	788	C	N1-C6	-5.15	1.34	1.37
1	A	2739	C	N1-C6	-5.13	1.34	1.37
1	A	924	G	N9-C8	-5.13	1.34	1.37
1	A	932	C	C4-C5	-5.12	1.38	1.43
1	A	2234	G	N9-C8	-5.12	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2830	C	C4-C5	-5.10	1.38	1.43
1	A	1856	C	N1-C6	-5.10	1.34	1.37
1	A	672	C	C4-C5	-5.10	1.38	1.43
1	A	667	A	C6-N6	-5.09	1.29	1.33
1	A	1124	C	N1-C6	-5.09	1.34	1.37
1	A	939	C	N1-C6	-5.08	1.34	1.37
1	A	2904	C	N1-C6	-5.08	1.34	1.37
1	A	2295	C	N1-C6	-5.07	1.34	1.37
1	A	807	C	C4-C5	-5.07	1.38	1.43
1	A	2253	A	N9-C4	-5.07	1.34	1.37
1	A	2666	C	N1-C6	-5.07	1.34	1.37
1	A	1445	C	N1-C6	-5.06	1.34	1.37
1	A	2848	C	C4-C5	-5.06	1.39	1.43
1	A	2004	A	C5-C6	-5.06	1.36	1.41
1	A	1124	C	C4-C5	-5.05	1.39	1.43
1	A	2915	C	N1-C6	-5.05	1.34	1.37
1	A	2279	C	N1-C6	-5.04	1.34	1.37
1	A	1429	C	C4-C5	-5.04	1.39	1.43
1	A	2290	C	C4-C5	-5.04	1.39	1.43
1	A	1413	C	N1-C6	-5.02	1.34	1.37
1	A	1104	C	N1-C6	-5.02	1.34	1.37
1	A	2289	C	C4-C5	-5.01	1.39	1.43
1	A	2004	A	N7-C5	-5.01	1.36	1.39
1	A	657	C	N1-C6	-5.00	1.34	1.37

All (330) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2509	C	O4'-C1'-N1	10.75	116.80	108.20
1	A	1012	C	C2-N1-C1'	10.49	130.34	118.80
1	A	2245	C	C2-N1-C1'	10.26	130.08	118.80
1	A	1012	C	N1-C2-O2	9.72	124.73	118.90
1	A	2245	C	N1-C2-O2	9.16	124.40	118.90
1	A	2274	C	N1-C2-O2	9.00	124.30	118.90
1	A	2025	C	C6-N1-C2	-8.95	116.72	120.30
1	A	2025	C	N3-C2-O2	-8.62	115.87	121.90
1	A	2025	C	N1-C2-O2	8.25	123.85	118.90
1	A	2245	C	C6-N1-C1'	-7.87	111.36	120.80
1	A	1441	C	C5-C4-N4	-7.83	114.72	120.20
2	B	87	U	N3-C2-O2	-7.76	116.77	122.20
1	A	2491	A	N1-C6-N6	-7.72	113.97	118.60
1	A	197	C	C6-N1-C2	-7.70	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2468	U	N3-C4-O4	7.63	124.74	119.40
1	A	1012	C	N3-C2-O2	-7.62	116.57	121.90
1	A	2511	A	O4'-C1'-N9	7.60	114.28	108.20
1	A	848	G	N1-C2-N2	-7.59	109.37	116.20
1	A	1421	C	C5-C4-N4	-7.56	114.91	120.20
1	A	336	C	N3-C2-O2	-7.51	116.64	121.90
1	A	2521	C	C6-N1-C2	-7.50	117.30	120.30
1	A	1012	C	C6-N1-C1'	-7.50	111.81	120.80
1	A	2248	C	N1-C2-O2	7.43	123.36	118.90
1	A	1747	C	N3-C2-O2	-7.39	116.73	121.90
1	A	3045	C	C5-C4-N4	-7.39	115.03	120.20
1	A	2944	U	C5-C4-O4	-7.35	121.49	125.90
1	A	1888	C	C5-C4-N4	-7.33	115.07	120.20
1	A	1992	U	C5-C4-O4	-7.32	121.51	125.90
1	A	962	U	C2-N1-C1'	7.30	126.47	117.70
1	A	2245	C	N3-C2-O2	-7.28	116.81	121.90
1	A	318	U	C2-N1-C1'	7.16	126.29	117.70
1	A	2185	C	C5-C4-N4	-7.16	115.19	120.20
1	A	318	U	N1-C2-O2	7.13	127.79	122.80
1	A	1277	C	C5-C4-N4	-7.13	115.21	120.20
1	A	1429	C	C6-N1-C2	-7.12	117.45	120.30
1	A	597	C	C5-C4-N4	-7.12	115.22	120.20
1	A	2730	U	C2-N1-C1'	7.10	126.22	117.70
1	A	2509	C	C6-N1-C2	-7.10	117.46	120.30
1	A	932	C	C5-C4-N4	-7.08	115.25	120.20
1	A	726	A	C5-C6-N6	-7.07	118.04	123.70
1	A	652	C	C5-C4-N4	-7.07	115.25	120.20
1	A	2944	U	N3-C4-O4	7.02	124.32	119.40
1	A	336	C	N1-C2-O2	6.95	123.07	118.90
1	A	2900	C	N1-C2-O2	6.90	123.04	118.90
1	A	879	A	C5-C6-N1	6.86	121.13	117.70
1	A	673	C	N1-C2-O2	6.81	122.99	118.90
1	A	557	G	C2-N3-C4	-6.80	108.50	111.90
1	A	1513	C	C5-C4-N4	-6.76	115.47	120.20
1	A	2766	A	C5-C6-N6	-6.76	118.29	123.70
1	A	197	C	C5-C6-N1	6.75	124.38	121.00
1	A	2519	C	C5-C4-N4	-6.73	115.49	120.20
1	A	318	U	N3-C2-O2	-6.69	117.52	122.20
1	A	1843	C	C5-C4-N4	-6.65	115.54	120.20
1	A	2468	U	C5-C4-O4	-6.64	121.92	125.90
1	A	2905	C	C5-C4-N4	-6.64	115.56	120.20
1	A	1030	C	C5-C4-N4	-6.63	115.56	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	93	ARG	C-N-CA	6.58	138.16	121.70
1	A	2825	C	C5-C4-N4	-6.57	115.60	120.20
1	A	2870	C	C5-C4-N4	-6.55	115.62	120.20
1	A	1272	C	N1-C2-O2	6.54	122.82	118.90
1	A	3046	C	C2-N1-C1'	6.53	125.98	118.80
1	A	1893	C	C5-C4-N4	-6.52	115.64	120.20
1	A	939	C	C5-C4-N4	-6.48	115.66	120.20
1	A	2676	C	C5-C4-N4	-6.47	115.67	120.20
16	P	24	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	804	A	C5-C6-N1	6.42	120.91	117.70
1	A	597	C	N3-C4-N4	6.41	122.49	118.00
1	A	2223	C	C5-C4-N4	-6.41	115.72	120.20
1	A	481	C	N1-C2-O2	6.40	122.74	118.90
1	A	1473	G	C2-N3-C4	-6.39	108.70	111.90
2	B	87	U	N1-C2-O2	6.38	127.27	122.80
1	A	197	C	N1-C2-O2	6.37	122.72	118.90
1	A	2288	C	C5-C4-N4	-6.37	115.74	120.20
1	A	2287	C	C5-C4-N4	-6.36	115.75	120.20
1	A	1562	C	C6-N1-C2	-6.36	117.76	120.30
1	A	2830	C	C5-C4-N4	-6.35	115.75	120.20
1	A	1429	C	C2-N1-C1'	6.35	125.78	118.80
3	C	221	VAL	C-N-CA	6.29	137.42	121.70
1	A	2915	C	C5-C4-N4	-6.27	115.81	120.20
1	A	1012	C	C6-N1-C2	-6.27	117.79	120.30
1	A	197	C	N3-C4-N4	6.26	122.38	118.00
1	A	2775	C	N1-C2-O2	6.25	122.65	118.90
1	A	1298	C	N1-C2-O2	6.24	122.64	118.90
1	A	1458	G	C4-N9-C1'	6.24	134.61	126.50
1	A	1311	C	C5-C4-N4	-6.19	115.87	120.20
32	g	4	GLY	N-CA-C	-6.17	97.68	113.10
1	A	1874	C	C5-C4-N4	-6.16	115.89	120.20
1	A	1992	U	N3-C4-O4	6.14	123.70	119.40
1	A	1458	G	C8-N9-C1'	-6.09	119.08	127.00
1	A	804	A	C5-C6-N6	-6.08	118.84	123.70
1	A	793	C	N1-C2-O2	6.08	122.55	118.90
1	A	1428	U	C2-N1-C1'	6.08	124.99	117.70
1	A	29	C	N1-C2-O2	6.06	122.54	118.90
1	A	1747	C	N1-C2-O2	6.04	122.52	118.90
1	A	853	C	N1-C2-O2	6.02	122.51	118.90
1	A	799	G	C2-N3-C4	-6.01	108.89	111.90
1	A	2023	C	N1-C2-O2	6.01	122.51	118.90
1	A	2870	C	C5-C6-N1	6.01	124.01	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2003	A	C5'-C4'-O4'	5.99	116.28	109.10
1	A	2725	C	N1-C2-O2	5.99	122.49	118.90
1	A	1234	U	C6-N1-C2	-5.98	117.41	121.00
1	A	556	G	C6-C5-N7	-5.97	126.82	130.40
1	A	2262	C	N1-C2-O2	5.96	122.48	118.90
1	A	2870	C	N3-C4-N4	5.96	122.17	118.00
1	A	848	G	C4-N9-C1'	5.96	134.25	126.50
2	B	87	U	C6-N1-C2	-5.95	117.43	121.00
1	A	1856	C	C5-C4-N4	-5.95	116.03	120.20
1	A	933	G	N1-C2-N2	-5.95	110.85	116.20
1	A	1843	C	N3-C4-N4	5.95	122.16	118.00
1	A	599	G	O4'-C1'-N9	5.95	112.96	108.20
1	A	2005	C	C5-C4-N4	-5.94	116.04	120.20
1	A	2869	C	C2-N1-C1'	5.94	125.33	118.80
1	A	1788	G	C8-N9-C1'	5.93	134.71	127.00
1	A	2925	C	N1-C2-O2	5.92	122.45	118.90
1	A	3074	C	C5-C4-N4	-5.92	116.06	120.20
1	A	1492	G	C2-N3-C4	-5.91	108.94	111.90
1	A	2556	C	N1-C2-O2	5.91	122.45	118.90
1	A	2004	A	N1-C6-N6	5.88	122.13	118.60
1	A	1122	C	N1-C2-O2	5.88	122.43	118.90
1	A	1384	G	C6-C5-N7	-5.88	126.87	130.40
1	A	848	G	C6-C5-N7	-5.85	126.89	130.40
1	A	2235	C	C5-C4-N4	-5.84	116.11	120.20
1	A	799	G	N3-C4-C5	5.83	131.51	128.60
1	A	848	G	N3-C2-N2	5.82	123.97	119.90
1	A	1124	C	C5-C4-N4	-5.81	116.13	120.20
1	A	390	G	N1-C2-N2	-5.81	110.97	116.20
1	A	2047	C	N3-C4-N4	5.80	122.06	118.00
1	A	2874	C	C5-C4-N4	-5.80	116.14	120.20
1	A	556	G	C4-C5-N7	5.80	113.12	110.80
29	d	9	GLN	N-CA-C	-5.80	95.35	111.00
1	A	2749	G	N3-C4-N9	-5.79	122.53	126.00
1	A	1234	U	N3-C2-O2	-5.78	118.15	122.20
1	A	812	C	C5-C4-N4	-5.78	116.15	120.20
1	A	2734	C	C5-C4-N4	-5.78	116.15	120.20
1	A	848	G	C2-N3-C4	-5.76	109.02	111.90
1	A	851	C	N1-C2-O2	5.75	122.35	118.90
1	A	174	G	C5-C6-O6	-5.75	125.15	128.60
1	A	1788	G	C4-N9-C1'	-5.74	119.04	126.50
1	A	1571	C	N1-C2-O2	-5.74	115.46	118.90
1	A	1298	C	C2-N1-C1'	5.71	125.08	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2723	C	C5-C4-N4	-5.71	116.20	120.20
1	A	197	C	C2-N1-C1'	5.69	125.06	118.80
1	A	2841	C	C5-C4-N4	-5.69	116.22	120.20
1	A	1092	G	O4'-C1'-N9	5.68	112.75	108.20
1	A	2047	C	C5-C4-N4	-5.68	116.22	120.20
1	A	2749	G	N3-C4-C5	5.67	131.43	128.60
1	A	1260	C	C2-N1-C1'	5.66	125.02	118.80
1	A	386	C	C5-C4-N4	-5.65	116.25	120.20
1	A	1409	C	N3-C4-N4	5.65	121.95	118.00
1	A	912	C	N1-C2-O2	5.64	122.29	118.90
1	A	932	C	N1-C2-O2	5.64	122.29	118.90
1	A	2818	C	N1-C2-O2	5.64	122.28	118.90
1	A	472	C	C6-N1-C2	-5.63	118.05	120.30
1	A	2181	C	C5-C4-N4	-5.62	116.27	120.20
1	A	1089	C	N1-C2-O2	5.60	122.26	118.90
1	A	2725	C	N3-C2-O2	-5.59	117.98	121.90
1	A	2004	A	C5-C6-N6	-5.59	119.23	123.70
1	A	2274	C	N3-C2-O2	-5.58	117.99	121.90
1	A	2626	U	C2-N1-C1'	5.58	124.39	117.70
1	A	2218	C	C5-C4-N4	-5.57	116.30	120.20
1	A	1968	U	C5-C4-O4	-5.57	122.56	125.90
1	A	2198	C	C5-C4-N4	-5.55	116.31	120.20
3	C	213	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	1302	G	N1-C6-O6	5.54	123.22	119.90
1	A	336	C	C6-N1-C2	-5.54	118.08	120.30
1	A	726	A	N1-C6-N6	5.54	121.92	118.60
1	A	1830	C	C5-C4-N4	-5.53	116.33	120.20
1	A	852	C	C5-C4-N4	-5.52	116.33	120.20
1	A	2419	C	C6-N1-C2	-5.52	118.09	120.30
1	A	2005	C	N3-C4-N4	5.52	121.86	118.00
1	A	1119	A	N1-C6-N6	-5.52	115.29	118.60
1	A	898	A	C4-N9-C1'	5.51	136.22	126.30
1	A	1120	G	C4-C5-N7	5.51	113.00	110.80
1	A	1472	C	N1-C2-O2	5.51	122.20	118.90
1	A	2766	A	C5-C6-N1	5.50	120.45	117.70
1	A	848	G	C8-N9-C1'	-5.50	119.84	127.00
1	A	2230	C	C5-C4-N4	-5.50	116.35	120.20
1	A	2610	C	N1-C2-O2	5.50	122.20	118.90
1	A	2004	A	C4-C5-N7	5.49	113.45	110.70
1	A	657	C	C5-C4-N4	-5.49	116.36	120.20
1	A	1123	C	C6-N1-C2	-5.48	118.11	120.30
1	A	1486	G	C2-N3-C4	-5.48	109.16	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	C	N1-C2-O2	5.47	122.18	118.90
1	A	2508	C	N1-C2-O2	5.47	122.18	118.90
1	A	2605	C	C5-C4-N4	-5.46	116.38	120.20
1	A	3045	C	N3-C4-N4	5.45	121.82	118.00
1	A	472	C	C2-N1-C1'	5.45	124.79	118.80
1	A	501	C	C5-C4-N4	-5.45	116.39	120.20
1	A	546	G	O4'-C1'-N9	5.45	112.56	108.20
1	A	2290	C	N1-C2-O2	5.45	122.17	118.90
1	A	3046	C	N3-C2-O2	-5.45	118.09	121.90
1	A	1104	C	N1-C2-O2	5.44	122.17	118.90
1	A	1273	G	C2-N3-C4	-5.44	109.18	111.90
1	A	1311	C	N3-C4-N4	5.44	121.81	118.00
1	A	2185	C	N3-C4-N4	5.44	121.81	118.00
1	A	974	G	P-O3'-C3'	5.42	126.20	119.70
1	A	1413	C	C2-N1-C1'	5.42	124.76	118.80
1	A	2848	C	C5-C4-N4	-5.42	116.41	120.20
1	A	1384	G	N7-C8-N9	5.42	115.81	113.10
1	A	1823	C	N1-C2-O2	5.42	122.15	118.90
1	A	726	A	N9-C4-C5	-5.41	103.64	105.80
1	A	860	G	N1-C2-N2	-5.41	111.33	116.20
1	A	2184	A	N9-C4-C5	-5.41	103.64	105.80
1	A	191	G	C4-N9-C1'	5.41	133.53	126.50
25	Z	51	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	2249	G	N7-C8-N9	5.41	115.80	113.10
7	G	65	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	1035	G	C2-N3-C4	-5.40	109.20	111.90
1	A	851	C	C5-C4-N4	-5.39	116.43	120.20
1	A	1303	U	C5-C4-O4	-5.39	122.67	125.90
1	A	2260	C	N3-C4-N4	5.39	121.77	118.00
33	y	29	ASP	C-N-CD	5.39	139.71	128.40
1	A	2203	C	N1-C2-O2	5.38	122.13	118.90
1	A	2419	C	C2-N1-C1'	5.38	124.72	118.80
1	A	726	A	C4-C5-N7	5.38	113.39	110.70
1	A	1012	C	C5-C6-N1	5.37	123.69	121.00
1	A	2124	A	N1-C6-N6	5.37	121.82	118.60
1	A	2016	G	C2-N3-C4	-5.37	109.22	111.90
1	A	1902	C	C5-C4-N4	-5.37	116.44	120.20
1	A	467	C	C5-C4-N4	-5.36	116.45	120.20
1	A	1509	U	O4'-C1'-N1	-5.35	103.92	108.20
3	C	222	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	2521	C	C2-N1-C1'	5.34	124.68	118.80
1	A	1901	C	C5-C4-N4	-5.34	116.46	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1027	C	N1-C2-O2	5.34	122.10	118.90
1	A	1030	C	N3-C4-N4	5.34	121.74	118.00
1	A	2004	A	N9-C4-C5	-5.33	103.67	105.80
1	A	2561	G	N1-C6-O6	5.33	123.09	119.90
1	A	2249	G	C6-C5-N7	-5.32	127.21	130.40
1	A	896	A	C5'-C4'-O4'	5.32	115.48	109.10
1	A	2339	G	O4'-C1'-N9	-5.32	103.95	108.20
1	A	1409	C	C6-N1-C2	-5.31	118.18	120.30
1	A	799	G	N3-C4-N9	-5.30	122.82	126.00
1	A	2398	C	N1-C2-O2	-5.29	115.72	118.90
29	d	9	GLN	C-N-CD	5.29	139.51	128.40
1	A	974	G	C8-N9-C4	-5.29	104.28	106.40
1	A	1638	C	C5-C4-N4	-5.29	116.50	120.20
1	A	1298	C	N3-C2-O2	-5.28	118.20	121.90
1	A	1775	C	N1-C2-O2	5.27	122.06	118.90
1	A	1436	C	C6-N1-C2	-5.27	118.19	120.30
1	A	43	C	C5-C4-N4	-5.26	116.52	120.20
1	A	617	U	C2-N1-C1'	5.26	124.01	117.70
1	A	2230	C	C6-N1-C2	-5.26	118.20	120.30
1	A	390	G	N3-C2-N2	5.26	123.58	119.90
1	A	1413	C	N1-C2-O2	5.26	122.05	118.90
1	A	436	C	N3-C2-O2	-5.25	118.23	121.90
1	A	631	C	N1-C2-O2	5.24	122.05	118.90
1	A	1378	U	C5-C4-O4	-5.24	122.75	125.90
1	A	2818	C	C5-C4-N4	-5.24	116.53	120.20
1	A	2260	C	C5-C6-N1	5.24	123.62	121.00
1	A	81	A	C5'-C4'-O4'	5.23	115.38	109.10
1	A	2510	A	N1-C6-N6	5.23	121.74	118.60
1	A	1561	C	C6-N1-C2	-5.23	118.21	120.30
1	A	2169	G	C5-C6-O6	-5.23	125.46	128.60
1	A	939	C	N3-C4-N4	5.22	121.66	118.00
1	A	1276	G	C4-N9-C1'	5.22	133.29	126.50
1	A	2574	C	C5-C4-N4	-5.22	116.55	120.20
1	A	1570	C	C6-N1-C2	-5.21	118.22	120.30
14	N	45	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	1082	C	C5-C4-N4	-5.21	116.56	120.20
1	A	534	G	C2-N3-C4	-5.21	109.30	111.90
1	A	202	C	C5-C4-N4	-5.20	116.56	120.20
1	A	1788	G	N3-C4-N9	-5.20	122.88	126.00
1	A	2248	C	C2-N1-C1'	5.20	124.52	118.80
1	A	734	C	C5-C4-N4	-5.19	116.56	120.20
1	A	2899	A	C5-C6-N6	-5.19	119.55	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2843	C	C5-C4-N4	-5.19	116.57	120.20
1	A	1393	C	C5-C4-N4	-5.18	116.57	120.20
1	A	2005	C	C5'-C4'-O4'	5.17	115.31	109.10
1	A	2841	C	N3-C4-N4	5.17	121.62	118.00
1	A	1458	G	C6-C5-N7	-5.17	127.30	130.40
1	A	617	U	N1-C2-O2	5.17	126.42	122.80
1	A	2900	C	N3-C2-O2	-5.17	118.28	121.90
1	A	97	U	P-O3'-C3'	5.16	125.89	119.70
1	A	652	C	N3-C4-N4	5.16	121.61	118.00
1	A	1251	A	O4'-C1'-N9	5.16	112.33	108.20
1	A	1752	C	C5-C4-N4	-5.16	116.59	120.20
1	A	2775	C	C2-N1-C1'	5.16	124.47	118.80
1	A	357	U	P-O3'-C3'	5.16	125.89	119.70
2	B	87	U	C5-C6-N1	5.16	125.28	122.70
1	A	1022	C	N3-C2-O2	-5.15	118.29	121.90
4	D	160	VAL	N-CA-CB	-5.15	100.16	111.50
1	A	1874	C	N3-C4-N4	5.15	121.61	118.00
1	A	73	C	C5-C4-N4	-5.14	116.60	120.20
1	A	872	G	N3-C4-C5	5.14	131.17	128.60
1	A	1638	C	N3-C4-N4	5.13	121.59	118.00
1	A	667	A	C5-C6-N1	5.13	120.27	117.70
1	A	2665	C	C5-C4-N4	-5.13	116.61	120.20
1	A	1894	A	C5-N7-C8	-5.13	101.34	103.90
1	A	2730	U	N3-C2-O2	-5.13	118.61	122.20
1	A	1022	C	N1-C2-O2	5.12	121.97	118.90
1	A	853	C	C2-N1-C1'	5.12	124.43	118.80
1	A	869	U	C5-C4-O4	-5.12	122.83	125.90
1	A	902	C	N1-C2-O2	5.12	121.97	118.90
1	A	1171	C	C5-C4-N4	-5.12	116.62	120.20
1	A	962	U	C6-N1-C1'	-5.12	114.04	121.20
1	A	2561	G	C5-C6-O6	-5.11	125.53	128.60
2	B	85	C	C5-C4-N4	-5.11	116.62	120.20
1	A	161	U	N1-C2-O2	5.10	126.37	122.80
1	A	1793	G	C6-C5-N7	-5.10	127.34	130.40
5	E	101	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	2249	G	C4-C5-N7	5.09	112.84	110.80
27	b	3	VAL	C-N-CD	5.09	139.09	128.40
1	A	340	A	N9-C4-C5	-5.09	103.77	105.80
1	A	2230	C	C5-C6-N1	5.09	123.54	121.00
28	c	30	ASP	C-N-CD	5.08	139.07	128.40
1	A	115	A	C8-N9-C4	-5.08	103.77	105.80
1	A	1384	G	C4-N9-C1'	5.07	133.09	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	G	C4-C5-N7	5.06	112.82	110.80
1	A	853	C	C6-N1-C2	-5.06	118.28	120.30
1	A	1473	G	N1-C2-N2	-5.05	111.65	116.20
1	A	357	U	OP2-P-O3'	5.05	116.32	105.20
1	A	957	C	N1-C2-O2	5.05	121.93	118.90
1	A	139	U	C2-N1-C1'	5.05	123.76	117.70
1	A	197	C	C5-C4-N4	-5.03	116.68	120.20
1	A	113	C	N1-C2-O2	5.03	121.92	118.90
1	A	191	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	2794	G	C2-N3-C4	-5.03	109.39	111.90
1	A	501	C	N3-C4-N4	5.02	121.52	118.00
1	A	895	G	C2-N3-C4	-5.02	109.39	111.90
1	A	946	G	N1-C2-N2	-5.02	111.68	116.20
1	A	2626	U	N1-C2-O2	5.02	126.31	122.80
1	A	847	C	C5-C4-N4	-5.01	116.69	120.20
1	A	2003	A	C5'-C4'-C3'	5.01	124.02	116.00
1	A	2249	G	C5-N7-C8	-5.01	101.80	104.30
1	A	2313	A	N9-C4-C5	-5.01	103.80	105.80
1	A	2610	C	C2-N1-C1'	5.01	124.31	118.80
1	A	150	C	C5-C4-N4	-5.00	116.70	120.20
1	A	174	G	N1-C6-O6	5.00	122.90	119.90
1	A	902	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	147	ARG	Peptide
10	J	21	ASN	Peptide
23	W	153	ALA	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	273/278 (98%)	232 (85%)	41 (15%)	0	100	100
4	D	212/217 (98%)	182 (86%)	28 (13%)	2 (1%)	17	53
5	E	207/214 (97%)	192 (93%)	15 (7%)	0	100	100
6	F	180/186 (97%)	165 (92%)	14 (8%)	1 (1%)	25	61
7	G	174/179 (97%)	157 (90%)	17 (10%)	0	100	100
8	H	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
9	I	124/175 (71%)	117 (94%)	6 (5%)	1 (1%)	19	56
10	J	131/142 (92%)	116 (88%)	15 (12%)	0	100	100
11	K	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
12	L	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
13	M	143/147 (97%)	120 (84%)	21 (15%)	2 (1%)	11	43
14	N	134/138 (97%)	119 (89%)	15 (11%)	0	100	100
15	O	116/199 (58%)	107 (92%)	9 (8%)	0	100	100
16	P	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
17	Q	111/113 (98%)	94 (85%)	15 (14%)	2 (2%)	8	38
18	R	122/129 (95%)	117 (96%)	5 (4%)	0	100	100
19	S	98/102 (96%)	93 (95%)	5 (5%)	0	100	100
20	T	112/152 (74%)	105 (94%)	7 (6%)	0	100	100
21	U	95/99 (96%)	81 (85%)	14 (15%)	0	100	100
22	V	93/105 (89%)	87 (94%)	6 (6%)	0	100	100
23	W	190/215 (88%)	169 (89%)	20 (10%)	1 (0%)	29	65
24	X	77/88 (88%)	69 (90%)	8 (10%)	0	100	100
25	Z	62/77 (80%)	62 (100%)	0	0	100	100
26	a	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
27	b	52/57 (91%)	47 (90%)	4 (8%)	1 (2%)	8	37
28	c	51/54 (94%)	26 (51%)	15 (29%)	10 (20%)	0	1
29	d	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
30	e	61/64 (95%)	56 (92%)	5 (8%)	0	100	100
31	f	35/37 (95%)	31 (89%)	4 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	62/82 (76%)	43 (69%)	14 (23%)	5 (8%)	1	8
33	y	75/78 (96%)	56 (75%)	8 (11%)	11 (15%)	0	2
34	3	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
All	All	3649/4003 (91%)	3255 (89%)	358 (10%)	36 (1%)	20	51

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	156	THR
6	F	131	GLY
27	b	9	SER
28	c	10	LYS
28	c	12	ARG
28	c	33	ARG
28	c	34	ILE
28	c	36	LEU
32	g	3	PRO
33	y	16	SER
33	y	24	THR
33	y	27	ARG
33	y	31	ASN
28	c	32	ASP
28	c	37	ARG
28	c	46	HIS
33	y	23	ARG
33	y	30	PRO
9	I	125	ASP
32	g	47	PRO
33	y	14	GLY
33	y	15	ASN
13	M	45	ASN
28	c	43	LEU
32	g	30	THR
4	D	162	LYS
13	M	70	ARG
17	Q	93	ARG
28	c	35	VAL
33	y	4	CYS
33	y	26	ARG
33	y	29	ASP
17	Q	3	THR

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Mol	Chain	Res	Type
32	g	5	ILE
23	W	154	GLY
32	g	11	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	215/218 (99%)	215 (100%)	0	100	100
4	D	160/163 (98%)	159 (99%)	1 (1%)	86	94
5	E	169/172 (98%)	168 (99%)	1 (1%)	86	94
6	F	151/155 (97%)	149 (99%)	2 (1%)	69	86
7	G	148/150 (99%)	148 (100%)	0	100	100
8	H	116/116 (100%)	115 (99%)	1 (1%)	78	90
9	I	89/120 (74%)	89 (100%)	0	100	100
10	J	102/108 (94%)	101 (99%)	1 (1%)	76	88
11	K	119/119 (100%)	119 (100%)	0	100	100
12	L	100/100 (100%)	100 (100%)	0	100	100
13	M	112/114 (98%)	112 (100%)	0	100	100
14	N	114/116 (98%)	113 (99%)	1 (1%)	78	90
15	O	97/158 (61%)	97 (100%)	0	100	100
16	P	93/93 (100%)	92 (99%)	1 (1%)	73	87
17	Q	100/100 (100%)	99 (99%)	1 (1%)	76	88
18	R	97/99 (98%)	97 (100%)	0	100	100
19	S	81/82 (99%)	80 (99%)	1 (1%)	71	87
20	T	90/116 (78%)	87 (97%)	3 (3%)	38	69
21	U	83/84 (99%)	83 (100%)	0	100	100
22	V	81/86 (94%)	80 (99%)	1 (1%)	71	87
23	W	155/168 (92%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	X	58/63 (92%)	56 (97%)	2 (3%)	37	68
25	Z	58/66 (88%)	58 (100%)	0	100	100
26	a	52/54 (96%)	52 (100%)	0	100	100
27	b	43/46 (94%)	42 (98%)	1 (2%)	50	77
28	c	49/50 (98%)	48 (98%)	1 (2%)	55	79
29	d	35/36 (97%)	35 (100%)	0	100	100
30	e	53/54 (98%)	53 (100%)	0	100	100
31	f	35/35 (100%)	35 (100%)	0	100	100
32	g	55/70 (79%)	54 (98%)	1 (2%)	59	81
33	y	64/65 (98%)	61 (95%)	3 (5%)	26	60
34	3	18/18 (100%)	18 (100%)	0	100	100
All	All	2992/3194 (94%)	2970 (99%)	22 (1%)	84	93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	201	ARG
5	E	46	ARG
6	F	78	ARG
6	F	95	ARG
8	H	57	LYS
10	J	52	ARG
14	N	10	ARG
16	P	26	ARG
17	Q	38	ARG
19	S	81	LYS
20	T	90	LYS
20	T	93	ARG
20	T	104	ARG
22	V	1	MET
24	X	14	ARG
24	X	85	ARG
27	b	6	ARG
28	c	12	ARG
32	g	64	SER
33	y	26	ARG
33	y	45	ARG
33	y	56	LYS

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

Mol	Chain	Res	Type
3	C	53	HIS
3	C	91	ASN
5	E	182	GLN
6	F	31	ASN
8	H	46	GLN
16	P	41	ASN
27	b	12	ASN
32	g	58	HIS
33	y	19	HIS
33	y	21	HIS
33	y	33	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3118/3119 (99%)	770 (24%)	32 (1%)
2	B	117/118 (99%)	23 (19%)	1 (0%)
All	All	3235/3237 (99%)	793 (24%)	33 (1%)

All (793) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	U
1	A	11	A
1	A	19	U
1	A	20	G
1	A	23	G
1	A	25	A
1	A	29	C
1	A	31	U
1	A	32	G
1	A	43	C
1	A	47	U
1	A	60	A
1	A	68	A
1	A	71	A
1	A	72	G
1	A	81	A
1	A	82	G
1	A	85	G

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Mol	Chain	Res	Type
1	A	94	G
1	A	98	U
1	A	99	G
1	A	107	G
1	A	115	A
1	A	117	U
1	A	125	C
1	A	126	C
1	A	128	G
1	A	136	U
1	A	138	A
1	A	148	A
1	A	150	C
1	A	151	A
1	A	159	A
1	A	161	U
1	A	162	A
1	A	180	A
1	A	188	G
1	A	195	A
1	A	198	A
1	A	203	A
1	A	204	G
1	A	212	A
1	A	214	G
1	A	215	A
1	A	220	A
1	A	221	A
1	A	227	A
1	A	229	U
1	A	230	G
1	A	232	G
1	A	233	A
1	A	241	A
1	A	248	G
1	A	265	A
1	A	267	G
1	A	279	U
1	A	282	A
1	A	285	U
1	A	286	G
1	A	287	A

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Mol	Chain	Res	Type
1	A	288	U
1	A	289	A
1	A	290	C
1	A	291	C
1	A	292	G
1	A	298	G
1	A	299	G
1	A	300	G
1	A	301	U
1	A	303	G
1	A	305	G
1	A	315	U
1	A	316	U
1	A	317	G
1	A	318	U
1	A	319	G
1	A	323	C
1	A	324	C
1	A	327	U
1	A	329	U
1	A	330	U
1	A	331	U
1	A	335	G
1	A	336	C
1	A	337	U
1	A	338	C
1	A	340	A
1	A	342	C
1	A	348	G
1	A	351	G
1	A	352	G
1	A	357	U
1	A	358	G
1	A	361	A
1	A	363	A
1	A	369	G
1	A	370	U
1	A	376	G
1	A	383	U
1	A	384	G
1	A	391	G
1	A	393	U

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Mol	Chain	Res	Type
1	A	404	A
1	A	412	A
1	A	413	G
1	A	417	C
1	A	428	A
1	A	433	C
1	A	434	G
1	A	437	G
1	A	441	G
1	A	444	U
1	A	445	U
1	A	446	G
1	A	448	U
1	A	449	G
1	A	450	G
1	A	452	G
1	A	460	G
1	A	467	C
1	A	474	G
1	A	475	U
1	A	482	U
1	A	489	A
1	A	491	U
1	A	493	U
1	A	494	G
1	A	500	A
1	A	505	C
1	A	509	U
1	A	512	G
1	A	514	C
1	A	517	A
1	A	523	U
1	A	531	A
1	A	539	C
1	A	543	U
1	A	544	U
1	A	552	U
1	A	553	G
1	A	556	G
1	A	561	G
1	A	562	G
1	A	563	U

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Mol	Chain	Res	Type
1	A	565	A
1	A	566	A
1	A	567	A
1	A	569	G
1	A	578	G
1	A	585	G
1	A	589	A
1	A	591	G
1	A	592	A
1	A	594	U
1	A	595	A
1	A	596	C
1	A	597	C
1	A	605	G
1	A	614	C
1	A	617	U
1	A	618	C
1	A	619	C
1	A	620	G
1	A	633	A
1	A	634	C
1	A	636	U
1	A	637	G
1	A	638	U
1	A	639	C
1	A	640	G
1	A	642	G
1	A	644	G
1	A	646	U
1	A	648	A
1	A	654	U
1	A	655	G
1	A	661	U
1	A	665	G
1	A	666	A
1	A	667	A
1	A	679	G
1	A	684	G
1	A	685	G
1	A	696	A
1	A	697	G
1	A	706	G

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Mol	Chain	Res	Type
1	A	707	G
1	A	708	G
1	A	714	U
1	A	721	A
1	A	725	A
1	A	731	A
1	A	740	A
1	A	747	A
1	A	756	A
1	A	757	G
1	A	758	A
1	A	760	U
1	A	763	G
1	A	764	U
1	A	766	G
1	A	767	U
1	A	768	G
1	A	784	G
1	A	801	U
1	A	830	A
1	A	832	G
1	A	845	C
1	A	862	U
1	A	863	G
1	A	868	C
1	A	880	G
1	A	890	G
1	A	897	A
1	A	898	A
1	A	899	G
1	A	905	U
1	A	907	A
1	A	909	A
1	A	915	U
1	A	920	G
1	A	927	C
1	A	942	U
1	A	943	U
1	A	945	G
1	A	954	U
1	A	960	G
1	A	961	U

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Mol	Chain	Res	Type
1	A	973	G
1	A	974	G
1	A	975	U
1	A	976	A
1	A	981	U
1	A	982	A
1	A	983	C
1	A	995	U
1	A	997	G
1	A	1001	C
1	A	1002	C
1	A	1003	A
1	A	1004	C
1	A	1005	A
1	A	1006	G
1	A	1007	G
1	A	1008	G
1	A	1011	A
1	A	1012	C
1	A	1013	U
1	A	1015	A
1	A	1025	A
1	A	1027	C
1	A	1028	U
1	A	1029	C
1	A	1030	C
1	A	1034	U
1	A	1046	C
1	A	1047	A
1	A	1049	G
1	A	1058	A
1	A	1062	A
1	A	1063	G
1	A	1075	U
1	A	1076	A
1	A	1078	G
1	A	1084	U
1	A	1085	G
1	A	1091	A
1	A	1092	G
1	A	1101	A
1	A	1103	C

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Mol	Chain	Res	Type
1	A	1114	G
1	A	1121	G
1	A	1130	C
1	A	1131	G
1	A	1140	G
1	A	1141	U
1	A	1143	G
1	A	1144	A
1	A	1151	U
1	A	1152	G
1	A	1153	U
1	A	1157	G
1	A	1164	A
1	A	1165	G
1	A	1173	G
1	A	1178	U
1	A	1179	U
1	A	1180	G
1	A	1184	U
1	A	1185	A
1	A	1186	G
1	A	1187	A
1	A	1188	A
1	A	1189	G
1	A	1190	C
1	A	1191	A
1	A	1192	G
1	A	1200	U
1	A	1201	G
1	A	1202	A
1	A	1203	A
1	A	1205	G
1	A	1206	A
1	A	1207	G
1	A	1208	U
1	A	1209	G
1	A	1212	U
1	A	1213	A
1	A	1214	A
1	A	1215	U
1	A	1216	A
1	A	1219	U

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Mol	Chain	Res	Type
1	A	1223	U
1	A	1224	G
1	A	1226	U
1	A	1230	G
1	A	1234	U
1	A	1235	U
1	A	1238	G
1	A	1240	G
1	A	1244	A
1	A	1246	A
1	A	1251	A
1	A	1253	C
1	A	1260	C
1	A	1261	A
1	A	1267	A
1	A	1270	G
1	A	1290	C
1	A	1292	U
1	A	1293	G
1	A	1294	U
1	A	1320	U
1	A	1325	U
1	A	1332	G
1	A	1339	G
1	A	1343	G
1	A	1344	A
1	A	1345	G
1	A	1352	A
1	A	1353	G
1	A	1359	G
1	A	1362	A
1	A	1365	G
1	A	1370	U
1	A	1371	G
1	A	1380	A
1	A	1386	G
1	A	1387	A
1	A	1389	U
1	A	1404	C
1	A	1408	C
1	A	1415	A
1	A	1416	A

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Mol	Chain	Res	Type
1	A	1435	C
1	A	1437	A
1	A	1440	C
1	A	1444	U
1	A	1445	C
1	A	1456	G
1	A	1457	A
1	A	1462	G
1	A	1465	C
1	A	1480	A
1	A	1481	C
1	A	1499	A
1	A	1501	C
1	A	1507	G
1	A	1508	A
1	A	1510	A
1	A	1511	U
1	A	1518	A
1	A	1522	G
1	A	1524	G
1	A	1525	U
1	A	1529	U
1	A	1530	G
1	A	1531	C
1	A	1534	C
1	A	1536	A
1	A	1537	U
1	A	1538	G
1	A	1540	U
1	A	1544	U
1	A	1546	A
1	A	1547	G
1	A	1550	G
1	A	1551	U
1	A	1552	A
1	A	1553	C
1	A	1554	U
1	A	1555	A
1	A	1556	A
1	A	1558	C
1	A	1559	A
1	A	1561	C

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Mol	Chain	Res	Type
1	A	1564	A
1	A	1565	A
1	A	1567	C
1	A	1570	C
1	A	1571	C
1	A	1572	G
1	A	1574	G
1	A	1579	C
1	A	1580	A
1	A	1584	U
1	A	1587	G
1	A	1588	G
1	A	1589	G
1	A	1595	G
1	A	1598	U
1	A	1599	U
1	A	1600	G
1	A	1604	G
1	A	1605	G
1	A	1607	C
1	A	1608	U
1	A	1611	A
1	A	1616	A
1	A	1617	C
1	A	1623	U
1	A	1625	G
1	A	1627	U
1	A	1629	G
1	A	1630	U
1	A	1631	A
1	A	1632	G
1	A	1637	G
1	A	1638	C
1	A	1639	G
1	A	1640	A
1	A	1648	A
1	A	1649	C
1	A	1650	G
1	A	1658	G
1	A	1674	G
1	A	1679	A
1	A	1680	A

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Mol	Chain	Res	Type
1	A	1681	U
1	A	1688	G
1	A	1696	G
1	A	1703	G
1	A	1710	A
1	A	1711	G
1	A	1713	U
1	A	1716	A
1	A	1717	U
1	A	1720	G
1	A	1724	G
1	A	1727	A
1	A	1728	U
1	A	1730	U
1	A	1731	A
1	A	1736	G
1	A	1737	A
1	A	1738	G
1	A	1746	G
1	A	1751	G
1	A	1754	G
1	A	1755	A
1	A	1756	G
1	A	1757	U
1	A	1760	G
1	A	1767	U
1	A	1778	A
1	A	1787	A
1	A	1789	A
1	A	1791	A
1	A	1801	C
1	A	1802	G
1	A	1803	A
1	A	1813	C
1	A	1820	U
1	A	1825	C
1	A	1834	A
1	A	1835	C
1	A	1852	A
1	A	1857	U
1	A	1864	U
1	A	1865	A

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Mol	Chain	Res	Type
1	A	1866	C
1	A	1871	G
1	A	1872	A
1	A	1878	G
1	A	1890	C
1	A	1892	G
1	A	1895	A
1	A	1909	C
1	A	1912	C
1	A	1916	A
1	A	1917	G
1	A	1918	A
1	A	1921	G
1	A	1925	A
1	A	1931	A
1	A	1946	U
1	A	1947	U
1	A	1948	A
1	A	1950	G
1	A	1973	C
1	A	1975	A
1	A	1979	A
1	A	1980	G
1	A	1981	U
1	A	1990	A
1	A	1998	C
1	A	2003	A
1	A	2004	A
1	A	2017	C
1	A	2018	G
1	A	2024	G
1	A	2025	C
1	A	2026	A
1	A	2027	A
1	A	2033	U
1	A	2036	A
1	A	2046	A
1	A	2047	C
1	A	2050	C
1	A	2052	G
1	A	2064	A
1	A	2065	A

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Mol	Chain	Res	Type
1	A	2066	G
1	A	2086	U
1	A	2088	C
1	A	2089	C
1	A	2090	U
1	A	2092	U
1	A	2093	G
1	A	2094	G
1	A	2095	G
1	A	2096	G
1	A	2106	A
1	A	2107	G
1	A	2112	U
1	A	2130	G
1	A	2136	A
1	A	2138	C
1	A	2140	A
1	A	2141	U
1	A	2152	A
1	A	2153	G
1	A	2154	G
1	A	2155	U
1	A	2161	A
1	A	2162	A
1	A	2163	U
1	A	2164	U
1	A	2165	C
1	A	2166	C
1	A	2167	U
1	A	2178	G
1	A	2179	U
1	A	2191	C
1	A	2194	A
1	A	2195	U
1	A	2196	G
1	A	2197	G
1	A	2199	G
1	A	2215	U
1	A	2217	U
1	A	2221	A
1	A	2241	U
1	A	2246	U

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Mol	Chain	Res	Type
1	A	2255	A
1	A	2256	G
1	A	2257	A
1	A	2267	C
1	A	2276	G
1	A	2279	C
1	A	2280	G
1	A	2284	A
1	A	2285	G
1	A	2286	A
1	A	2293	G
1	A	2300	A
1	A	2315	U
1	A	2316	G
1	A	2325	U
1	A	2327	C
1	A	2329	G
1	A	2331	U
1	A	2334	U
1	A	2335	G
1	A	2336	U
1	A	2338	G
1	A	2339	G
1	A	2341	U
1	A	2342	A
1	A	2343	G
1	A	2346	G
1	A	2347	G
1	A	2348	G
1	A	2350	G
1	A	2351	A
1	A	2352	C
1	A	2353	U
1	A	2354	G
1	A	2355	U
1	A	2356	G
1	A	2358	A
1	A	2359	G
1	A	2363	A
1	A	2367	G
1	A	2368	C
1	A	2373	G

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Mol	Chain	Res	Type
1	A	2375	G
1	A	2380	G
1	A	2381	A
1	A	2382	G
1	A	2383	U
1	A	2384	C
1	A	2385	G
1	A	2387	U
1	A	2388	G
1	A	2389	U
1	A	2390	U
1	A	2392	A
1	A	2394	A
1	A	2395	U
1	A	2399	A
1	A	2401	U
1	A	2402	C
1	A	2403	U
1	A	2407	C
1	A	2408	G
1	A	2411	U
1	A	2413	G
1	A	2421	A
1	A	2434	A
1	A	2436	A
1	A	2437	U
1	A	2449	A
1	A	2450	C
1	A	2454	G
1	A	2462	G
1	A	2463	G
1	A	2490	A
1	A	2492	A
1	A	2503	G
1	A	2507	C
1	A	2508	C
1	A	2510	A
1	A	2511	A
1	A	2520	U
1	A	2521	C
1	A	2528	G
1	A	2529	A

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Mol	Chain	Res	Type
1	A	2530	C
1	A	2532	G
1	A	2534	A
1	A	2549	G
1	A	2559	A
1	A	2566	C
1	A	2571	C
1	A	2574	C
1	A	2585	U
1	A	2596	G
1	A	2601	A
1	A	2607	G
1	A	2609	A
1	A	2626	U
1	A	2627	C
1	A	2639	G
1	A	2643	U
1	A	2647	U
1	A	2649	A
1	A	2653	G
1	A	2654	A
1	A	2655	U
1	A	2658	A
1	A	2659	A
1	A	2664	C
1	A	2665	C
1	A	2672	A
1	A	2673	U
1	A	2693	A
1	A	2694	G
1	A	2699	C
1	A	2707	C
1	A	2715	U
1	A	2722	C
1	A	2726	G
1	A	2728	U
1	A	2729	G
1	A	2730	U
1	A	2742	A
1	A	2749	G
1	A	2750	G
1	A	2753	G

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Mol	Chain	Res	Type
1	A	2755	A
1	A	2759	G
1	A	2767	G
1	A	2778	U
1	A	2788	A
1	A	2790	A
1	A	2791	G
1	A	2796	A
1	A	2797	C
1	A	2802	G
1	A	2806	G
1	A	2810	U
1	A	2826	A
1	A	2827	G
1	A	2833	U
1	A	2835	U
1	A	2837	U
1	A	2853	C
1	A	2854	A
1	A	2857	A
1	A	2860	U
1	A	2862	G
1	A	2870	C
1	A	2871	U
1	A	2878	A
1	A	2884	A
1	A	2893	G
1	A	2906	U
1	A	2912	A
1	A	2913	U
1	A	2926	A
1	A	2929	A
1	A	2936	C
1	A	2937	G
1	A	2938	G
1	A	2957	A
1	A	2959	A
1	A	2963	U
1	A	2968	G
1	A	2972	A
1	A	2974	A
1	A	2979	C

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Mol	Chain	Res	Type
1	A	2982	A
1	A	2985	G
1	A	2989	A
1	A	2990	A
1	A	3002	A
1	A	3013	C
1	A	3014	A
1	A	3015	C
1	A	3020	U
1	A	3021	A
1	A	3023	G
1	A	3024	A
1	A	3029	U
1	A	3039	C
1	A	3042	A
1	A	3047	A
1	A	3053	U
1	A	3054	U
1	A	3055	G
1	A	3068	U
1	A	3070	G
1	A	3079	U
1	A	3080	A
1	A	3082	U
1	A	3087	G
1	A	3088	C
1	A	3089	A
1	A	3093	A
1	A	3095	C
1	A	3100	A
1	A	3101	C
1	A	3104	A
1	A	3105	C
1	A	3106	C
1	A	3107	G
1	A	3112	A
1	A	3115	A
1	A	3117	U
2	B	4	A
2	B	5	C
2	B	9	G
2	B	11	U

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Mol	Chain	Res	Type
2	B	12	C
2	B	13	C
2	B	14	A
2	B	26	A
2	B	30	G
2	B	36	U
2	B	37	C
2	B	41	U
2	B	42	C
2	B	43	C
2	B	45	G
2	B	56	C
2	B	67	A
2	B	87	U
2	B	89	C
2	B	90	G
2	B	103	G
2	B	107	A
2	B	114	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	81	A
1	A	97	U
1	A	228	A
1	A	316	U
1	A	336	C
1	A	357	U
1	A	445	U
1	A	552	U
1	A	641	U
1	A	643	G
1	A	899	G
1	A	974	G
1	A	1002	C
1	A	1004	C
1	A	1006	G
1	A	1014	G
1	A	1046	C
1	A	1084	U
1	A	1186	G

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Mol	Chain	Res	Type
1	A	1293	G
1	A	1436	C
1	A	1510	A
1	A	2003	A
1	A	2005	C
1	A	2088	C
1	A	2094	G
1	A	2139	U
1	A	2165	C
1	A	2350	G
1	A	2384	C
1	A	2389	U
1	A	2626	U
2	B	10	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 monosaccharides 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.

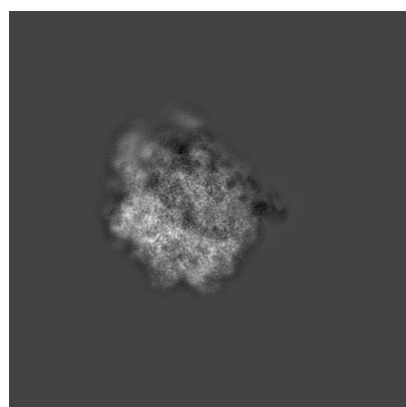
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8937. These allow visual inspection of the internal detail of the map and identification of artifacts.

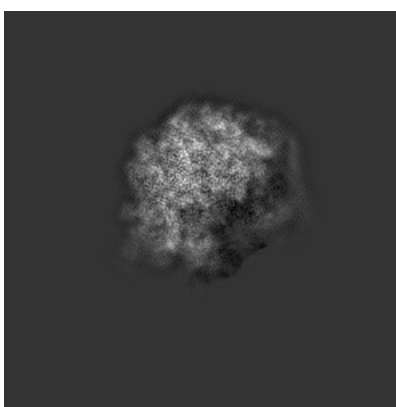
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

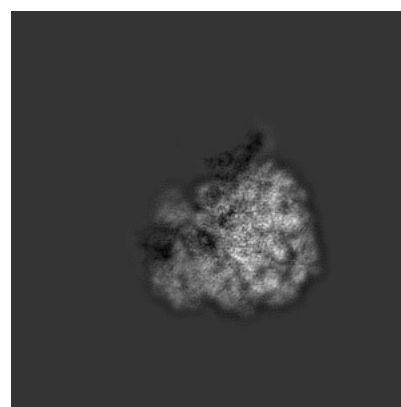
6.1.1 Primary map



X



Y

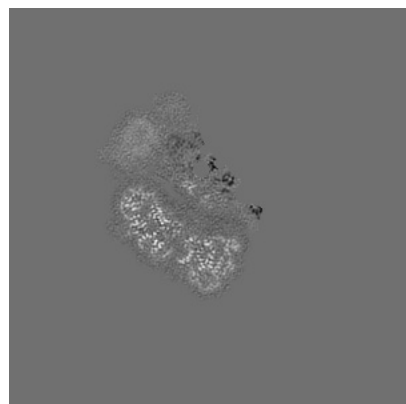


Z

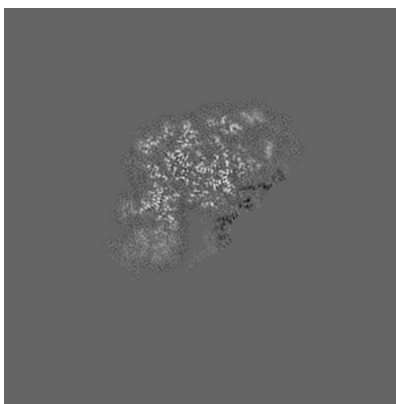
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

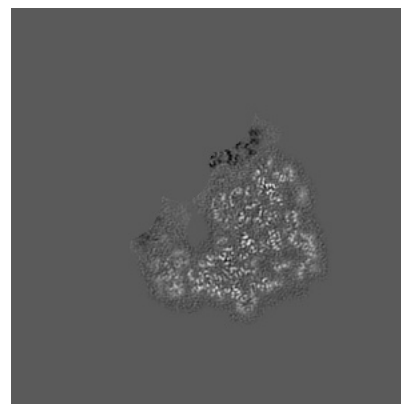
6.2.1 Primary map



X Index: 227



Y Index: 227

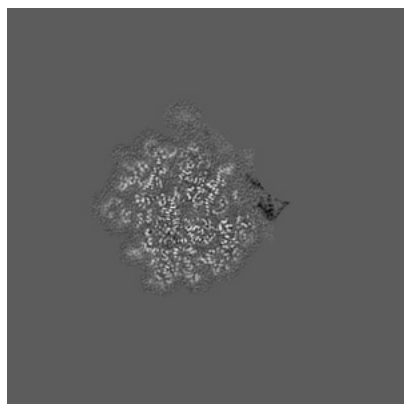


Z Index: 227

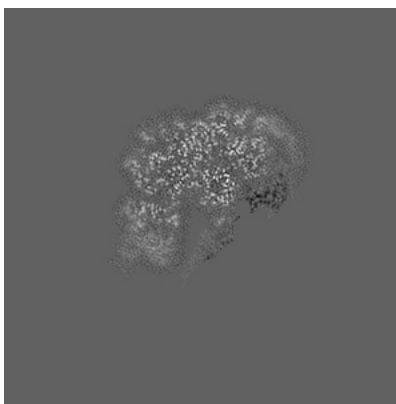
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

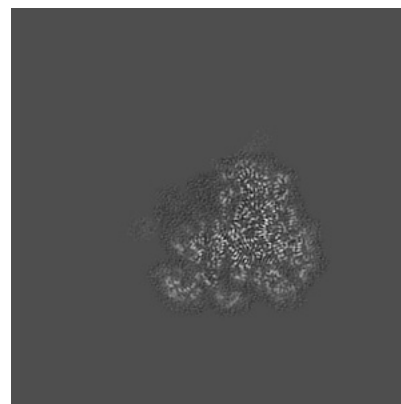
6.3.1 Primary map



X Index: 270



Y Index: 216



Z Index: 201

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

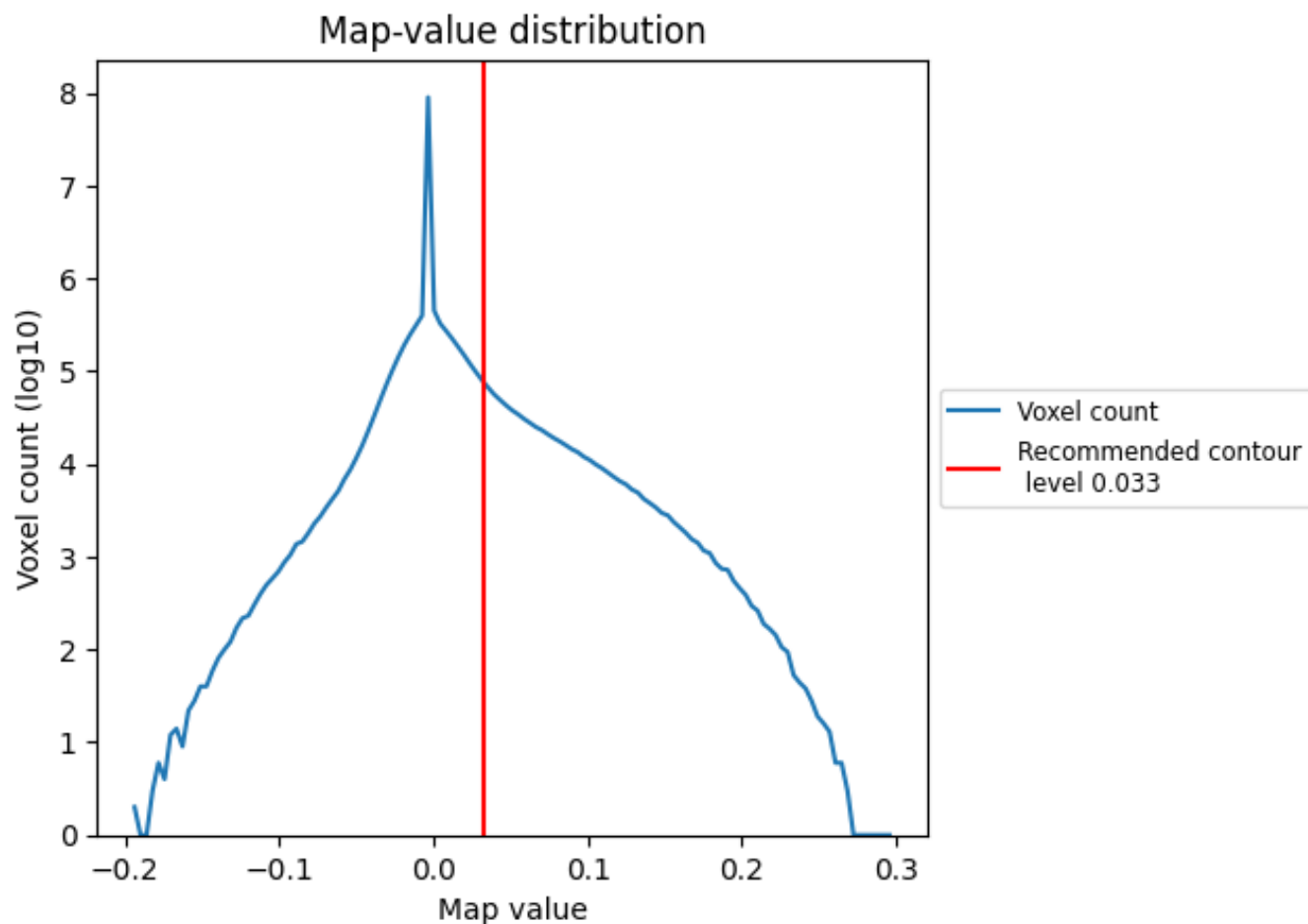
6.5 Mask visualisation

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

7 Map analysis [i](#)

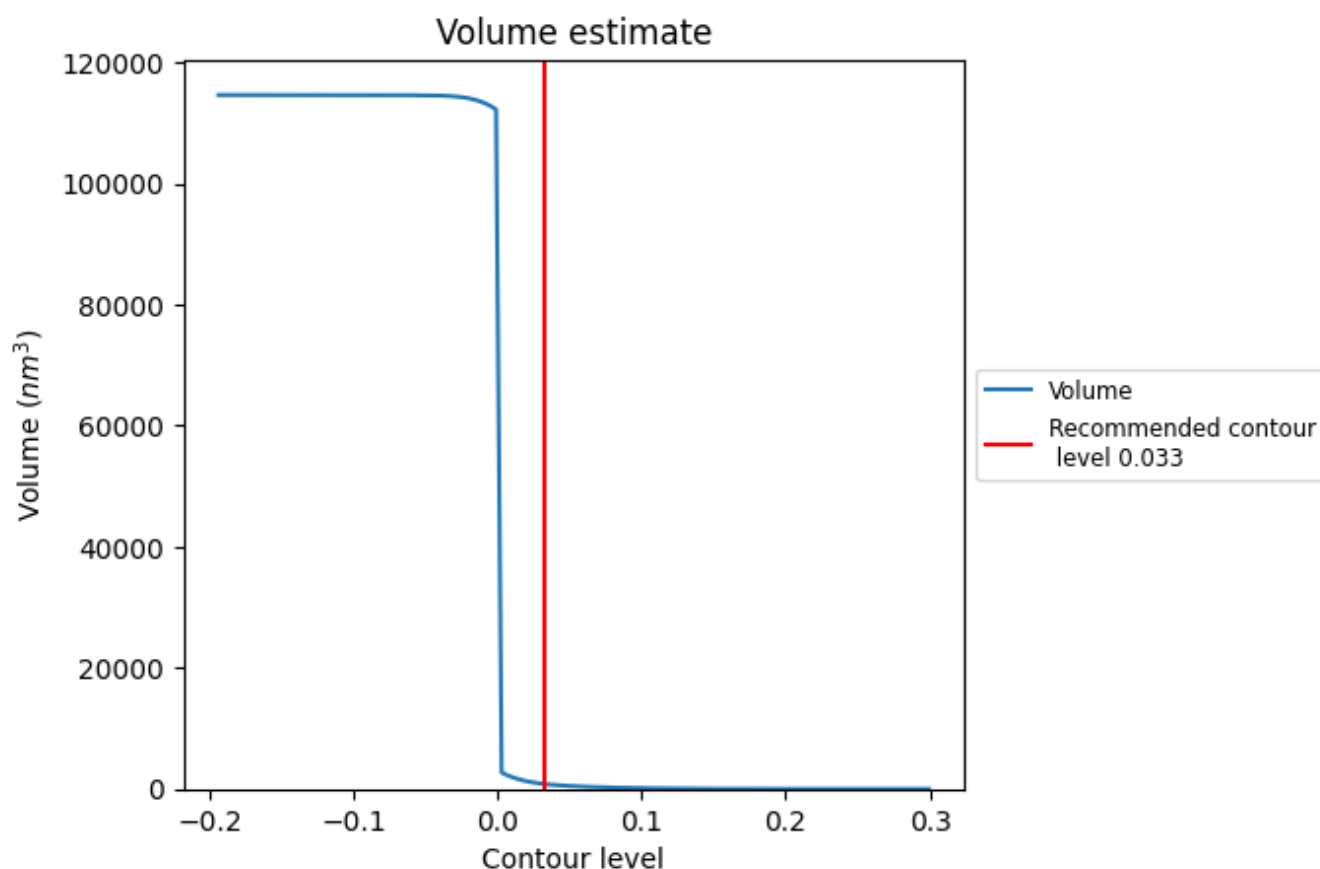
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

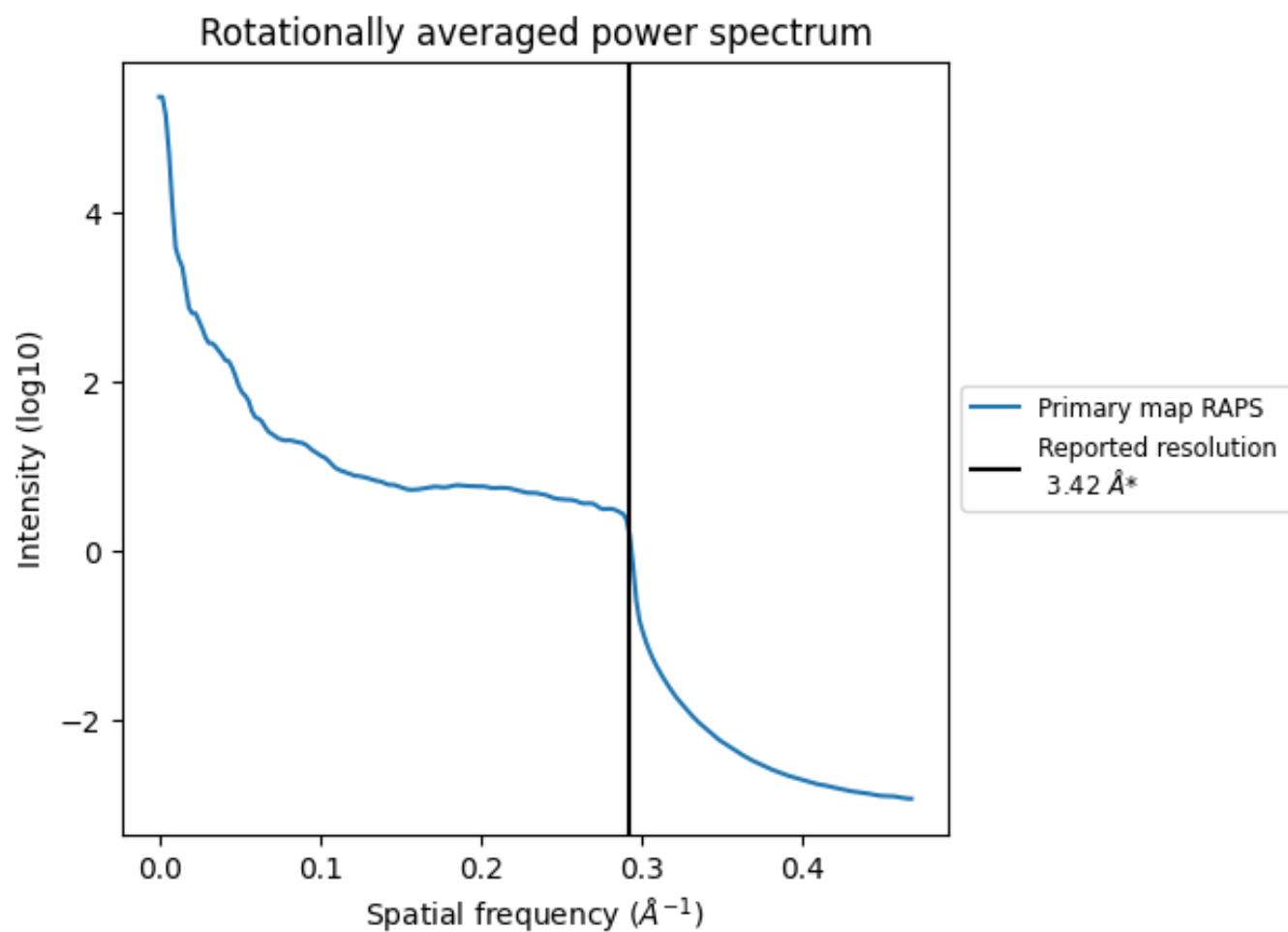
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 804 nm³; this corresponds to an approximate mass of 726 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 ⓘ

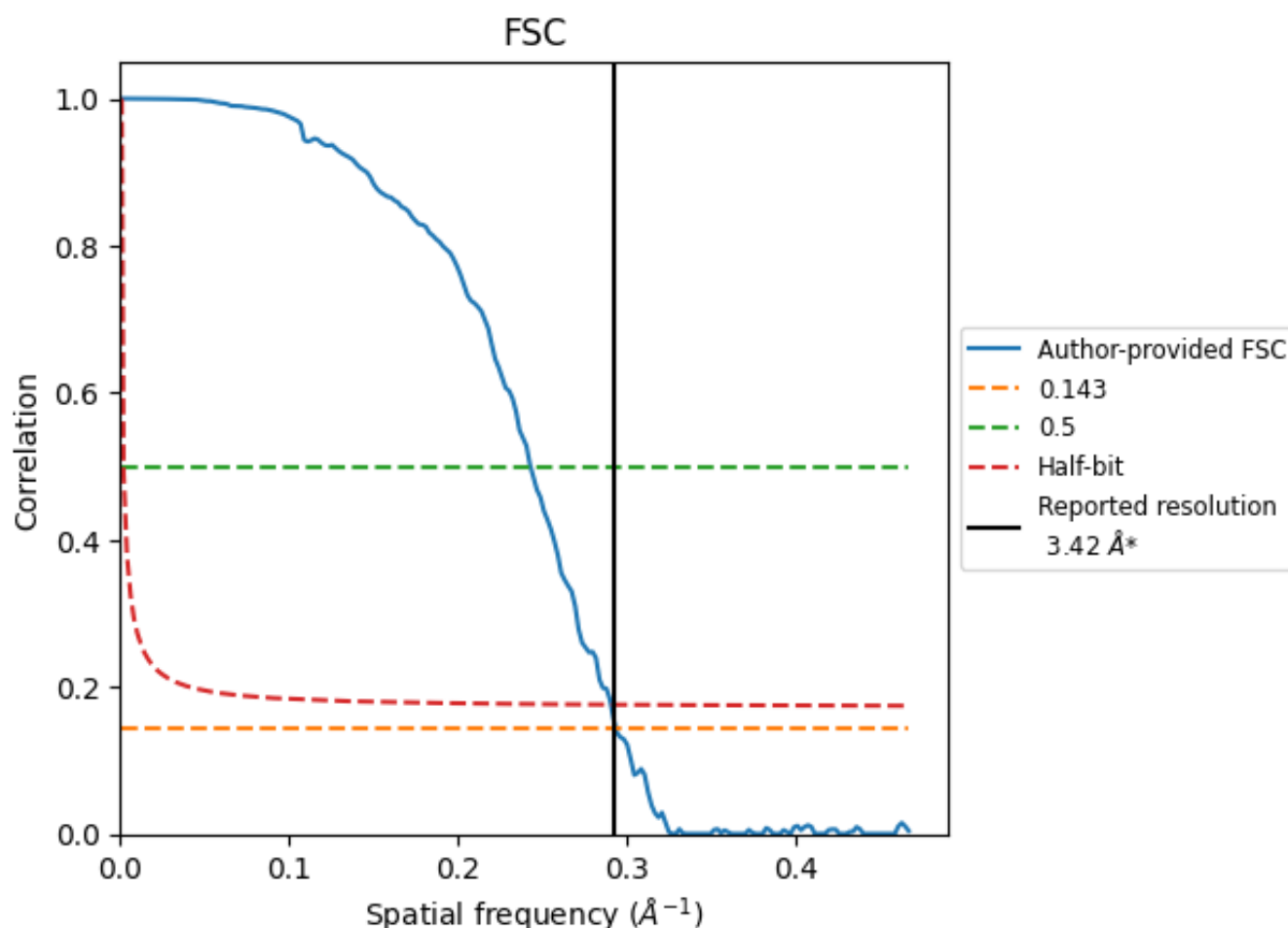


*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

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 0.292 \AA^{-1}

8.2 Resolution estimates [i](#)

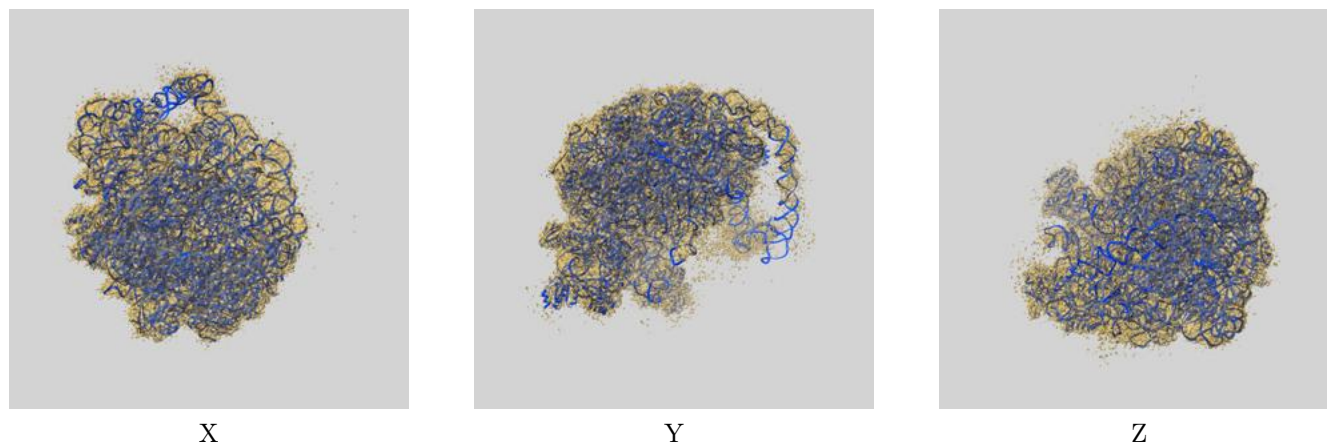
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.40	4.11	3.44
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

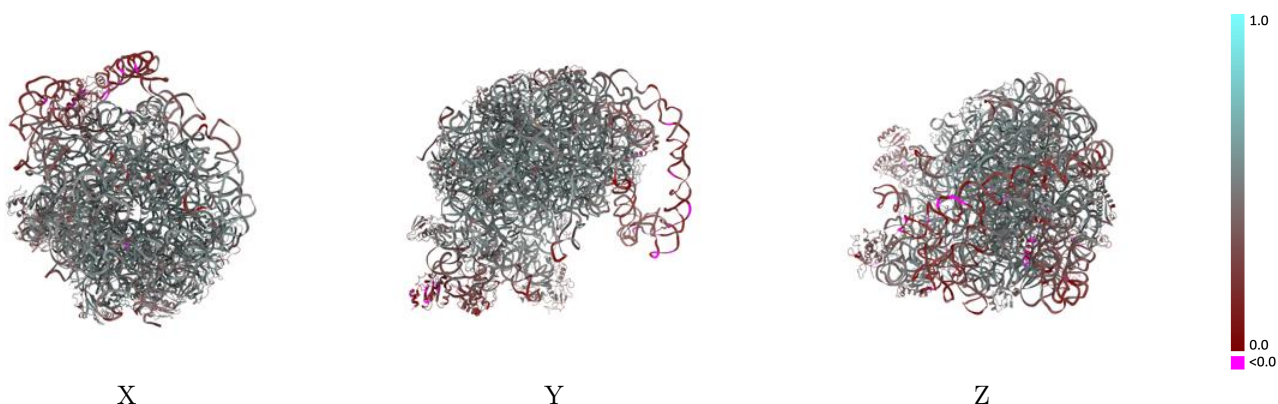
This section contains information regarding the fit between EMDB map EMD-8937 and PDB model 6DZP. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



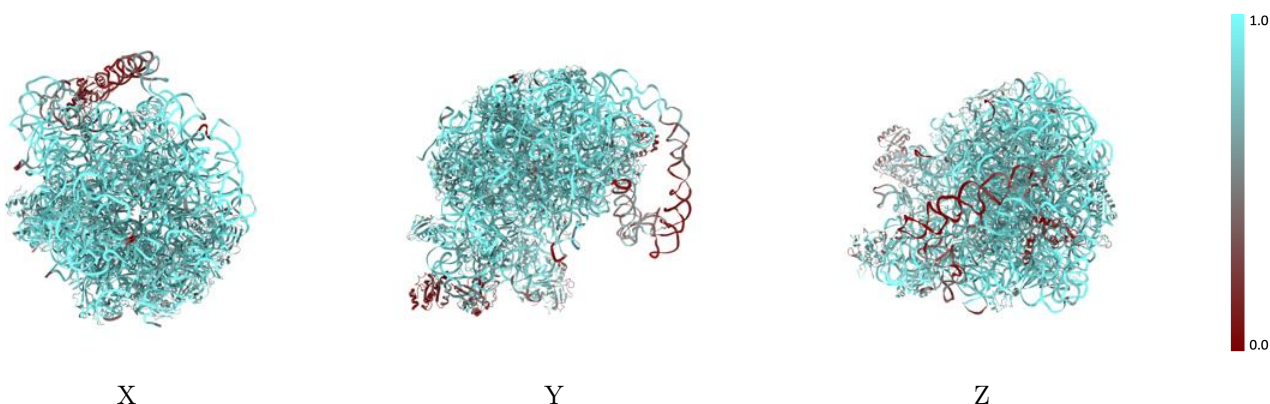
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



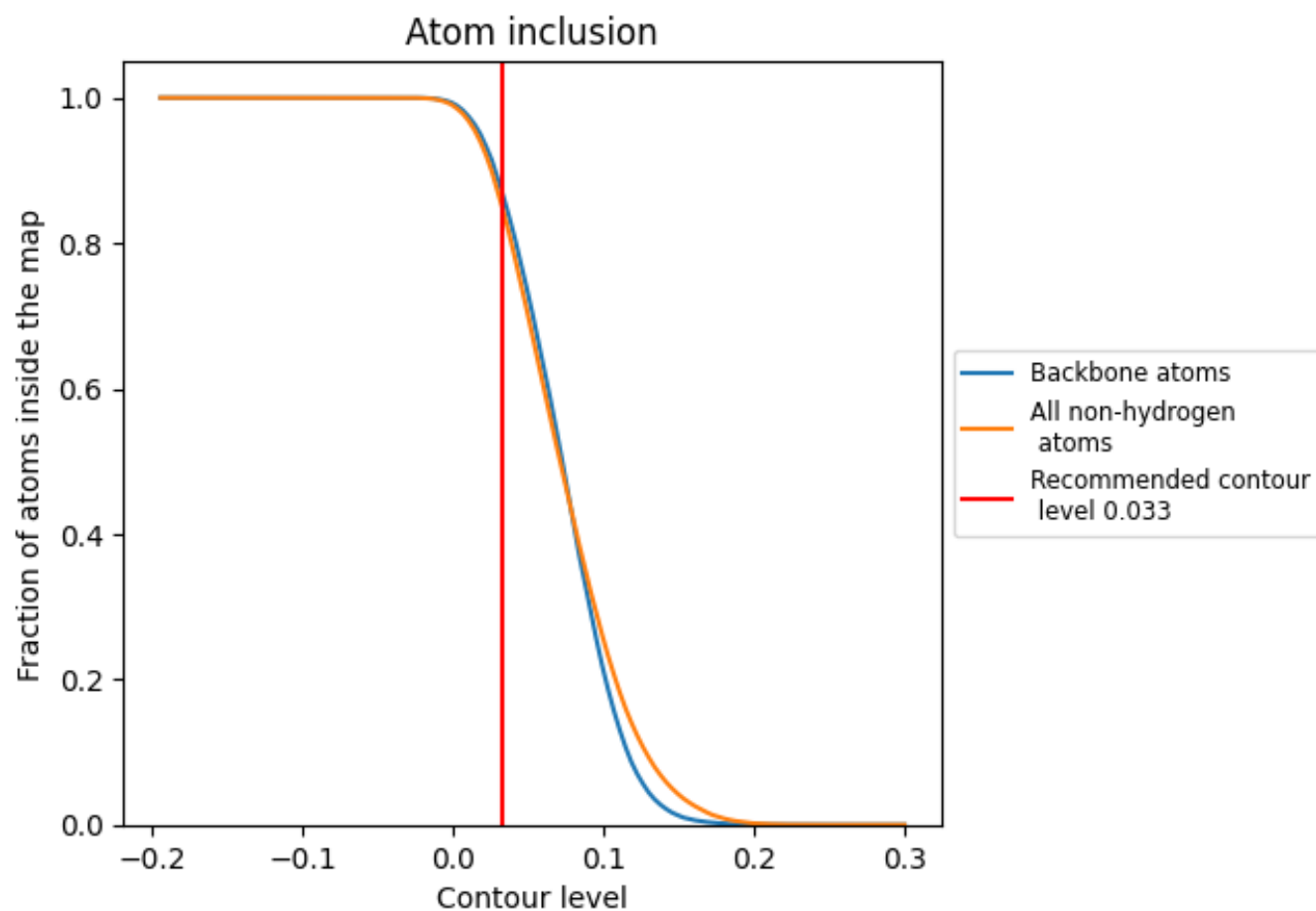
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.033).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8476	 0.4640
3	 0.8101	 0.5200
A	 0.8923	 0.4710
B	 0.9445	 0.4600
C	 0.7410	 0.4900
D	 0.8324	 0.5100
E	 0.8016	 0.4780
F	 0.6995	 0.3860
G	 0.7753	 0.4300
H	 0.2948	 0.2840
I	 0.2238	 0.2020
J	 0.4178	 0.2760
K	 0.8366	 0.5050
L	 0.7462	 0.4880
M	 0.8055	 0.4890
N	 0.8034	 0.5030
O	 0.8427	 0.4980
P	 0.8384	 0.4540
Q	 0.7352	 0.4610
R	 0.8436	 0.5080
S	 0.8617	 0.5060
T	 0.8135	 0.4880
U	 0.7743	 0.4620
V	 0.7403	 0.4210
W	 0.7335	 0.4470
X	 0.8216	 0.5170
Z	 0.8078	 0.4390
a	 0.8126	 0.5030
b	 0.8060	 0.4800
c	 0.6014	 0.3370
d	 0.7994	 0.5120
e	 0.8187	 0.5110
f	 0.8432	 0.5200
g	 0.5617	 0.2850
y	 0.7496	 0.4270

