



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 06:39 PM UTC

PDB ID : 6QUL / pdb_00006qul
EMDB ID : EMD-4638
Title : Structure of a bacterial 50S ribosomal subunit in complex with the novel quinoxolidinone antibiotic cadazolid
Authors : Scaiola, A.; Leibundgut, M.; Boehringer, D.; Ritz, D.
Deposited on : 2019-02-27
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

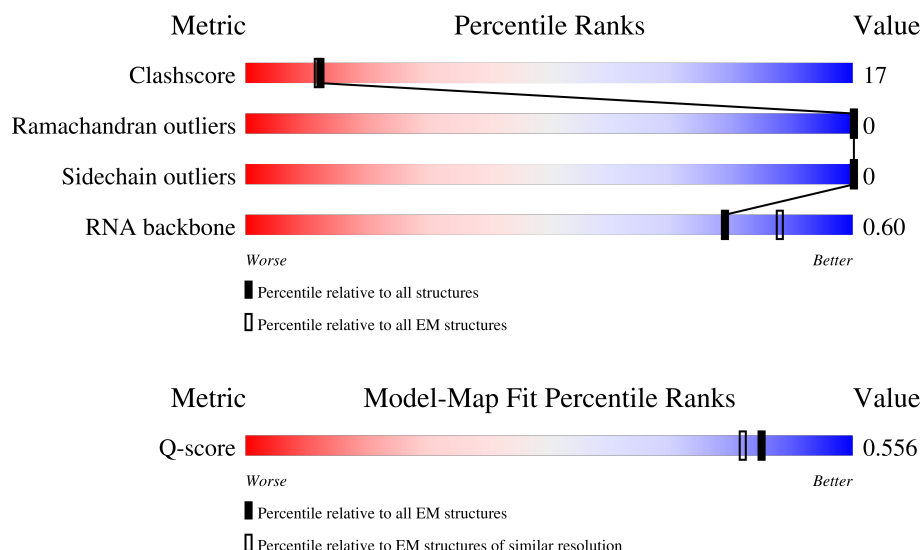
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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	14081 (2.50 - 3.50)

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	1	4	
2	A	2795	
3	B	120	

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Mol	Chain	Length	Quality of chain
4	C	273	
5	D	209	
6	E	201	
7	F	179	
8	G	177	
9	H	149	
10	K	142	
11	L	123	
12	M	144	
13	N	136	
14	O	127	
15	P	117	
16	Q	115	
17	R	118	
18	S	103	
19	T	110	
20	U	100	
21	V	104	
22	W	94	
23	X	85	
24	Y	78	
25	Z	63	
26	a	59	
27	b	57	
28	c	55	

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Mol	Chain	Length	Quality of chain
29	d	46	7% 63% 37%
30	e	65	6% 45% 54%
31	f	38	18% 58% 42%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 87635 atoms, of which 28 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 P-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	4	Total	C	N	O	P	0	0
			84	38	16	26	4		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2795	Total	C	N	O	P	3	0
			60085	26803	11076	19408	2798		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	209	Total	C	N	O	S	0	0
			1564	979	288	293	4		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	201	Total	C	N	O	S	0	0
			1551	974	283	289	5		

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	176	Total	C	N	O	S	0	0
			1322	832	243	245	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	142	Total	C	N	O	S	0	0
			1128	714	212	198	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	144	Total	C	N	O	S	0	0
			1052	654	207	189	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	136	Total	C	N	O	S	0	0
			1073	686	205	176	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	117	Total	C	N	O	S	0	0
			899	557	179	162	1		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	114	Total	C	N	O	S	0	0
			916	574	179	162	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	117	Total	C	N	O		0	0
			946	604	192	150			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	103	Total	C	N	O	S	0	0
			815	516	153	144	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	110	Total	C	N	O	S	0	0
			856	532	166	155	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	94	Total	C	N	O	S	
			752	479	137	133	3	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	76	Total	C	N	O	S	
			579	359	117	102	1	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	77	Total	C	N	O	S	
			624	388	129	105	2	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	62	Total	C	N	O	S	
			500	308	98	93	1	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
26	a	58	Total	C	N	O	S	
			448	281	87	78	2	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
27	b	56	Total	C	N	O	S	
			443	269	94	79	1	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	51	Total	C	N	O	0	0
			414	266	76	72		

- 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
			376	228	90	56	2		

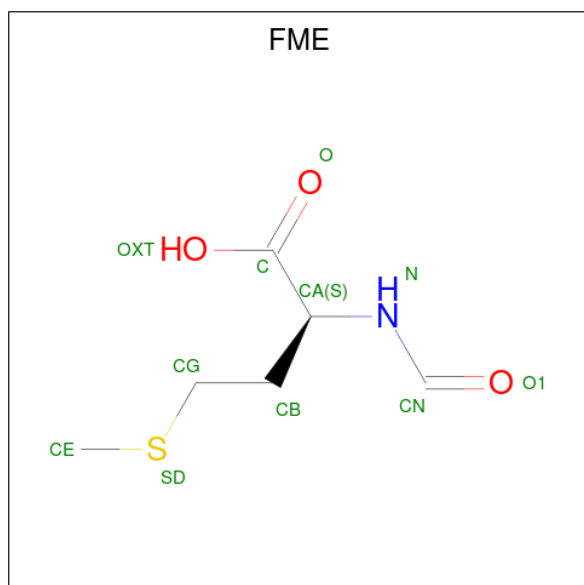
- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	64	Total	C	N	O	S	0	0
			503	323	105	73	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 32 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).

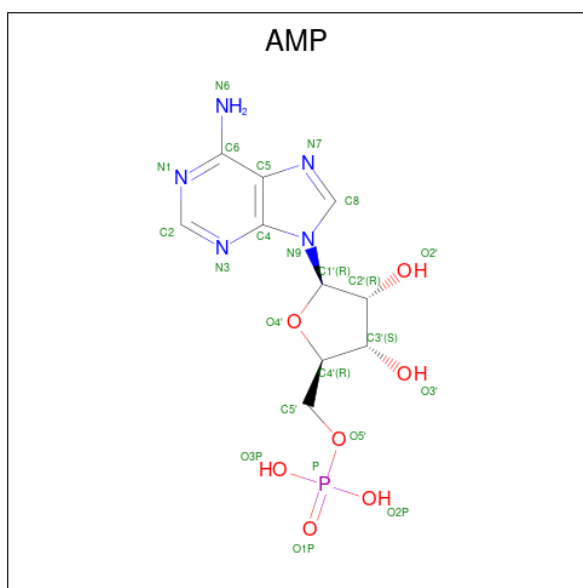


Mol	Chain	Residues	Atoms					AltConf
32	1	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	1	1	Total	Mg	0
			1	1	
33	A	369	Total	Mg	0
			369	369	
33	B	8	Total	Mg	0
			8	8	
33	C	1	Total	Mg	0
			1	1	
33	O	1	Total	Mg	0
			1	1	
33	R	1	Total	Mg	0
			1	1	
33	b	1	Total	Mg	0
			1	1	

- Molecule 34 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 35 is cadazolid (CCD ID: JJH) (formula: C₂₉H₂₉F₂N₃O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
35	A	1	Total 70	C 29	F 2	H 28	N 3	O 8	0

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
36	f	1	Total Zn 1 1	0

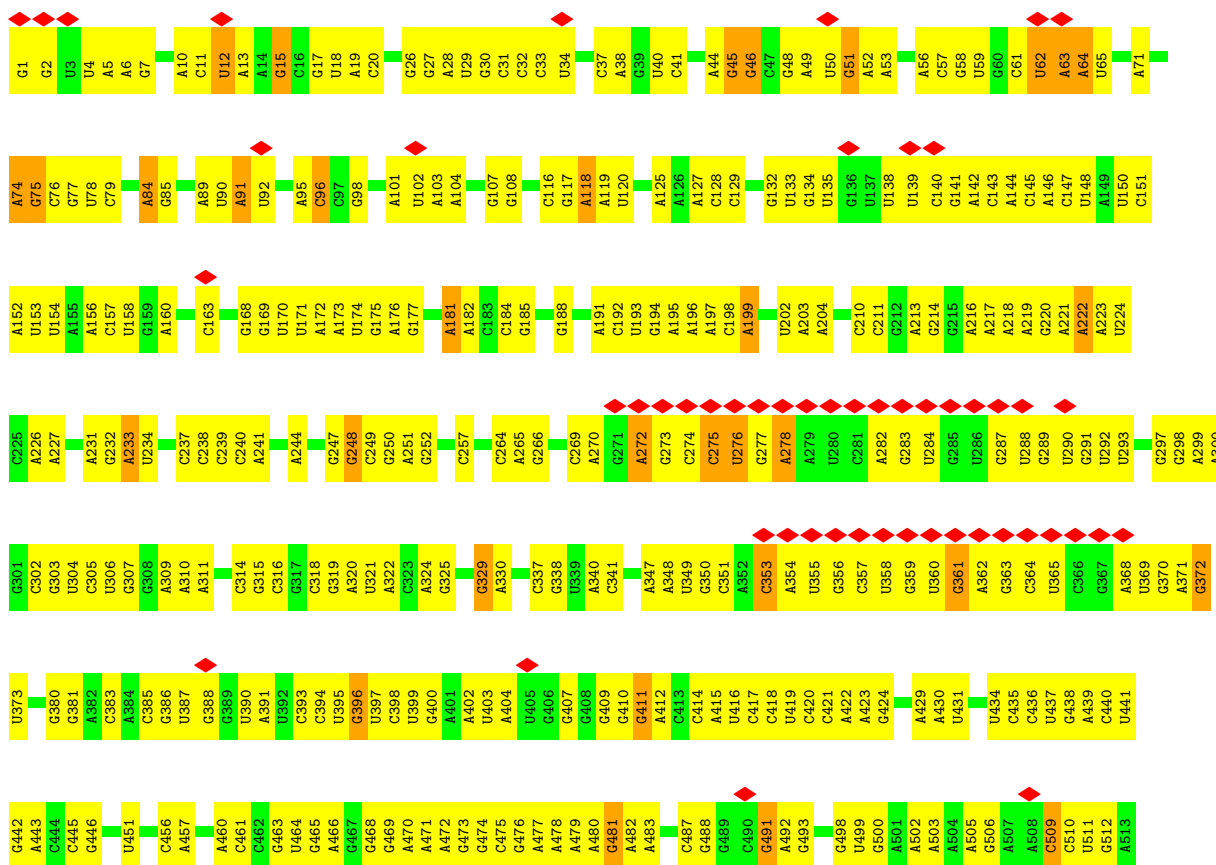
3 Residue-property plots

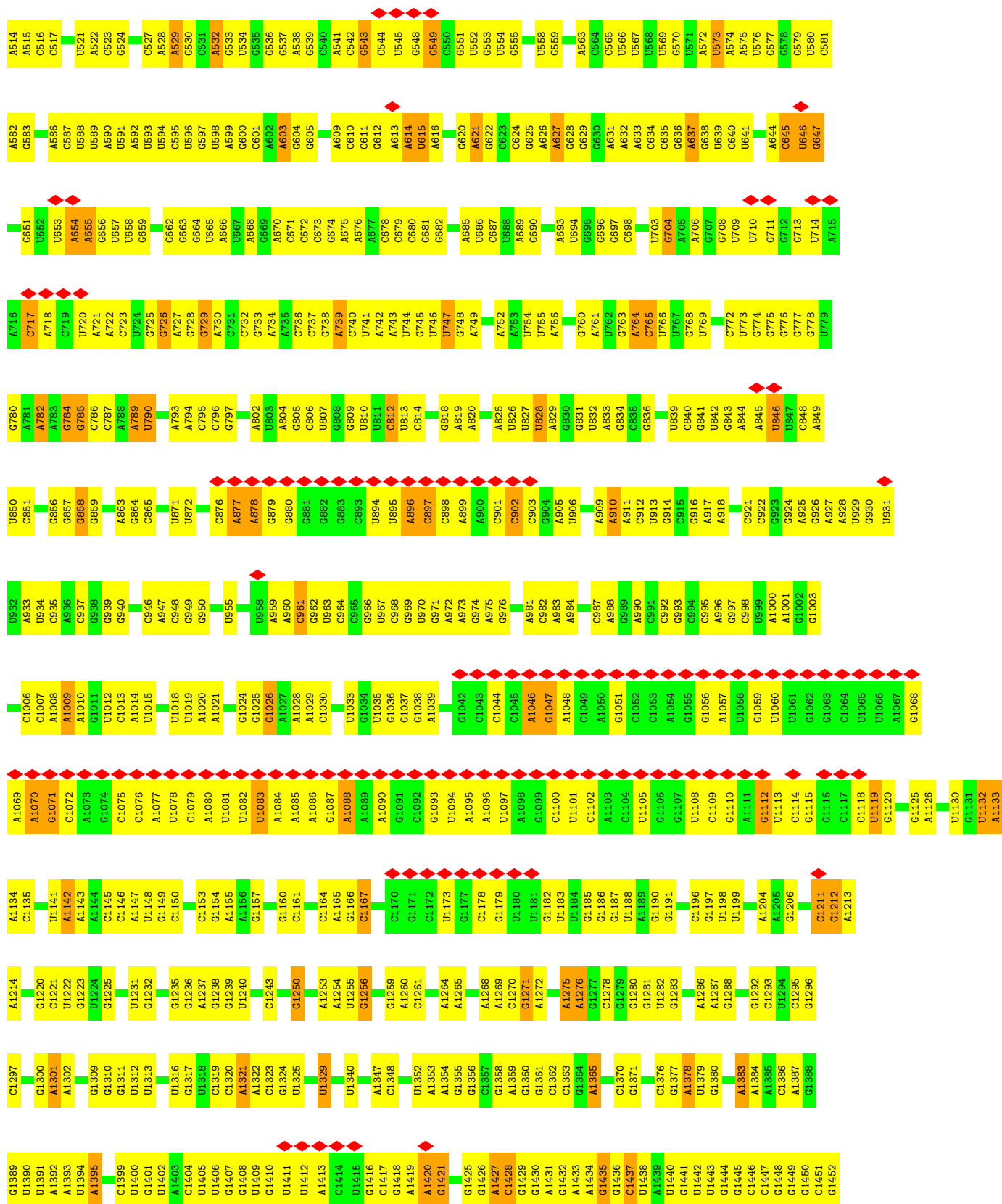
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: P-site fMet-tRNA(fMet)

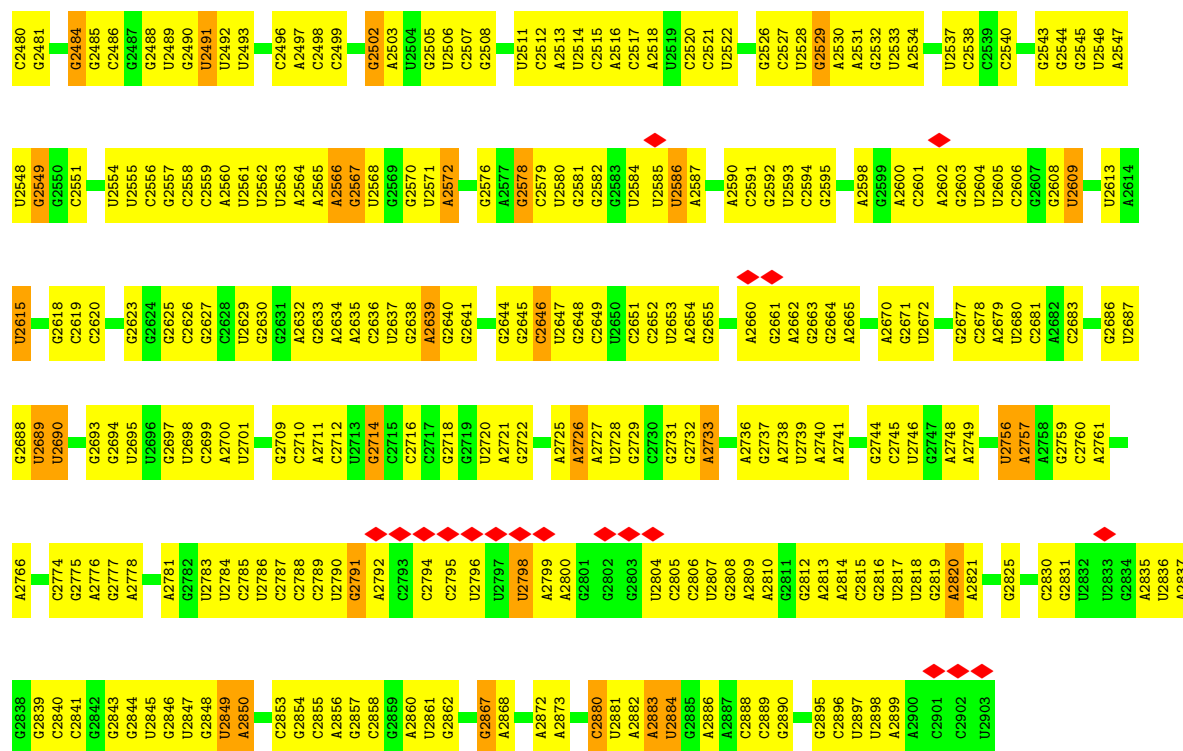


• Molecule 2: 23S rRNA

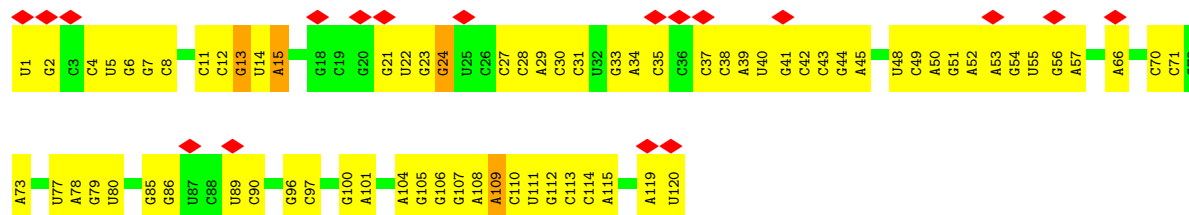




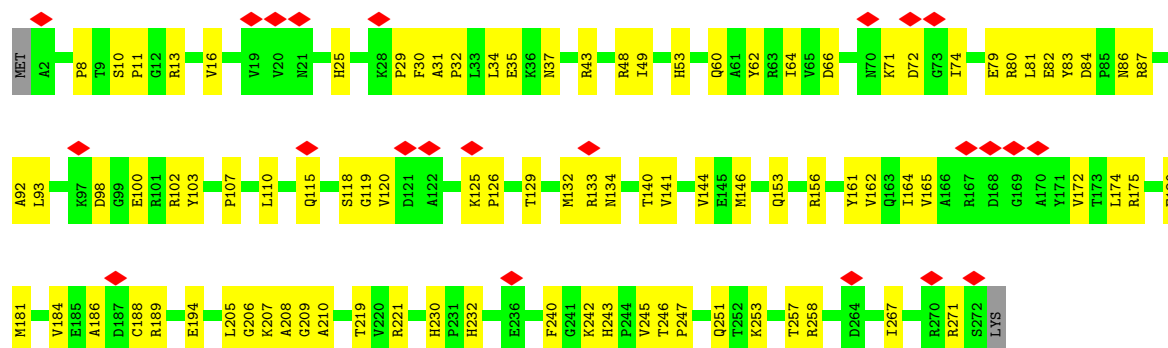
U2401	A1453	C1526	C1604	G1682	A1757	C1830	C1894	A1966	U2039	U2194	G2271	A2336	U2401
U2402	C1454	G1527	C1605	U1682	U1758	G1831	G1897	C1967	G2040	U2195	U2272	G2341	U2402
U2403	G1455	A1528	C1606	C1684	A1759	C1832	U1898	G1968	U2041	C2196	A2273	C2342	U2403
U2404	C1456	G1529	C1607	C1685	C1760	C1833	U1901	A1969	A2042	U2197	A2274	C2343	U2404
G2405	U1457	G1530	A1608	C1686	A1761	C1834	A1901	U1970	C2043	A2198	G2279	U2344	G2405
A2406	U1458	C1531	A1609	G1687	A1762	C1835	U1902	U1971	G2044	A2199	G2280	G2345	A2406
A2407	U1459	A1540	A1610	U1688	C1763	C1836	G1906	G1972	A2050	G2204	A2281	A2346	A2407
G2410	U1460	U1542	A1614	U1693	C1771	C1838	U1907	G1973	A2052	A2205	G2282	C2347	G2410
A2411	G1464	U1543	U1624	C1694	A1772	G1839	C1908	U1974	G2056	C2206	A2283	U2348	A2411
A2412	U1465	G1544	C1625	G1697	A1773	G1842	C1909	U1975	G2055	C2207	A2284	G2349	A2412
G2413	U1466	A1545	A1626	A1698	C1774	C1843	G1910	U1976	G2056	C2208	G2285	C2350	G2413
G2418	U1467	U1546	G1627	G1703	U1777	C1844	U1911	U1979	A2060	C2209	A2287	G2351	G2418
U2419	U1468	C1547	G1628	G1704	U1778	G1845	A1912	G1980	G2061	U2210	A2288	A2352	U2419
C2420	A1469	A1548	U1629	U1778	U1779	A1846	A1913	G1989	G2062	A2211	G2289	C2353	U2420
G2425	A1470	A1549	A1630	C1706	U1782	A1847	A1914	U1990	C2064	U2212	A2290	G2354	G2425
A2426	U1474	C1556	G1631	G1710	U1783	A1848	U1915	U1991	C2065	U2213	G2291	C2355	A2426
A2426	U1475	C1557	A1632	G1711	A1784	U1851	U1916	U1992	G2066	U2214	U2292	U2356	A2426
C2427	C1480	C1558	G1633	U1712	A1785	U1852	U1917	U1993	C2067	U2215	G2293	G2359	C2427
G2428	U1481	U1559	A1634	U1713	A1786	U1853	A1918	U1994	G2068	G2216	C2294	C2360	G2428
G2429	G1482	G1560	A1713	U1714	A1789	U1854	U1919	U1995	U2069	G2217	A2295	G2361	G2429
A2430	G1483	C1561	A1637	G1715	C1790	U1855	A1920	U1996	C2070	A2218	C2296	C2362	A2430
U2431	U1484	U1562	C1638	G1716	A1791	U1856	G1922	U1997	C2071	G2219	A2297	G2363	U2431
A2435	U1485	U1563	G1642	U1720	C1791	U1857	U1923	U1998	U2072	G2220	C2298	C2364	A2435
G2436	U1486	C1564	G1643	G1721	A1794	U1858	A1927	U2000	U2073	A2225	G2299	G2365	G2436
G2437	U1487	C1565	G1644	G1722	A1795	U1859	A1928	U2007	U2074	G2226	U2300	A2366	G2437
G2438	U1488	A1566	C1645	A1723	A1796	G1862	G1929	U2008	U2075	A2227	G2301	G2367	U2438
U2441	C1488	G1567	G1646	G1724	U1796	U1863	U1932	U2009	U2076	G2228	G2302	A2368	U2441
A2448	C1489	U1569	U1647	U1725	U1797	U1864	A1933	A2011	U2077	G2229	U2303	G2370	A2448
U2449	A1490	A1570	G1649	C1726	U1798	U1865	G1934	G2012	U2078	U2230	G2304	G2371	U2449
A2450	G1491	A1571	A1650	C1727	G1799	U1866	A1935	A2013	U2079	U2231	U2305	C2372	A2450
G2457	G1492	U1572	G1651	G1728	A1800	C1867	U1936	A2014	A2080	U2232	C2306	G2373	G2457
G2458	C1493	U1578	G1652	U1729	A1801	C1868	A1937	A2015	A2081	U2233	C2307	C2374	G2458
A2461	U1494	A1579	G1653	C1730	A1802	C1869	U1938	A2016	U2082	U2234	G2308	G2375	A2461
C2462	A1495	A1580	G1654	U1731	A1803	C1870	U1939	U2017	C2088	U2235	U2309	A2376	C2462
G2463	U1496	G1581	U1657	G1732	A1808	U1862	C1942	A2018	A2089	U2236	U2310	G2377	G2463
G2464	C1498	C1582	C1658	U1733	A1809	U1863	U1943	A2019	C2090	U2237	C2311	A2378	G2464
C2465	C1499	A1583	G1659	G1734	A1810	U1864	U1944	A2020	C2091	U2238	G2312	G2379	C2465
C2466	G1500	U1584	G1660	U1735	A1812	U1865	U1945	A2021	C2092	U2239	C2313	C2380	C2466
C2467	G1501	C1585	G1661	U1736	G1812	U1866	U1946	U2022	U2092	U2240	A2314	A2381	C2467
A2468	A1502	U1586	G1662	U1737	G1813	U1867	U1947	C2023	C2093	U2241	U2315	G2382	A2468
A2469	A1503	G1587	A1664	G1738	G1814	C1874	C1948	G2024	A2094	U2242	U2316	U2383	A2469
G2470	A1504	G1588	U1665	U1739	C1815	C1875	G1949	U2025	A2095	U2243	U2317	U2384	G2470
A2471	A1505	U1589	G1666	G1740	C1816	C1876	G1950	G2026	C2096	U2244	G2318	C2385	A2471
G2472	U1506	U1590	G1667	A1669	U1817	C1877	U1951	U2027	A2097	U2245	U2319	A2386	G2472
U2473	C1507	A1591	A1668	U1672	U1818	C1878	U1952	G2028	C2098	U2246	U2320	G2387	U2473
U2474	A1508	C1592	A1673	A1744	A1821	U1880	A1953	G2029	U2098	U2247	U2321	U2388	U2474
C2475	U1509	U1594	G1674	A1745	G1822	U1881	G1954	A2030	U2099	U2248	U2322	U2389	C2475
A2476	C1593	C1595	U1675	A1746	G1823	U1882	U1955	A2031	C2100	U2249	U2323	G2390	A2476
U2477	U1585	A1596	U1680	C1748	G1824	U1883	U1956	G2032	A2101	U2250	U2324	U2391	U2477
	G1524	U1597	U1681	A1749	G1825	U1884	C1957	U2033	U2188	U2251	U2325	U2392	
	A1525	A1598	G1681	A1751	U1827	U1885	G1958	G2034	U2189	U2252	U2326	U2393	
				C1752	G1828	U1886	U1959	G2035	G2190	A2191	A2333	U2394	
				A1752	U1751	C1887	A1889	A2037	A2191	U1963	U2334	A2335	
				A1601	G1752	U1888	A1890	A2038	U1964	G1963	U2335		
				U1602	A1754	G1889	G1891	G2038	C1965	G1964	U2192		
				A1603	A1755	C1892	C1893			C1965	G2193		



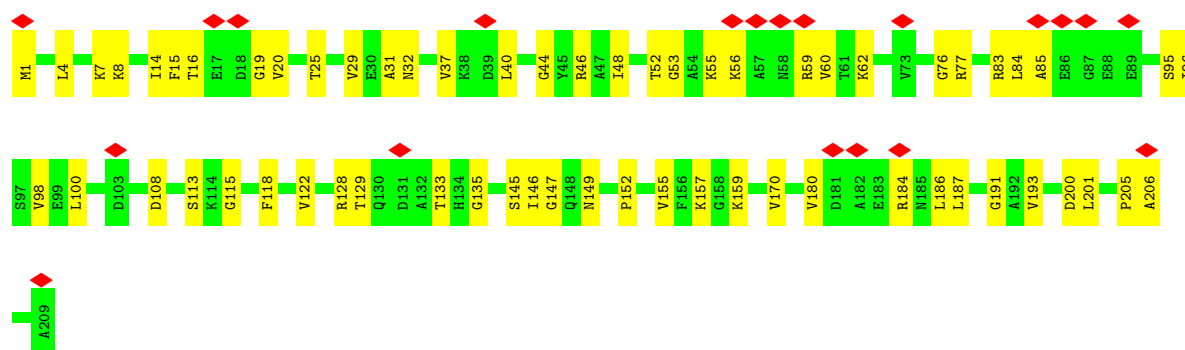
• Molecule 3: 5S rRNA



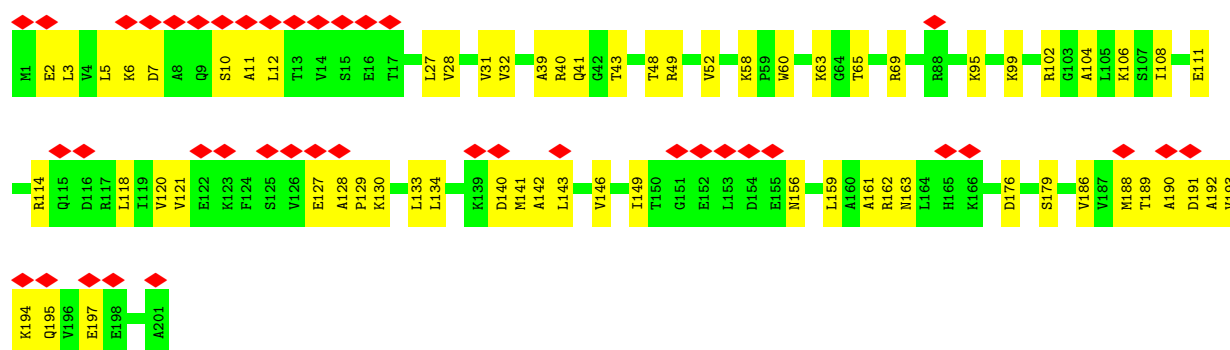
• Molecule 4: 50S ribosomal protein L2



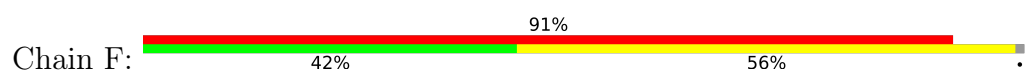
• Molecule 5: 50S ribosomal protein L3



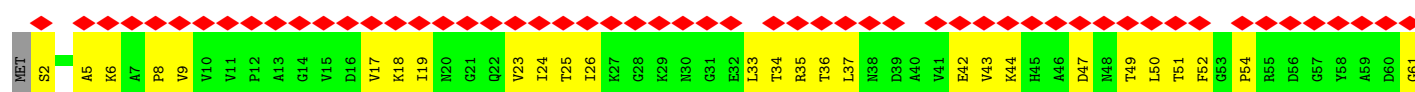
• Molecule 6: 50S ribosomal protein L4

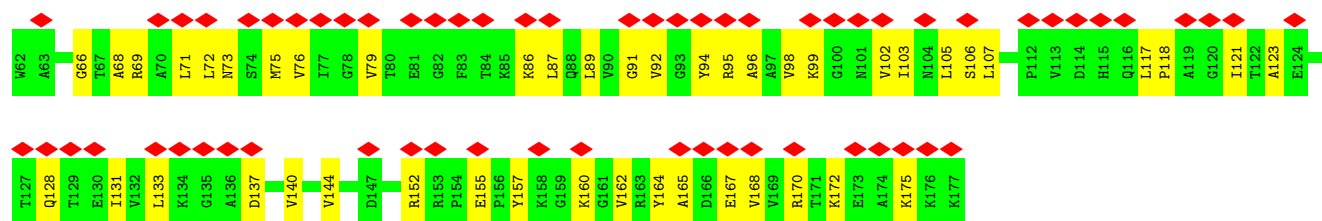


• Molecule 7: 50S ribosomal protein L5

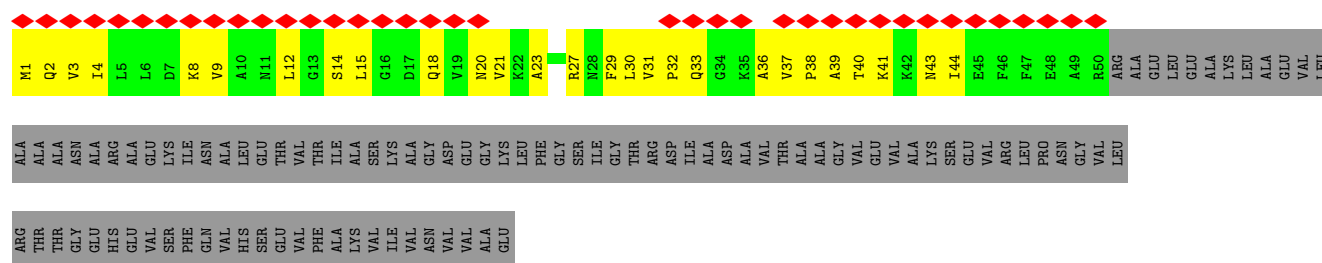


• Molecule 8: 50S ribosomal protein L6

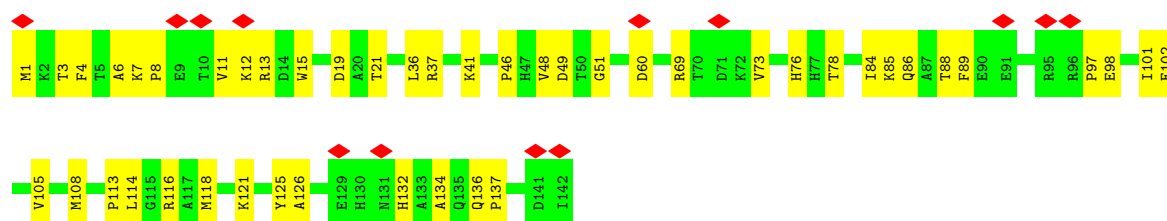




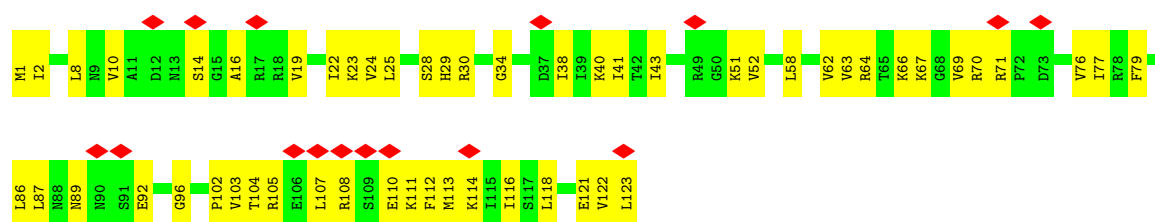
• Molecule 9: 50S ribosomal protein L9



• Molecule 10: 50S ribosomal protein L13

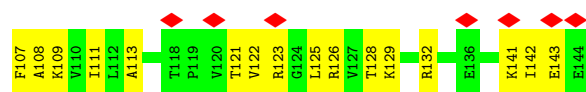


• Molecule 11: 50S ribosomal protein L14

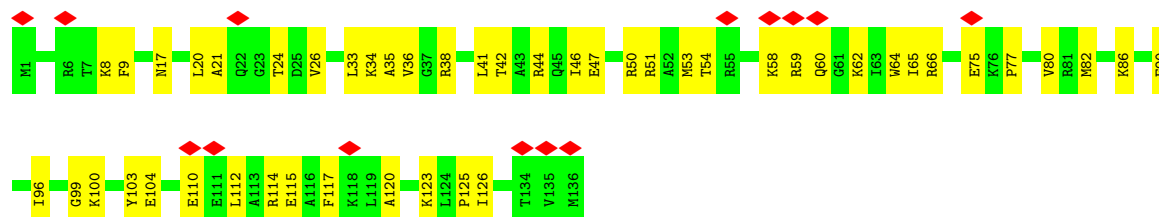


• Molecule 12: 50S ribosomal protein L15

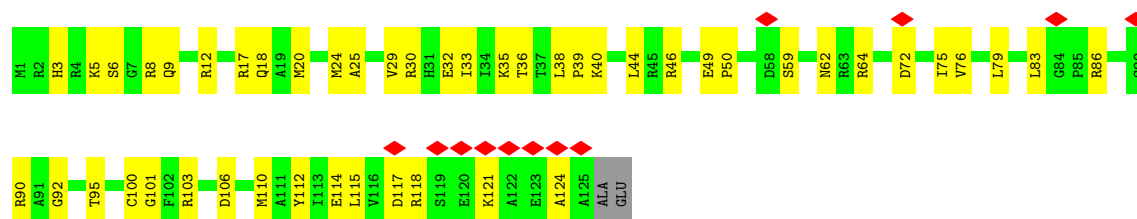




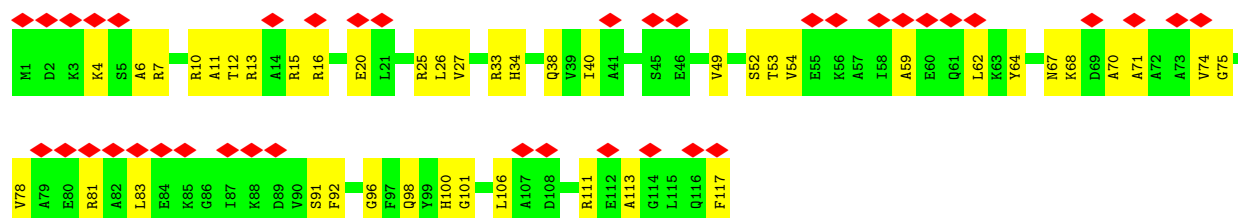
- Molecule 13: 50S ribosomal protein L16



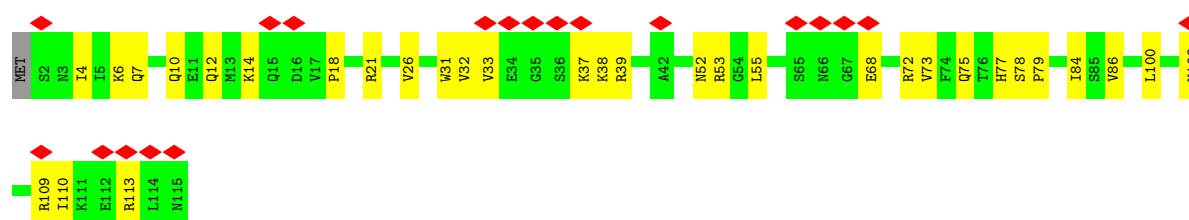
- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18

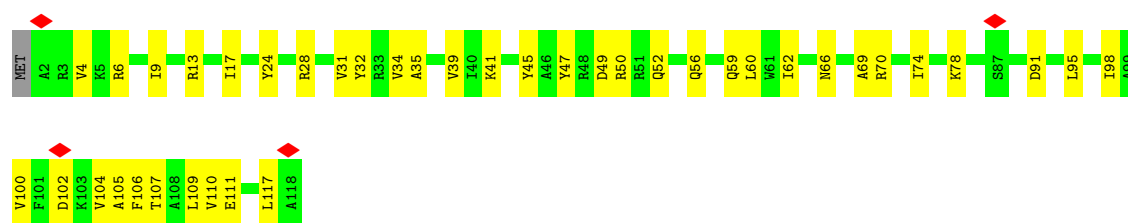


- Molecule 16: 50S ribosomal protein L19



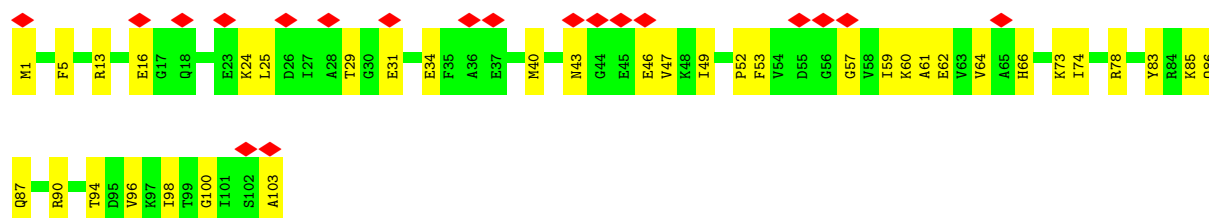
- Molecule 17: 50S ribosomal protein L20

Chain R:  65% 34%



- Molecule 18: 50S ribosomal protein L21

Chain S:  18% 65% 35%



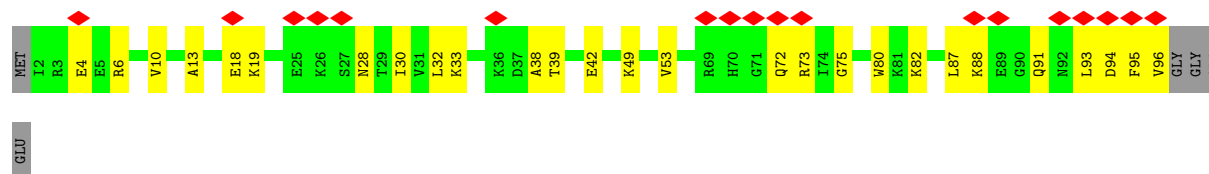
- Molecule 19: 50S ribosomal protein L22

Chain T:  12% 64% 36%



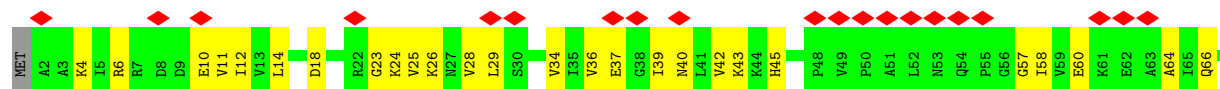
- Molecule 20: 50S ribosomal protein L23

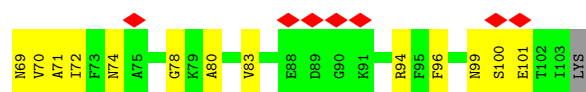
Chain U:  18% 68% 27% 5%



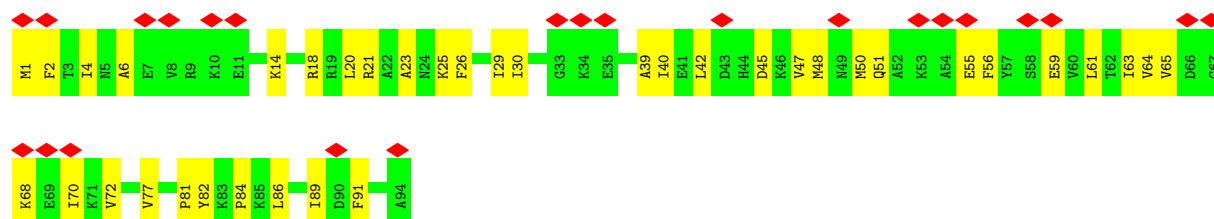
- Molecule 21: 50S ribosomal protein L24

Chain V:  26% 61% 38%

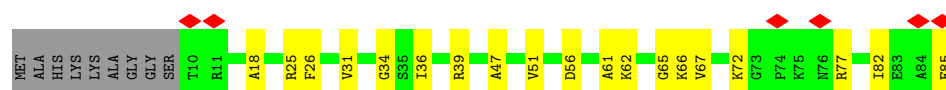




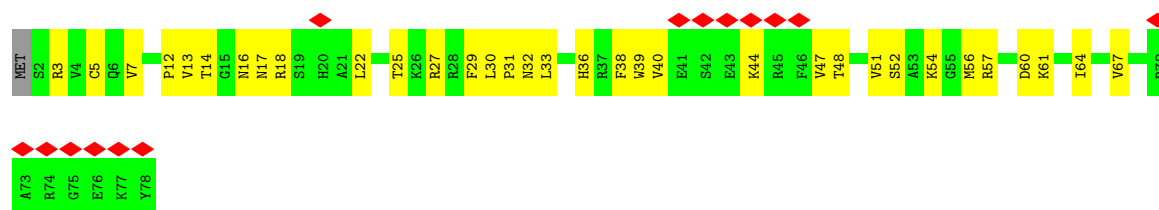
- Molecule 22: 50S ribosomal protein L25



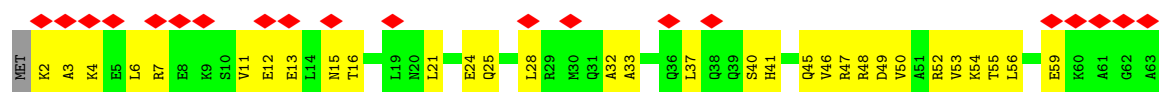
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28



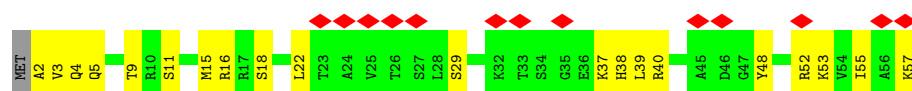
- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L32



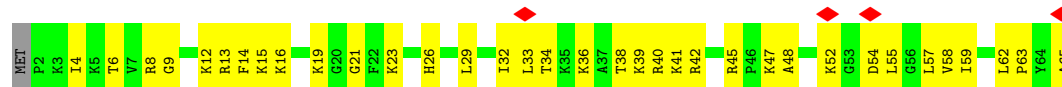
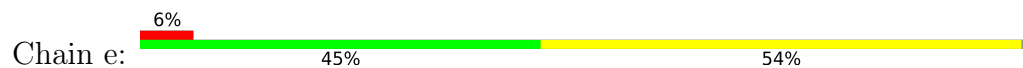
- Molecule 28: 50S ribosomal protein L33



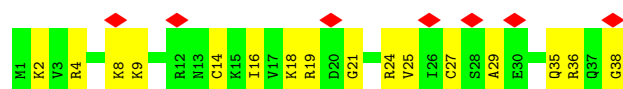
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	59148	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 ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.616	Depositor
Minimum map value	-0.384	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	312.91, 312.91, 302.12	wwPDB
Map dimensions	290, 290, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.079, 1.079, 1.079	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, MG, JJH, FME, ZN

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	1	0.10	0/93	0.35	0/142
2	A	0.10	0/67296	0.20	0/104979
3	B	0.08	0/2872	0.16	0/4478
4	C	0.14	0/2121	0.36	0/2852
5	D	0.12	0/1585	0.34	0/2134
6	E	0.12	0/1570	0.32	0/2113
7	F	0.14	0/1434	0.39	0/1926
8	G	0.13	0/1342	0.35	0/1816
9	H	0.14	0/389	0.41	0/523
10	K	0.12	0/1151	0.30	0/1551
11	L	0.14	0/955	0.33	0/1279
12	M	0.15	0/1061	0.39	0/1413
13	N	0.13	0/1092	0.32	0/1460
14	O	0.13	0/1006	0.37	0/1345
15	P	0.11	0/909	0.31	0/1219
16	Q	0.13	0/928	0.34	0/1242
17	R	0.13	0/959	0.34	0/1278
18	S	0.12	0/828	0.30	0/1107
19	T	0.12	0/863	0.32	0/1156
20	U	0.10	0/763	0.30	0/1021
21	V	0.12	0/787	0.33	0/1051
22	W	0.13	0/765	0.33	0/1025
23	X	0.13	0/586	0.36	0/776
24	Y	0.12	0/634	0.35	0/848
25	Z	0.10	0/501	0.32	0/667
26	a	0.11	0/452	0.29	0/605
27	b	0.12	0/449	0.32	0/599
28	c	0.12	0/421	0.31	0/561
29	d	0.13	0/379	0.38	0/498
30	e	0.13	0/512	0.36	0/676
31	f	0.12	0/302	0.30	0/397
All	All	0.11	0/95005	0.24	0/142737

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1	84	0	44	2	0
2	A	60085	0	30220	1583	0
3	B	2569	0	1301	66	0
4	C	2082	0	2154	83	0
5	D	1564	0	1616	61	0
6	E	1551	0	1619	53	0
7	F	1410	0	1444	102	0
8	G	1322	0	1371	68	0
9	H	384	0	405	21	0
10	K	1128	0	1162	36	0
11	L	946	0	1023	50	0
12	M	1052	0	1129	43	0
13	N	1073	0	1157	35	0
14	O	993	0	1034	41	0
15	P	899	0	935	38	0
16	Q	916	0	962	31	0
17	R	946	0	1019	33	0
18	S	815	0	839	28	0
19	T	856	0	922	32	0
20	U	756	0	817	22	0
21	V	779	0	831	32	0
22	W	752	0	780	40	0
23	X	579	0	594	14	0
24	Y	624	0	652	34	0
25	Z	500	0	531	28	0
26	a	448	0	488	26	0
27	b	443	0	458	22	0
28	c	414	0	442	16	0
29	d	376	0	418	15	0
30	e	503	0	572	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	f	301	0	340	16	0
32	1	10	0	10	0	0
33	1	1	0	0	0	0
33	A	369	0	0	0	0
33	B	8	0	0	0	0
33	C	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	b	1	0	0	0	0
34	A	22	0	12	1	0
35	A	42	28	0	0	0
36	f	1	0	0	0	0
All	All	87607	28	57301	2423	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 17.

The worst 5 of 2423 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)
2:A:775:G:H4'	2:A:776:G:H5'	1.45	0.97
13:N:77:PRO:HG2	13:N:80:VAL:HG21	1.47	0.96
20:U:53:VAL:HG11	20:U:87:LEU:HD13	1.48	0.94
7:F:108:VAL:HG11	7:F:176:PRO:HG2	1.47	0.93
8:G:164:TYR:HB2	8:G:167:GLU:HG2	1.50	0.91

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	
4	C	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
5	D	207/209 (99%)	203 (98%)	4 (2%)	0	100	100
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
7	F	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
8	G	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
9	H	48/149 (32%)	45 (94%)	3 (6%)	0	100	100
10	K	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	L	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
12	M	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
13	N	134/136 (98%)	134 (100%)	0	0	100	100
14	O	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
15	P	115/117 (98%)	115 (100%)	0	0	100	100
16	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
17	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
18	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
19	T	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
20	U	93/100 (93%)	93 (100%)	0	0	100	100
21	V	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
22	W	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
24	Y	75/78 (96%)	75 (100%)	0	0	100	100
25	Z	60/63 (95%)	60 (100%)	0	0	100	100
26	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
27	b	54/57 (95%)	54 (100%)	0	0	100	100
28	c	49/55 (89%)	49 (100%)	0	0	100	100
29	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
30	e	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
31	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	3078/3267 (94%)	3010 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	216/218 (99%)	216 (100%)	0	100	100
5	D	164/164 (100%)	164 (100%)	0	100	100
6	E	165/165 (100%)	165 (100%)	0	100	100
7	F	148/150 (99%)	148 (100%)	0	100	100
8	G	137/138 (99%)	137 (100%)	0	100	100
9	H	40/114 (35%)	40 (100%)	0	100	100
10	K	116/116 (100%)	116 (100%)	0	100	100
11	L	104/104 (100%)	104 (100%)	0	100	100
12	M	103/103 (100%)	103 (100%)	0	100	100
13	N	109/109 (100%)	109 (100%)	0	100	100
14	O	102/103 (99%)	102 (100%)	0	100	100
15	P	87/87 (100%)	87 (100%)	0	100	100
16	Q	99/100 (99%)	99 (100%)	0	100	100
17	R	89/90 (99%)	89 (100%)	0	100	100
18	S	84/84 (100%)	84 (100%)	0	100	100
19	T	93/93 (100%)	93 (100%)	0	100	100
20	U	82/84 (98%)	82 (100%)	0	100	100
21	V	83/85 (98%)	83 (100%)	0	100	100
22	W	78/78 (100%)	78 (100%)	0	100	100
23	X	57/63 (90%)	57 (100%)	0	100	100
24	Y	67/68 (98%)	67 (100%)	0	100	100
25	Z	54/55 (98%)	54 (100%)	0	100	100
26	a	48/49 (98%)	48 (100%)	0	100	100
27	b	47/48 (98%)	47 (100%)	0	100	100
28	c	45/49 (92%)	45 (100%)	0	100	100
29	d	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	e	51/52 (98%)	51 (100%)	0	100	100
31	f	34/34 (100%)	34 (100%)	0	100	100
All	All	2540/2641 (96%)	2540 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
16	Q	12	GLN
24	Y	34	HIS
16	Q	56	HIS
22	W	78	GLN
29	d	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3/4 (75%)	1 (33%)	0
2	A	2786/2795 (99%)	327 (11%)	8 (0%)
3	B	119/120 (99%)	9 (7%)	0
All	All	2908/2919 (99%)	337 (11%)	8 (0%)

5 of 337 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	76	A
2	A	10	A
2	A	12	U
2	A	15	G
2	A	34	U

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	2756	U
2	A	2474	U
2	A	1757	A
2	A	1358	G
2	A	2211	A

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](#)

Of 386 ligands modelled in this entry, 383 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	JJH	A	3370	-	46,47,47	1.93	9 (19%)	66,71,71	2.59	20 (30%)
34	AMP	A	3001	-	21,24,25	0.24	0	30,35,38	0.32	0
32	FME	1	101	1	8,9,10	0.96	0	8,9,11	0.95	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	JJH	A	3370	-	-	11/24/50/50	0/6/6/6
34	AMP	A	3001	-	-	0/7/25/26	0/3/3/3
32	FME	1	101	1	-	2/7/9/11	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3370	JJH	CBB-CBF	-5.47	1.40	1.48
35	A	3370	JJH	CBJ-NAM	-4.97	1.33	1.43
35	A	3370	JJH	CBA-CBD	-4.47	1.39	1.48
35	A	3370	JJH	CAT-NAK	-3.92	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3370	JJH	CAX-NAK	3.54	1.40	1.34

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	3370	JJH	CBL-OAH-CBO	-11.45	100.96	110.10
35	A	3370	JJH	CBK-NAM-CBO	-8.28	105.05	111.17
35	A	3370	JJH	OAJ-CBO-NAM	-5.72	123.50	128.80
35	A	3370	JJH	OAH-CBL-CBK	-5.41	99.26	104.50
35	A	3370	JJH	CBL-CBK-NAM	-3.99	98.08	101.85

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

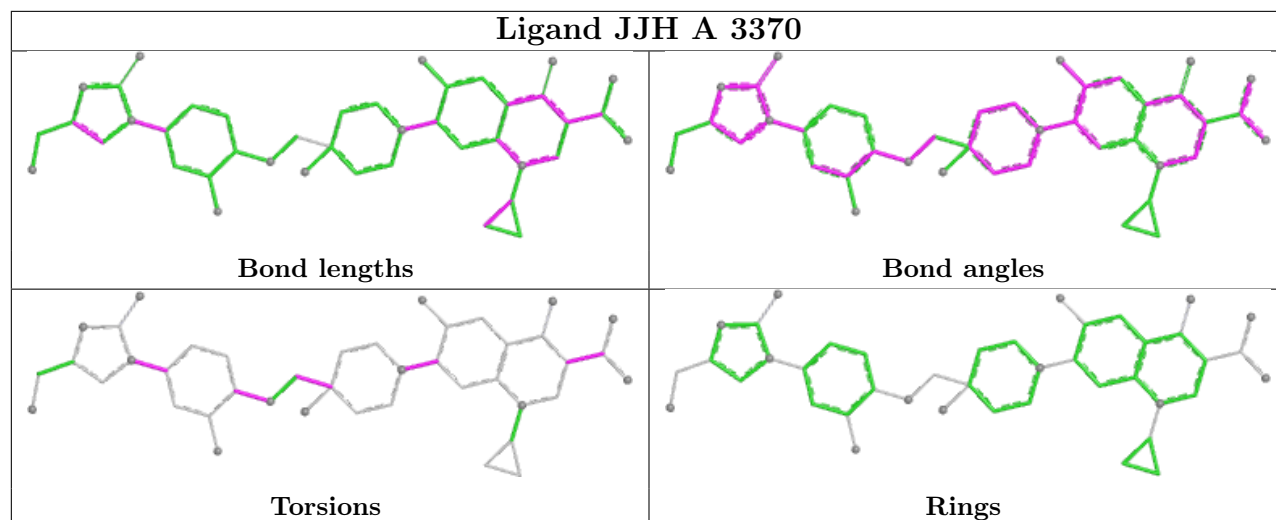
Mol	Chain	Res	Type	Atoms
32	1	101	FME	O1-CN-N-CA
32	1	101	FME	CB-CA-N-CN
35	A	3370	JJH	CAR-CAQ-CAY-OAD
35	A	3370	JJH	CAS-CAQ-CAY-OAD
35	A	3370	JJH	OAC-CAQ-CAY-OAD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	3001	AMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
2	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1531:C	O3'	1540:G	P	18.12
1	A	883:G	O3'	893:C	P	17.33
1	A	2101:A	O3'	2188:U	P	16.18
1	A	545:U	O3'	548:G	P	15.10
1	A	1173:U	O3'	1177:G	P	12.82

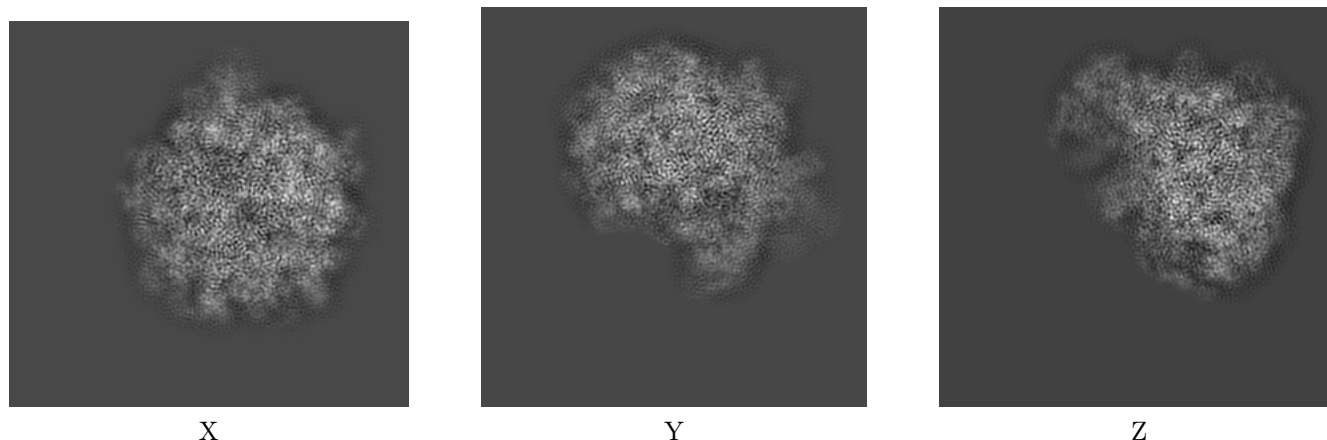
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4638. These allow visual inspection of the internal detail of the map and identification of artifacts.

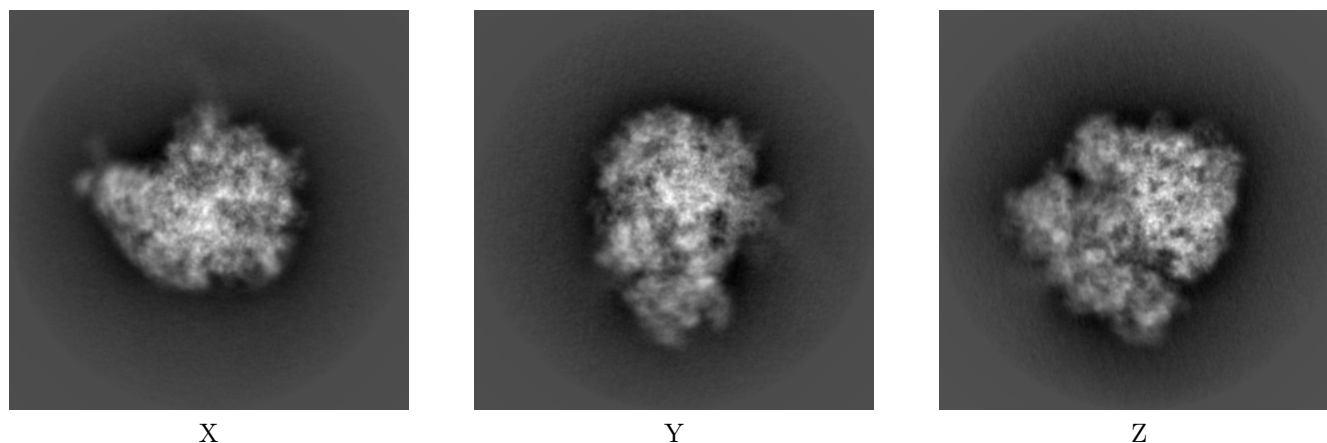
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



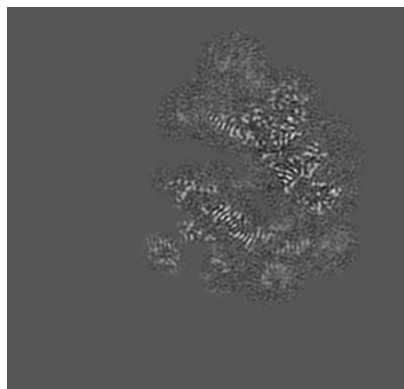
6.1.2 Raw map



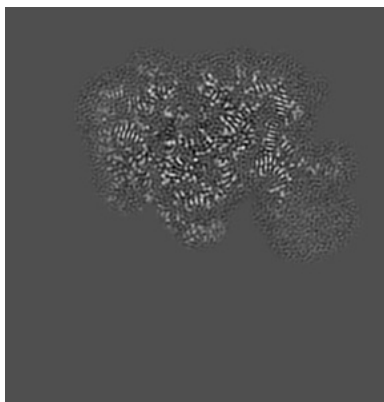
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

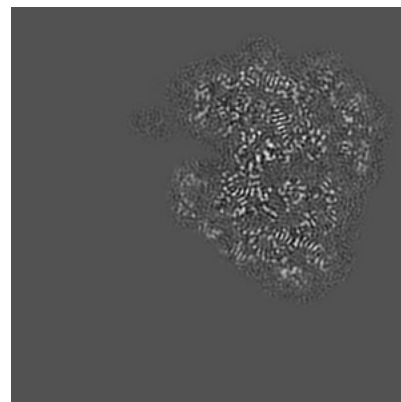
6.2.1 Primary map



X Index: 145

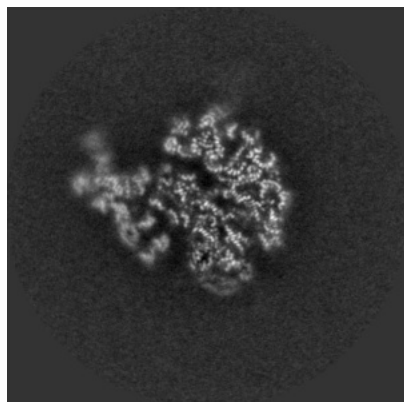


Y Index: 145

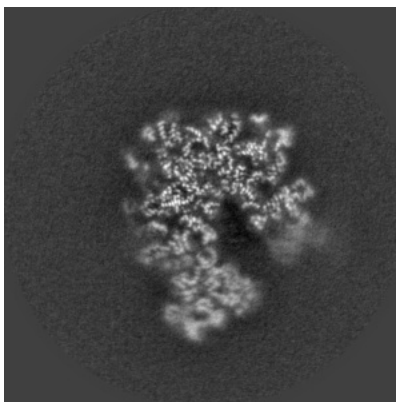


Z Index: 140

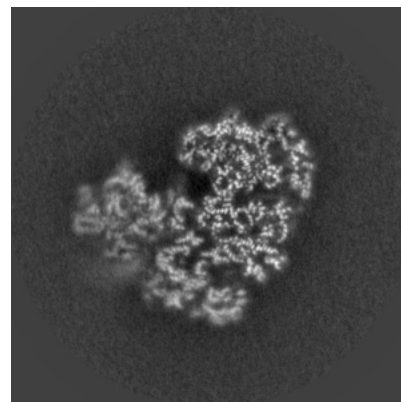
6.2.2 Raw map



X Index: 200



Y Index: 200

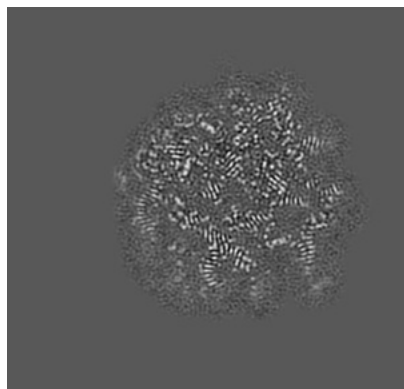


Z Index: 200

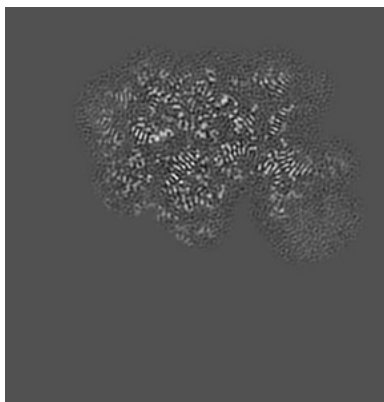
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

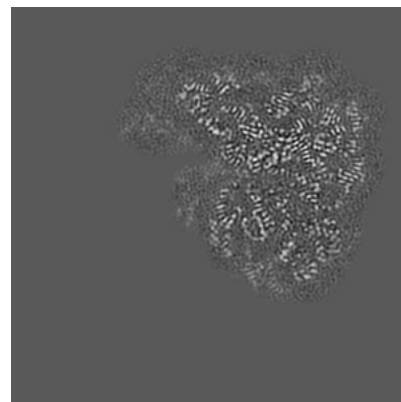
6.3.1 Primary map



X Index: 196

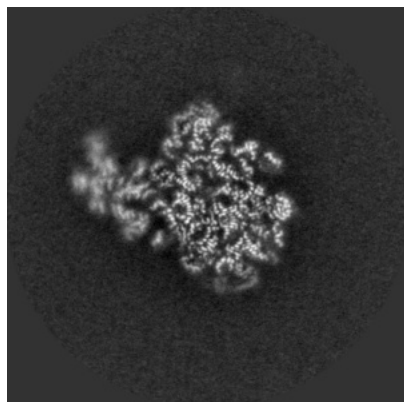


Y Index: 150

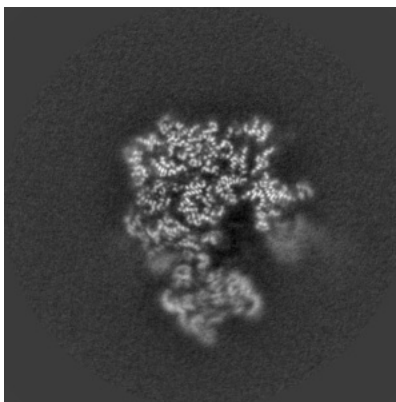


Z Index: 153

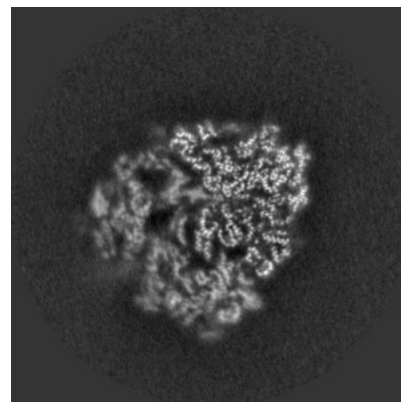
6.3.2 Raw map



X Index: 208



Y Index: 190

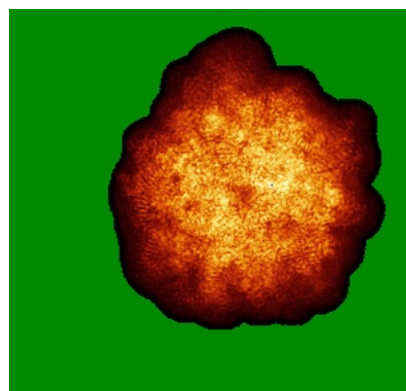


Z Index: 213

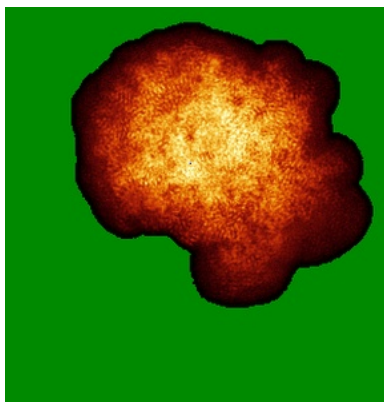
The images above show the largest variance slices of the map in three orthogonal directions.

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

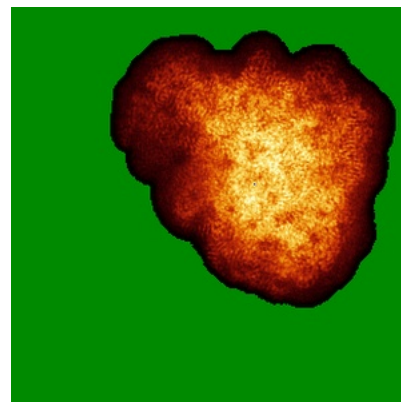
6.4.1 Primary map



X

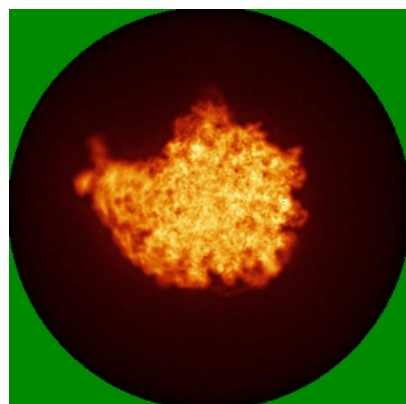


Y

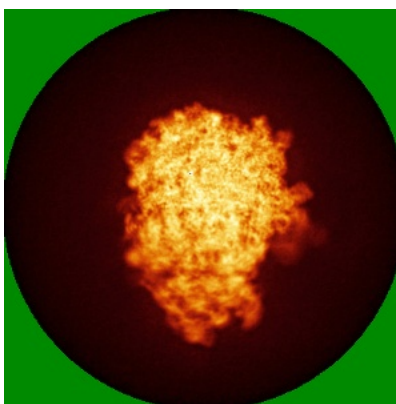


Z

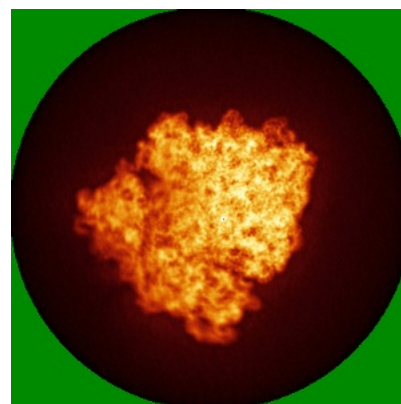
6.4.2 Raw map



X



Y

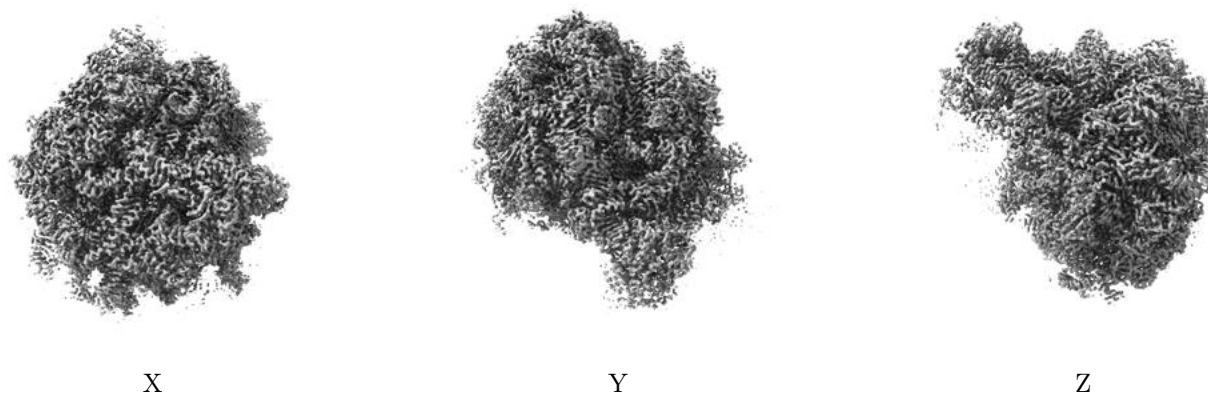


Z

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

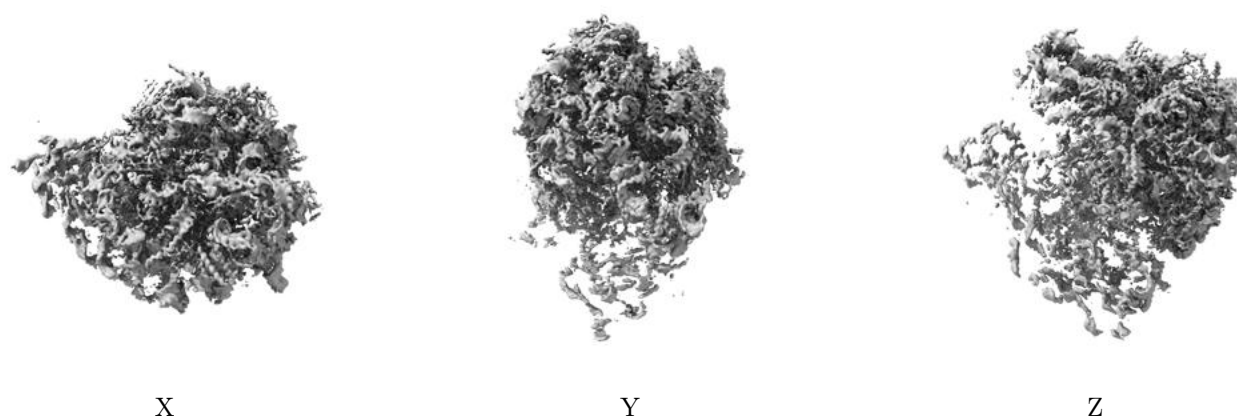
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

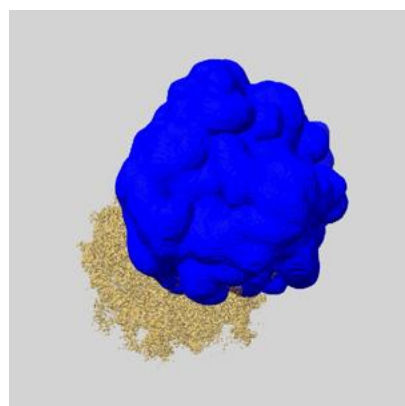
6.6 Mask visualisation [i](#)

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

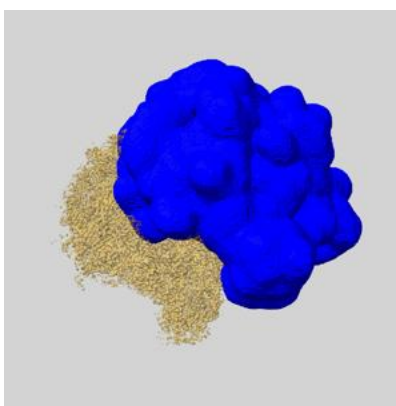
A mask typically either:

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

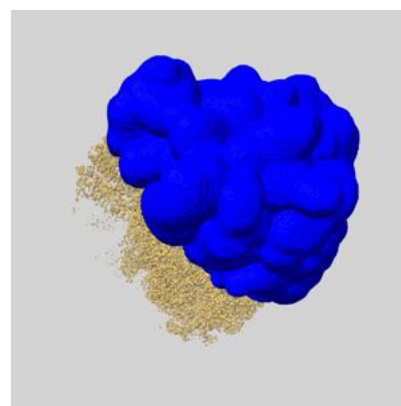
6.6.1 emd_4638_msk_1.map [i](#)



X



Y

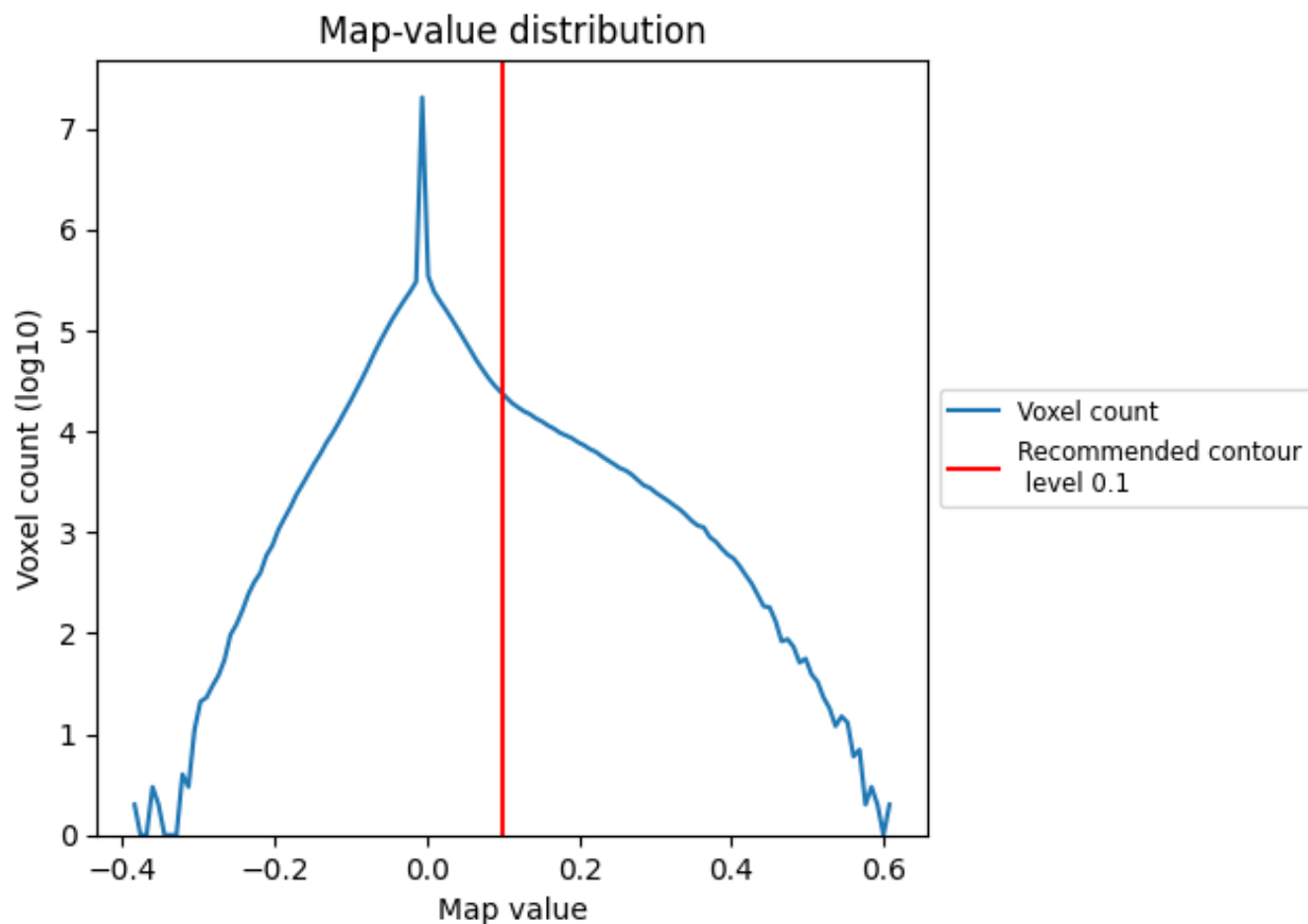


Z

7 Map analysis [i](#)

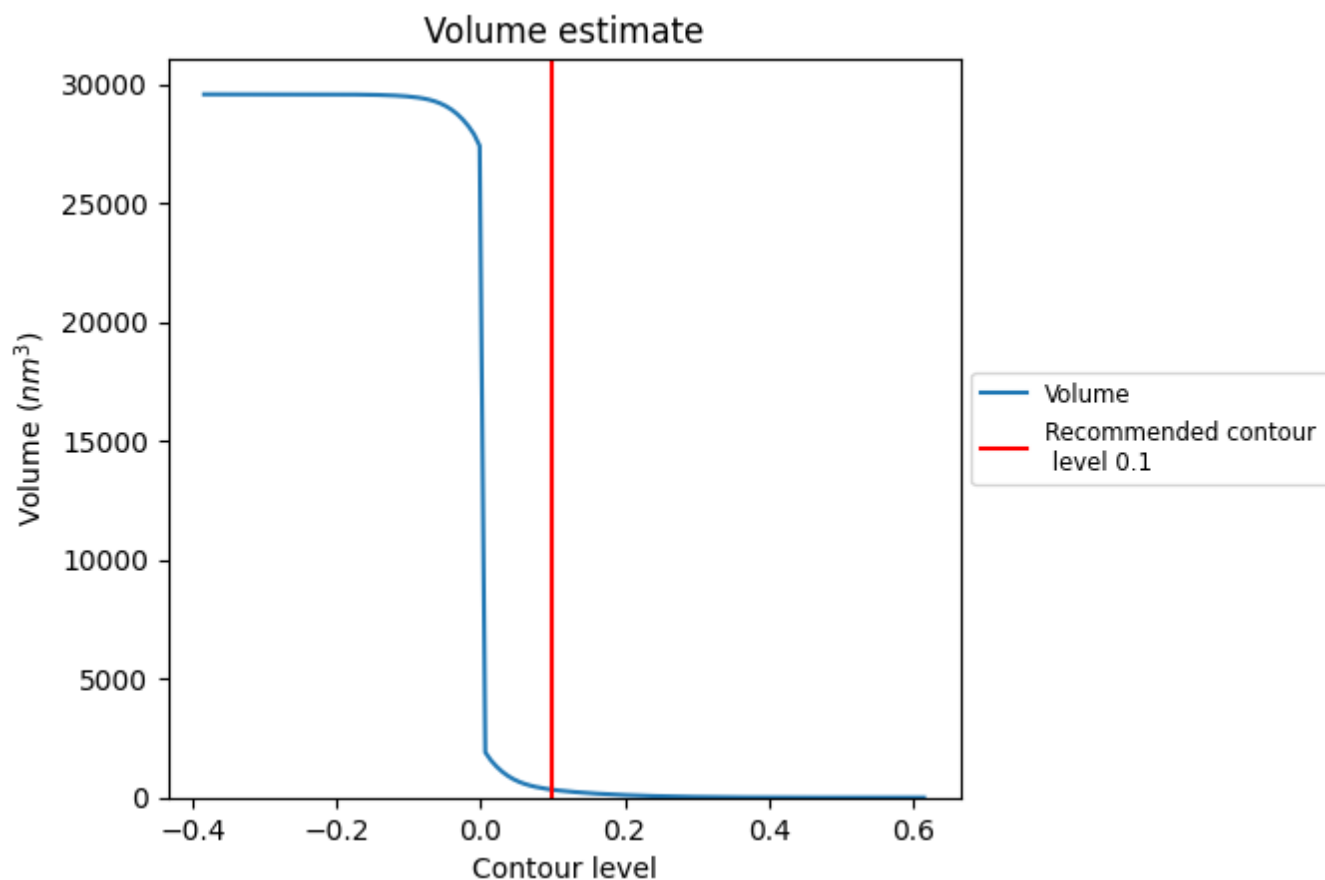
This section contains the results of statistical analysis of the map.

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 329 nm³; this corresponds to an approximate mass of 297 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.

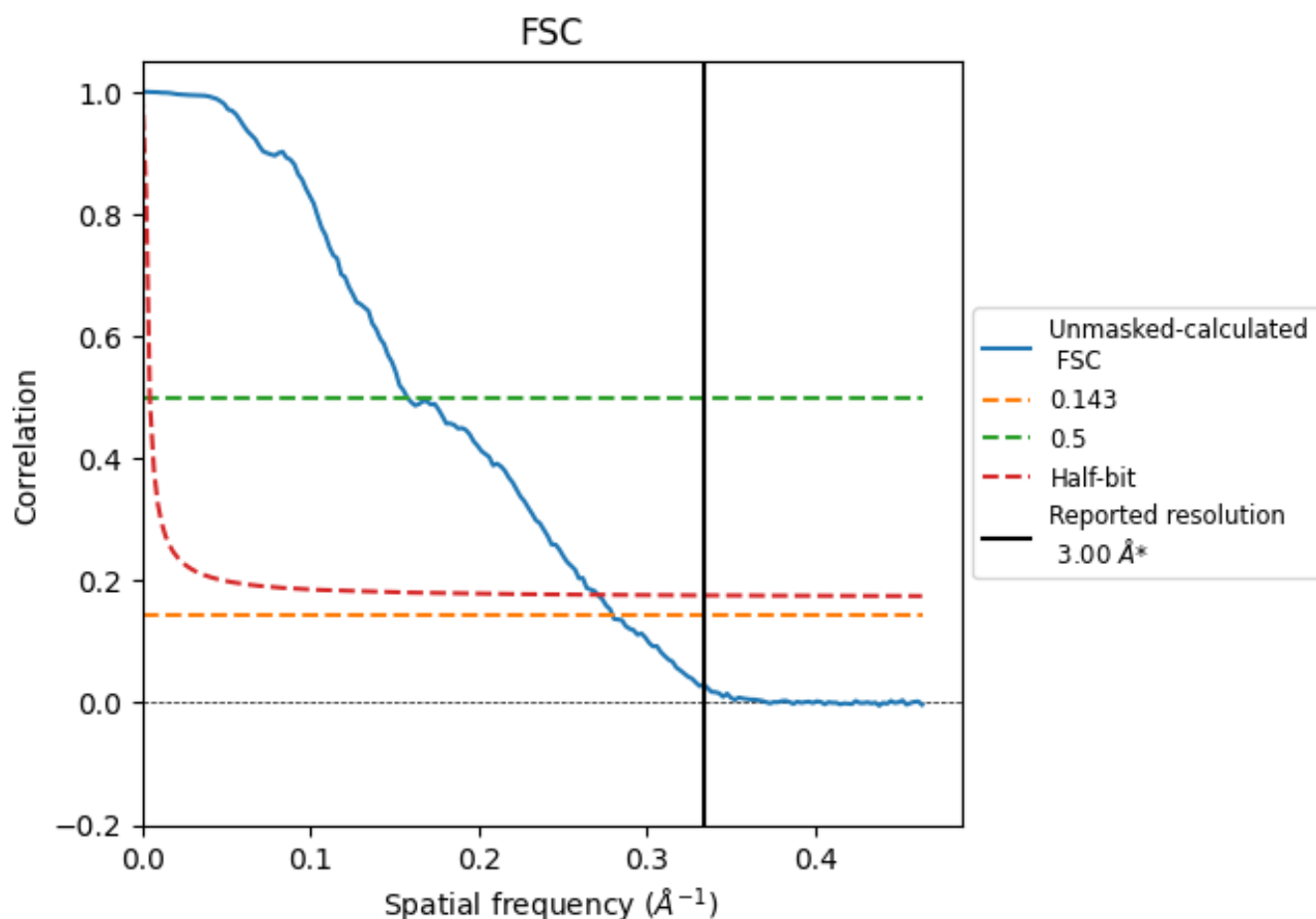
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

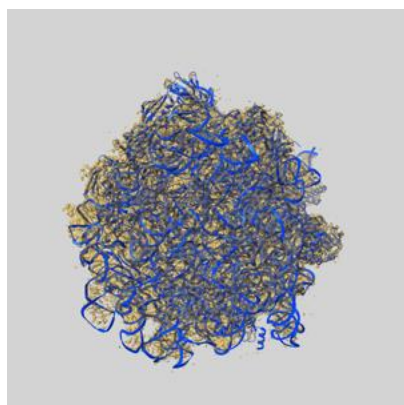
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	6.35	3.69

*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 3.58 differs from the reported value 3.0 by more than 10 %

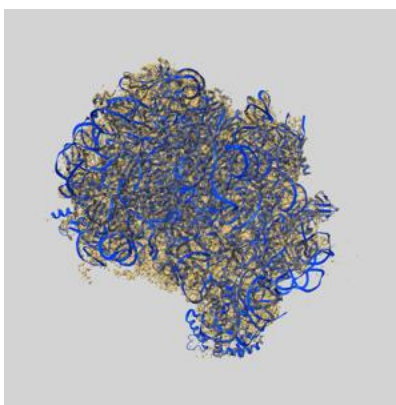
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4638 and PDB model 6QUL. Per-residue inclusion information can be found in section 3 on page 12.

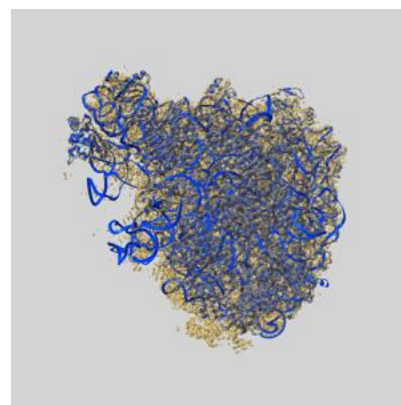
9.1 Map-model overlay [i](#)



X



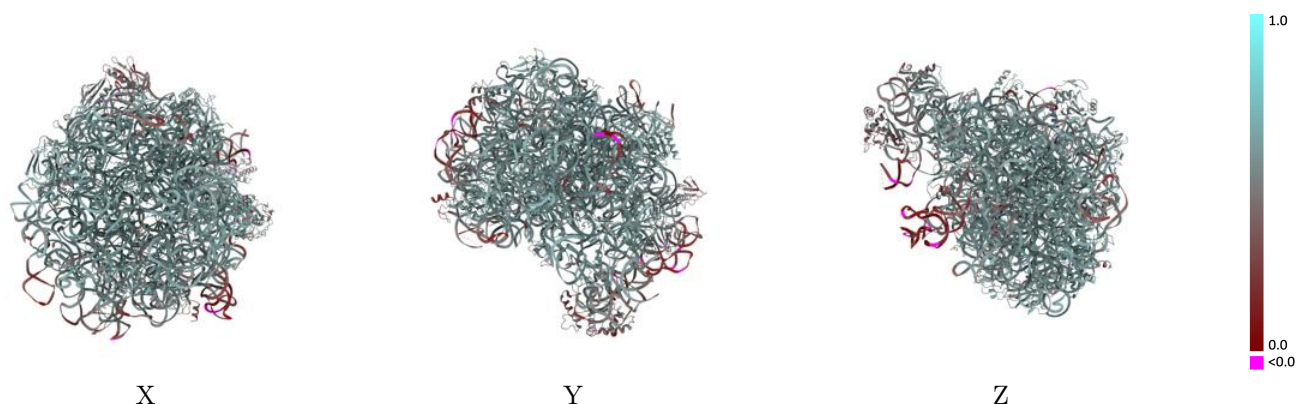
Y



Z

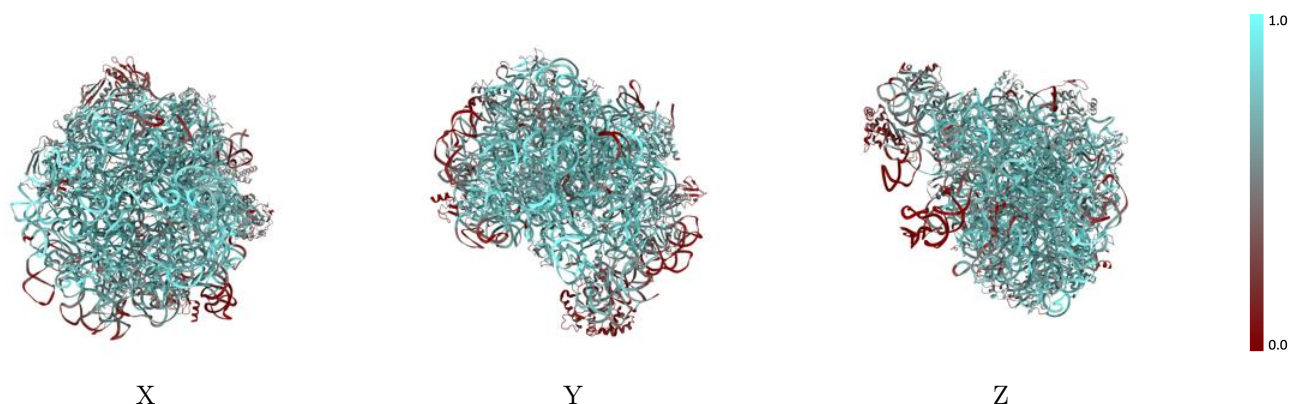
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



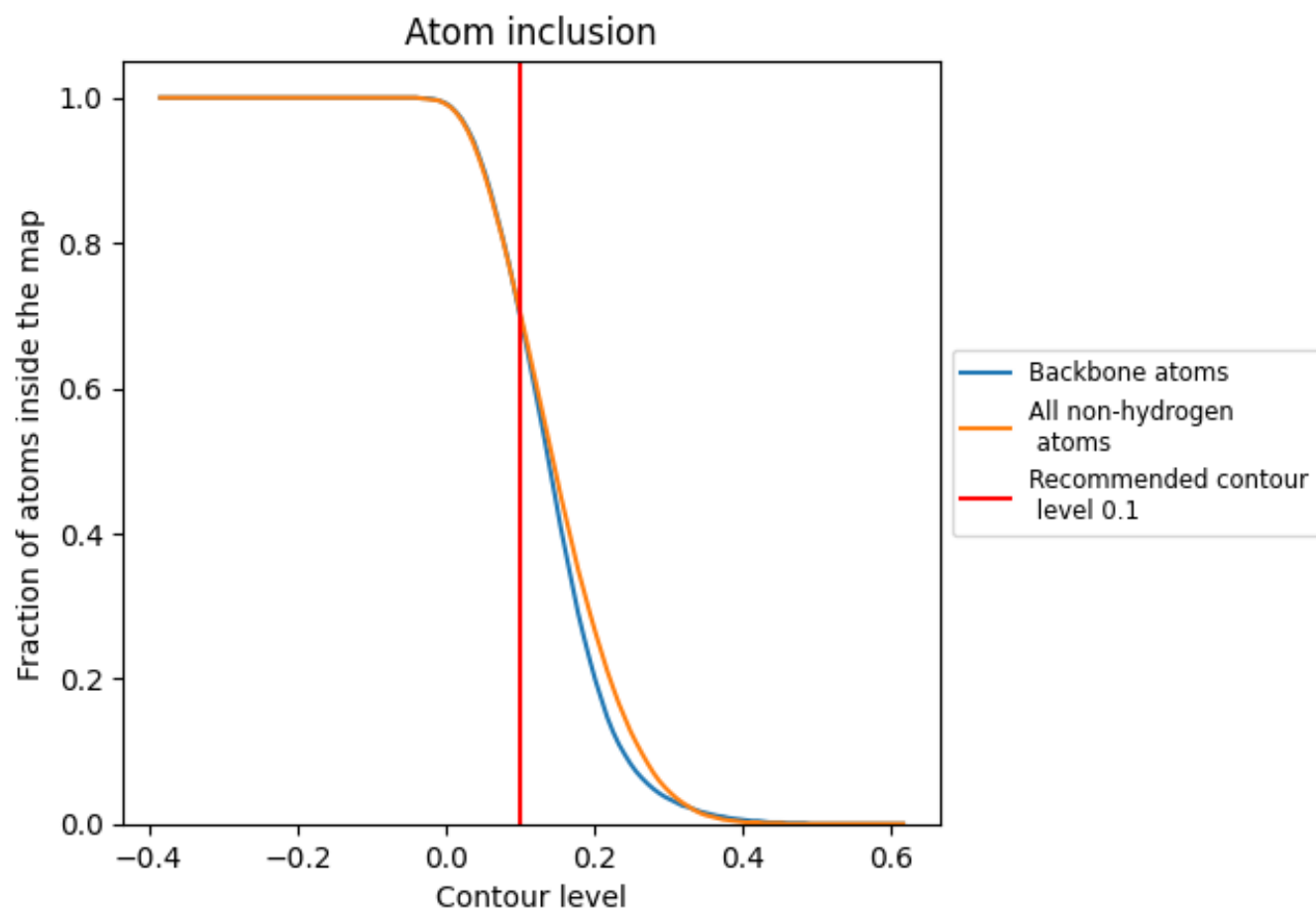
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.7050	 0.5560
1	 0.3900	 0.4680
A	 0.7570	 0.5590
B	 0.6120	 0.5120
C	 0.7030	 0.5940
D	 0.6840	 0.5880
E	 0.5980	 0.5610
F	 0.1780	 0.4100
G	 0.3240	 0.4600
H	 0.2240	 0.4210
K	 0.7030	 0.5900
L	 0.6440	 0.5840
M	 0.6620	 0.5720
N	 0.6600	 0.5830
O	 0.7020	 0.5810
P	 0.5070	 0.5260
Q	 0.6080	 0.5710
R	 0.7380	 0.5940
S	 0.6490	 0.5750
T	 0.6570	 0.5800
U	 0.5650	 0.5500
V	 0.5350	 0.5300
W	 0.5480	 0.5390
X	 0.6980	 0.5910
Y	 0.6230	 0.5760
Z	 0.5080	 0.5210
a	 0.6650	 0.5750
b	 0.6450	 0.5610
c	 0.5860	 0.5550
d	 0.7510	 0.6080
e	 0.7310	 0.5940
f	 0.6030	 0.5590

