



## wwPDB EM Validation Summary Report ⓘ

Sep 1, 2025 – 03:51 PM EDT

PDB ID : 9B50 / pdb\_00009b50  
EMDB ID : EMD-44193  
Title : E. coli 70S ribosome complex (unmethylated 16S A1408 + arbekacin)  
Authors : Mattingly, J.M.; Dey, D.; Zelinskaya, N.; Dunham, C.M.; Conn, G.L.  
Deposited on : 2024-03-21  
Resolution : 2.70 Å (reported)  
Based on initial models : 7K00, 5JTE

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

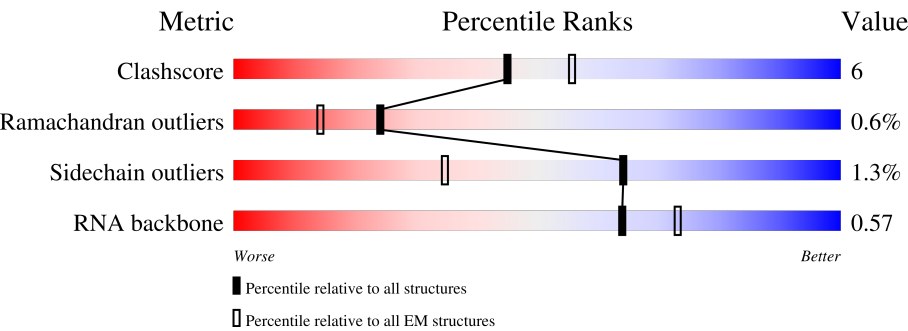
EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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





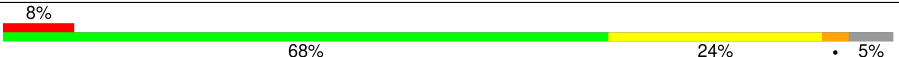
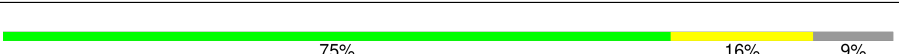
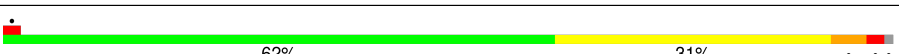
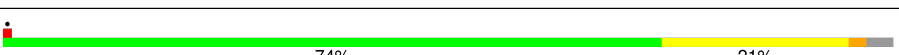
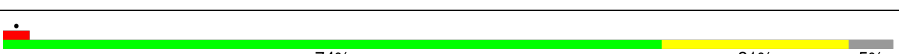
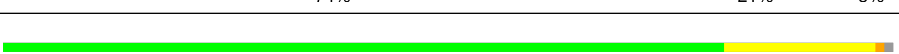

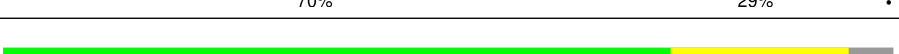
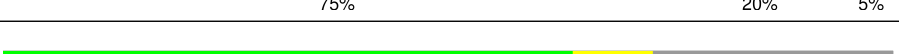
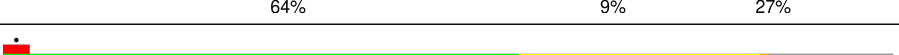
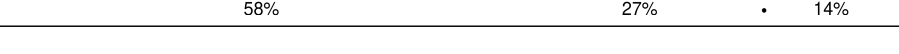
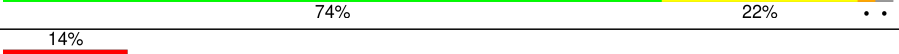




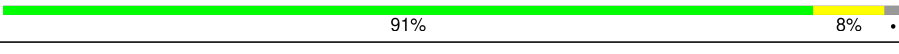
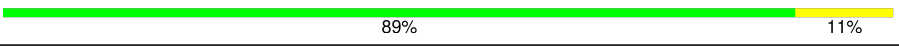

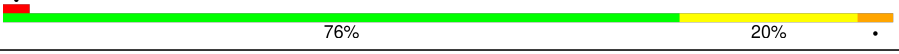



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AA	1539	<div><div>17%</div><div>68%25%7%</div></div>
2	AB	240	<div><div>67%23%9%</div></div>
3	AC	233	<div><div>73%16%12%</div></div>
4	AD	206	<div><div>17%</div><div>56%38%. .</div></div>
5	AE	167	<div><div>68%22%10%</div></div>
6	AF	135	<div><div>58%16%.26%</div></div>
7	AG	179	<div><div>68%16%.16%</div></div>











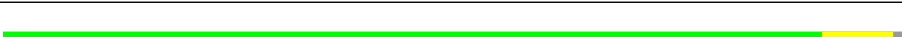


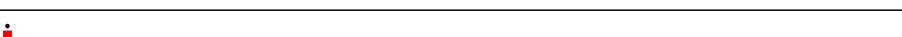
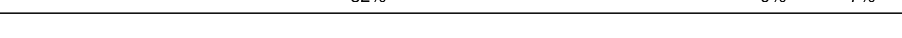
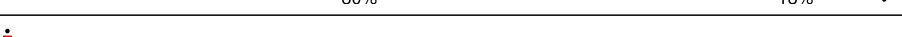
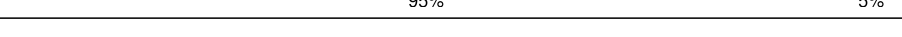
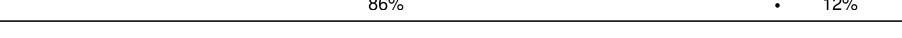

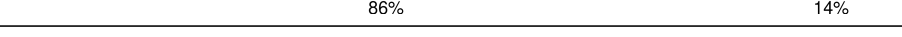
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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	B0	57	
23	B1	55	
24	B2	46	
25	B3	65	
26	B4	38	
27	B5	70	
28	BA	2903	
29	BB	120	
30	BC	273	
31	BD	209	
32	BE	201	

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Mol	Chain	Length	Quality of chain
33	BF	179	
34	BG	177	
35	BH	149	
36	BJ	142	
37	BK	123	
38	BL	144	
39	BM	136	
40	BN	127	
41	BO	117	
42	BP	115	
43	BQ	118	
44	BR	103	
45	BS	110	
46	BT	100	
47	BU	104	
48	BV	94	
49	BW	85	
50	BX	78	
51	BY	63	
52	BZ	59	

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 141469 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B5	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	120	A	U	conflict	GB 1370526515

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BH	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

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

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BW	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

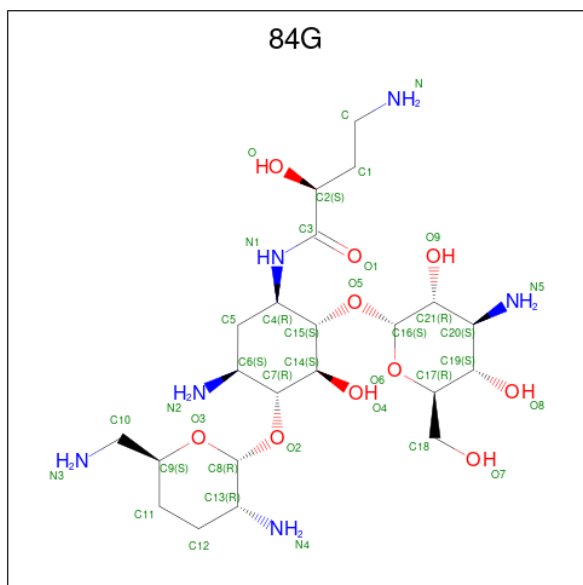
Mol	Chain	Residues	Atoms		AltConf
53	AA	93	Total	Mg	0
			93	93	
53	B0	1	Total	Mg	0
			1	1	
53	BA	207	Total	Mg	0
			207	207	
53	BB	5	Total	Mg	0
			5	5	
53	BC	1	Total	Mg	0
			1	1	
53	BN	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
53	BQ	1	Total	Mg	0
			1	1	

- Molecule 54 is Arbekacin (CCD ID: 84G) (formula:  $C_{22}H_{44}N_6O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
54	AA	1	Total	C	N	O	0
			38	22	6	10	
54	AA	1	Total	C	N	O	0
			38	22	6	10	

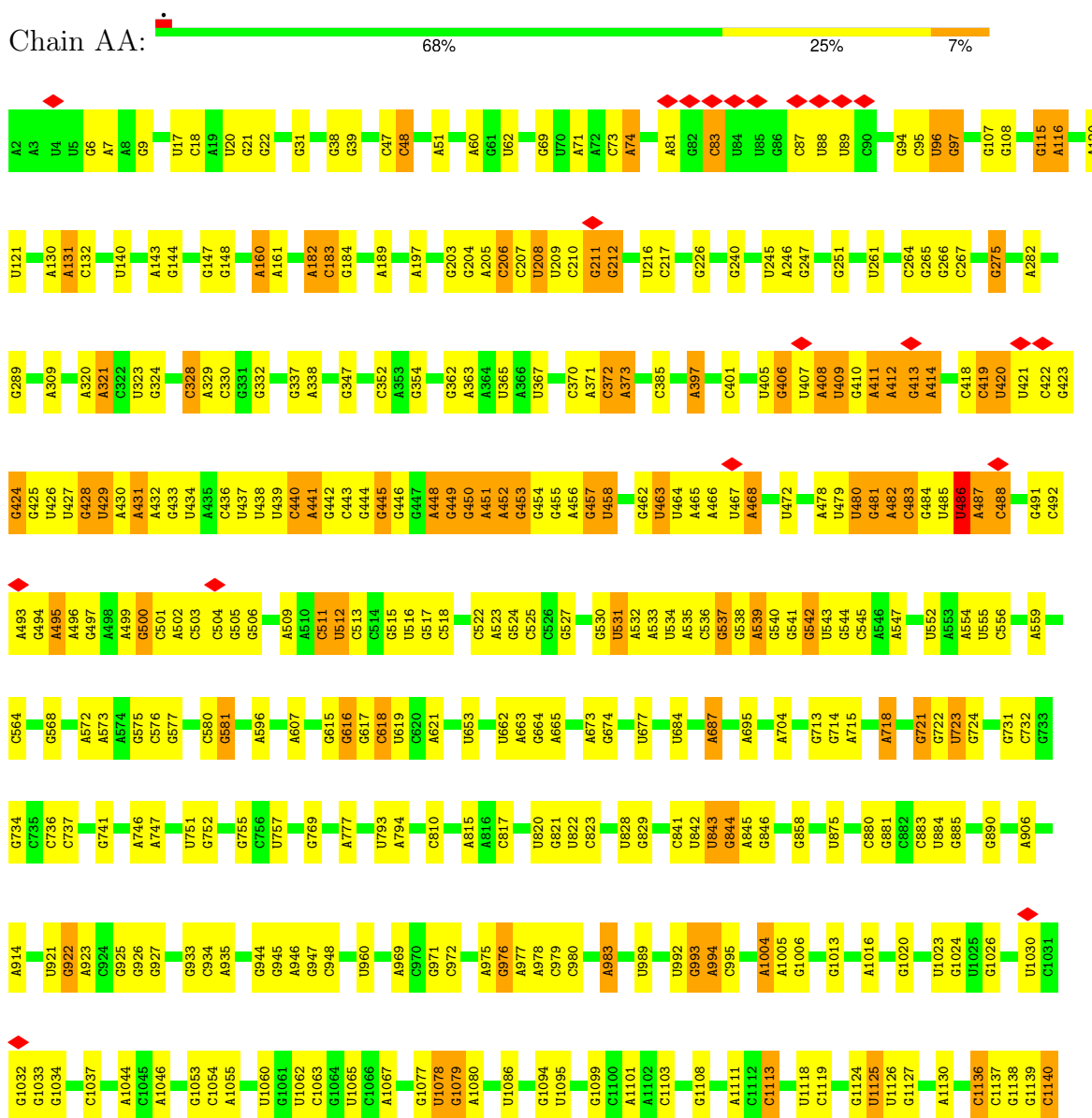
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

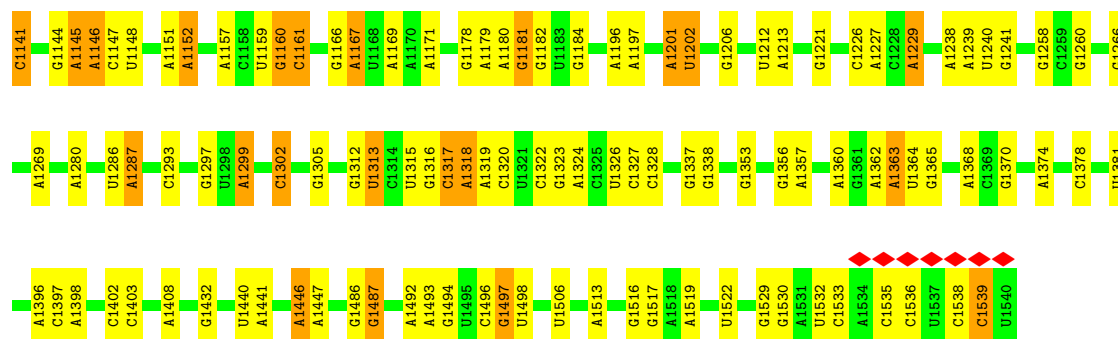
Mol	Chain	Residues	Atoms		AltConf
55	B4	1	Total	Zn	0
			1	1	
55	B5	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

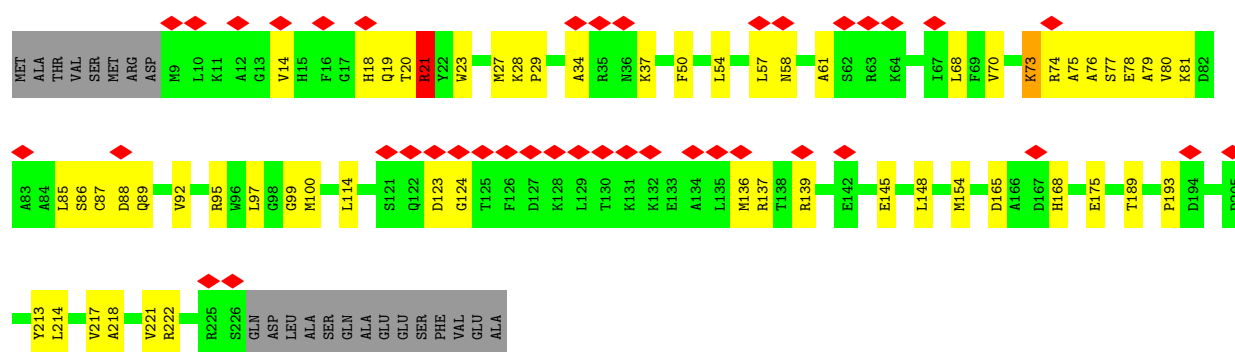
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

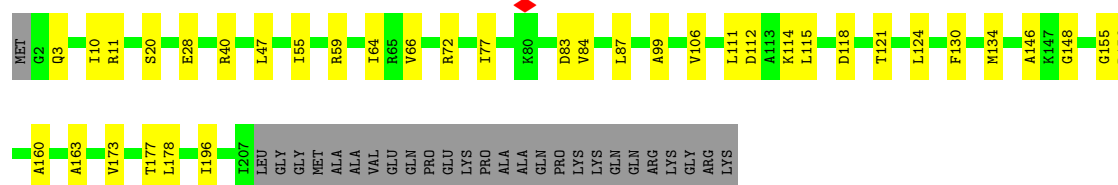




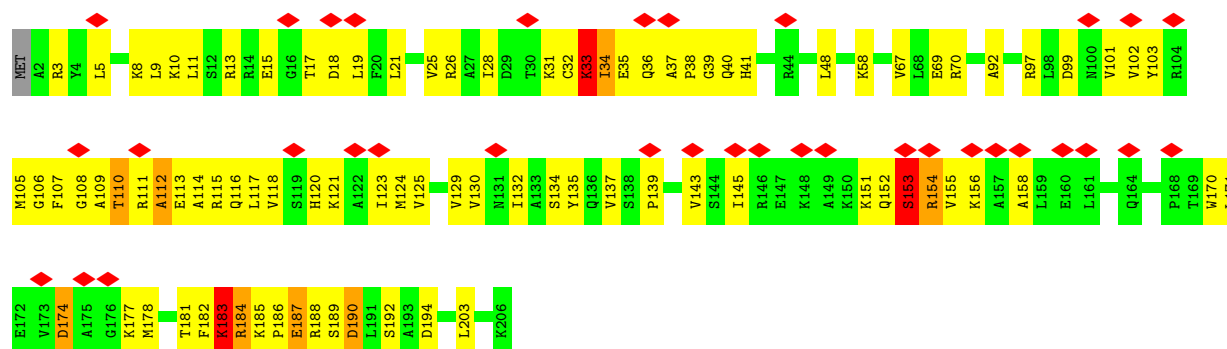
• Molecule 2: 30S ribosomal protein S2



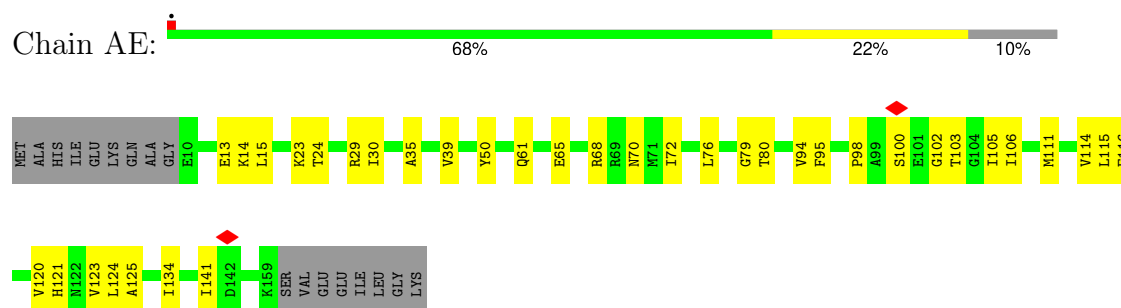
• Molecule 3: 30S ribosomal protein S3



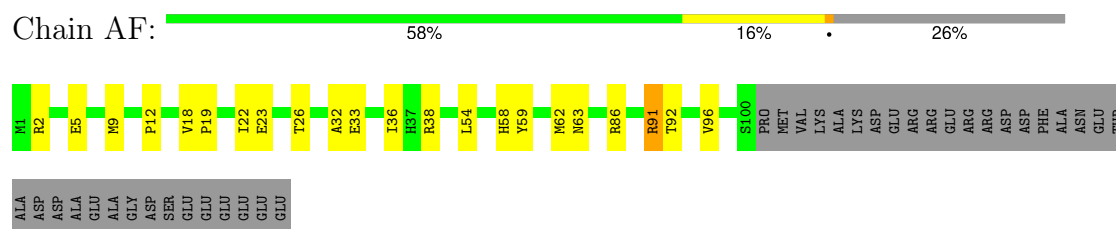
• Molecule 4: 30S ribosomal protein S4



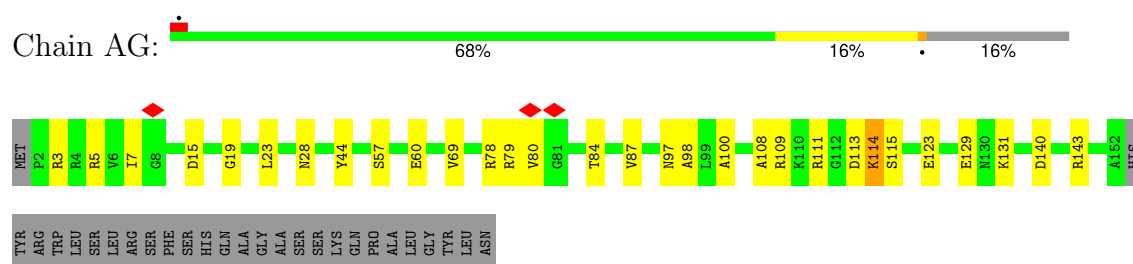
- Molecule 5: 30S ribosomal protein S5



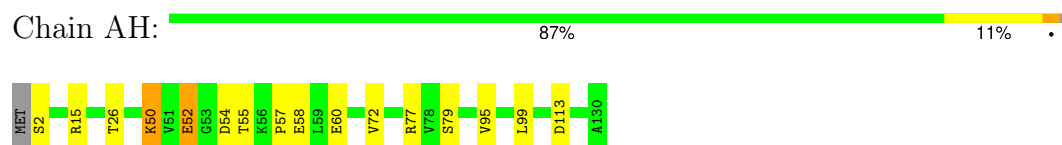
- Molecule 6: 30S ribosomal protein S6



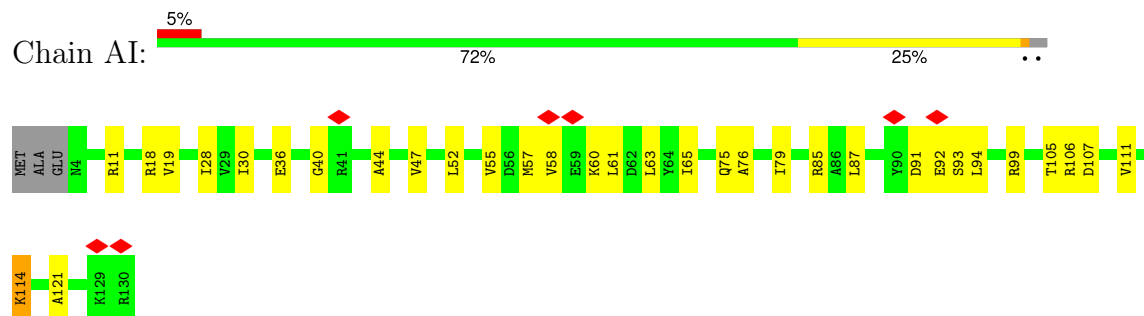
- Molecule 7: 30S ribosomal protein S7



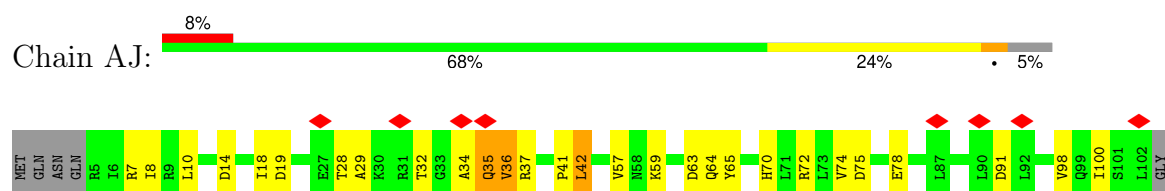
- Molecule 8: 30S ribosomal protein S8



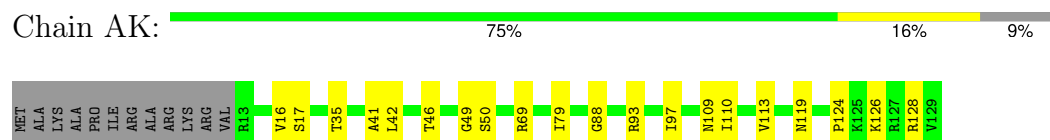
- Molecule 9: 30S ribosomal protein S9



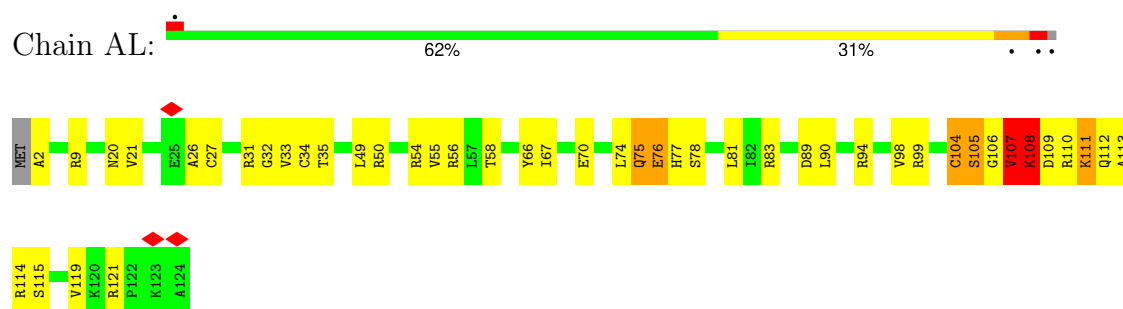
- Molecule 10: 30S ribosomal protein S10



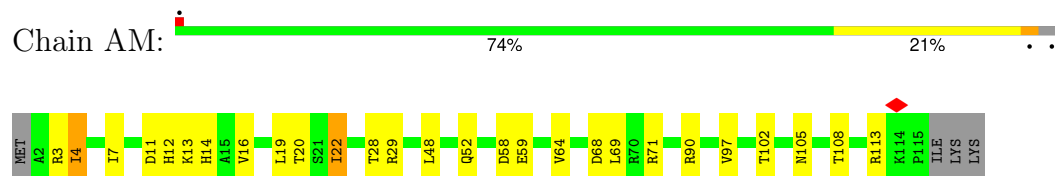
- Molecule 11: 30S ribosomal protein S11



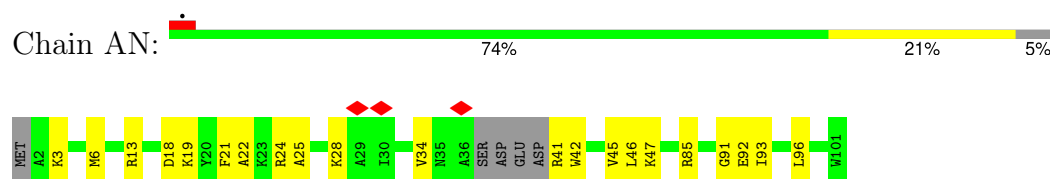
- Molecule 12: 30S ribosomal protein S12



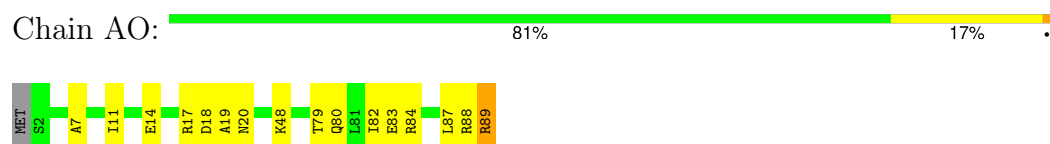
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

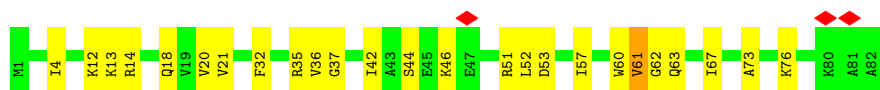


- Molecule 15: 30S ribosomal protein S15

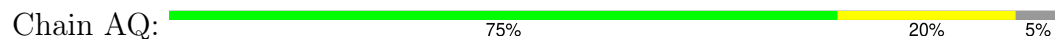


- Molecule 16: 30S ribosomal protein S16

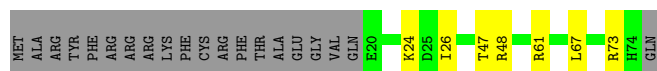




- Molecule 17: 30S ribosomal protein S17



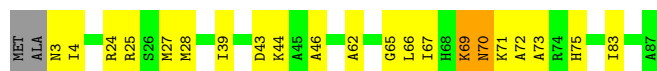
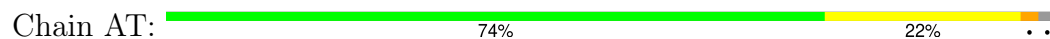
- Molecule 18: 30S ribosomal protein S18



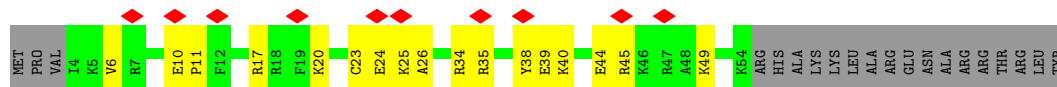
- Molecule 19: 30S ribosomal protein S19



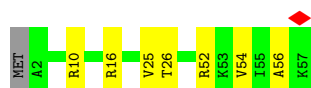
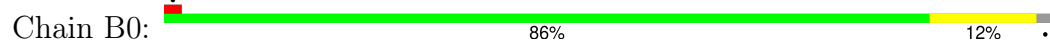
- Molecule 20: 30S ribosomal protein S20




- Molecule 21: 30S ribosomal protein S21

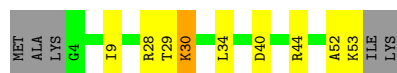


- Molecule 22: 50S ribosomal protein L32



- Molecule 23: 50S ribosomal protein L33

Chain B1:  75% 15% 9%



- Molecule 24: 50S ribosomal protein L34

Chain B2:  83% 17%



- Molecule 25: 50S ribosomal protein L35

Chain B3:  91% 8%



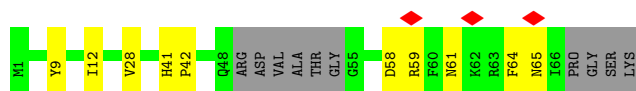
- Molecule 26: 50S ribosomal protein L36

Chain B4:  89% 11%




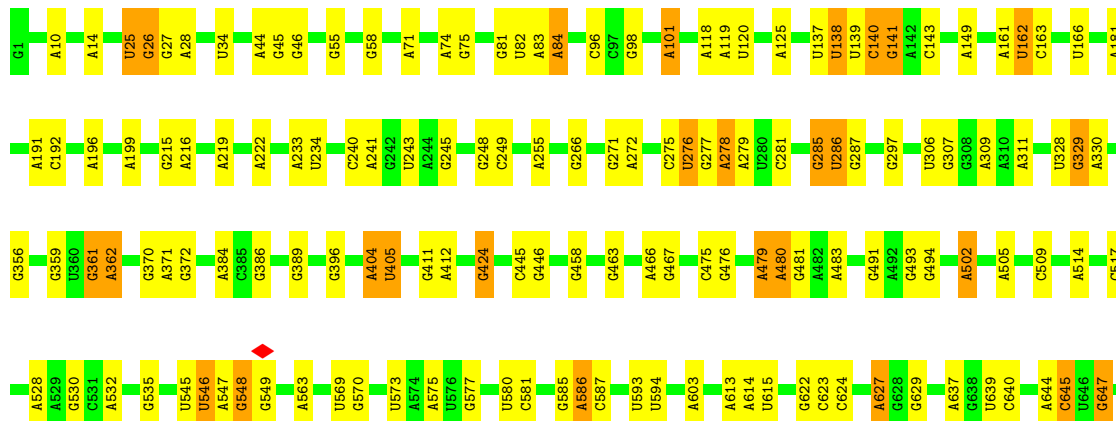
- Molecule 27: 50S ribosomal protein L31

Chain B5:  71% 14% 14%

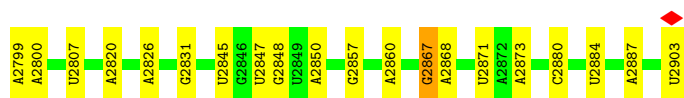


- Molecule 28: 23S ribosomal RNA

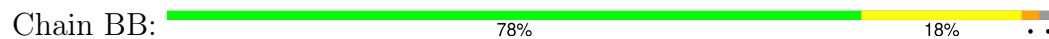
Chain BA:  76% 20%



G2567	G2581	G2582	G2599	A2602	U2609	U2613	A2614	U2615	G2623	U2629	G2630	C2636	A2639	C2646	G2663	G2683	U2684	U2687	U2688	U2690	G2714	G2715	G2716	U2720	A2726	G2732	A2733	A2748	A2765	U2778	U2779	G2780	C2788	G2789	C2794																		
U2402	A2406	A2407	G2413	U2423	C2424	A2425	G2428	G2429	A2430	A2435	U2441	A2448	A2459	A2469	C2475	A2476	G2481	U2491	C2496	G2502	A2503	U2504	G2505	U2506	C2507	A2516	C2517	U2518	U2519	C2520	G2529	G2532	A2547	U2548	U2554	G2557	C2558	A2566															
G2238	G2239	U2243	U2244	G2250	A2266	A2267	A2278	A2281	G2282	C2283	G2286	A2287	A2288	U2291	U2292	A2297	U2305	C2306	G2307	G2308	A2309	C2310	A2311	U2321	A2322	G2323	U2324	G2325	C2326	A2327	A2328	U2329	G2330	G2331	A2332	U2333	U2334	A2335	C2347	G2361	C2380	G2383	U2384	C2385									
C2143	G2144	C2145	C2146	A2147	G2148	U2149	C2150	G2157	A2158	G2159	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	G2170	A2171	U2172	A2173	C2174	C2177	C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2187	U2188	U2189	G2190	A2191	U2192	G2193	U2194	A2198	G2204	A2211	A2212	A2225	C2226	G2230						
G2056	A2060	G2061	A2062	C2063	C2064	C2065	G2069	A2070	A2071	C2072	U2092	U2098	U2099	G2100	A2101	C2102	C2103	U2104	U2105	U2106	U2109	G2110	U2111	G2112	U2113	A2114	G2115	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	U2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	U2138	U2139	G2140	G2141	A2142
C1920	A1927	A1928	G1929	G1930	U1937	C1942	U1943	U1944	G1954	U1955	U1956	C1965	A1966	C1967	U1970	U1971	C1972	C1990	U1991	G1992	U1993	C1997	G2002	G2012	A2013	A2014	A2015	U2022	C2023	G2027	U2028	G2029	A2030	A2031	G2032	A2033	C2036	A2037	G2038	U2039	C2043	A2052	C2055										
A1548	A1549	A1566	A1569	U1578	A1583	U1584	C1585	C1604	C1607	A1608	A1609	A1610	U1647	U1648	G1649	G1667	A1668	A1669	G1674	C1675	A1676	A1677	U1693	C1694	G1715	U1720	G1721	C1728	U1729	C1730	G1731	C1732	G1738	G1743	A1744	A1746	U1747	A1754	U1758	C1764													
A1773	C1774	U1775	G1776	U1779	A1784	A1785	U1786	C1787	A1788	U1789	C1790	A1791	A1794	C1795	U1796	C1797	C1800	A1801	A1802	A1803	U1808	C1816	G1826	A1829	A1847	A1848	A1853	A1854	A1858	G1869	C1870	A1871	A1872	C1881	U1882	G1903	U1906	A1913	C1914	A1918	A1919												
A1392	A1395	U1405	U1406	G1416	A1420	C1428	G1432	A1433	A1434	C1447	G1452	G1456	U1460	A1469	A1470	G1475	G1482	G1483	C1493	A1494	A1495	A1496	U1497	C1498	A1504	A1508	A1509	G1510	G1514	A1515	G1527	C1533	U1534	A1535	C1536	G1537	A1544																
G1216	G1236	A1237	G1238	U1240	A1241	U1249	G1250	A1253	A1254	U1255	G1266	G1271	A1272	U1273	U1282	G1283	G1300	A1301	C1315	C1319	C1320	A1328	U1329	C1330	C1345	C1351	U1352	G1360	G1361	A1365	G1368	G1369	C1370	G1371	U1379	A1383	A1384	C1385	C1386	A1387													
C994	C995	A996	A1009	U1012	C1013	G1025	G1026	A1027	A1028	A1029	U1033	C1045	A1046	G1047	G1056	A1057	U1058	U1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1070	A1071	C1072	U1073	G1074	C1075	C1076	A1077	U1078	U1079	U1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	A1089	C1092					
C948	A949	U950	G956	G957	G958	G959	U971	U972	C976	A977	A978	G983	U984	C985	A	U	C	C	A992	A996	C997	A900	A910	G914	C915	G916	G930	U931	A941	C946	A947	C948	C961	A972	A973	G974	A983	A984	C985	A990	G993												
G651	U652	U653	A654	A655	U657	A658	A677	U677	U686	U684	G695	U703	U704	A730	G738	A742	A743	U747	A764	G775	G776	A782	A783	G784	G785	A792	G805	G809	C812	A819	U826	U827	U828	A829	G830	C837	A844	A845	U846	U847													



- Molecule 29: 5S ribosomal RNA



- Molecule 30: 50S ribosomal protein L2



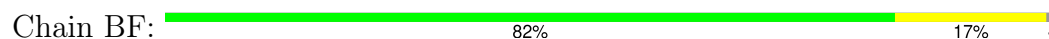
- Molecule 31: 50S ribosomal protein L3



- Molecule 32: 50S ribosomal protein L4



- Molecule 33: 50S ribosomal protein L5



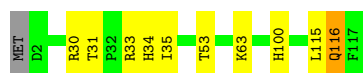
- Molecule 34: 50S ribosomal protein L6



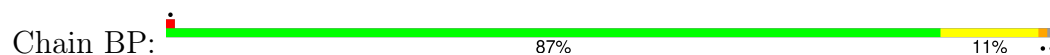
- Molecule 35: 50S ribosomal protein L9







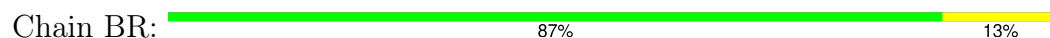
- Molecule 42: 50S ribosomal protein L19



- Molecule 43: 50S ribosomal protein L20



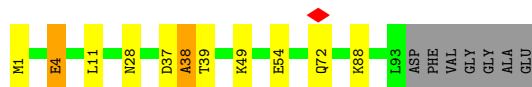
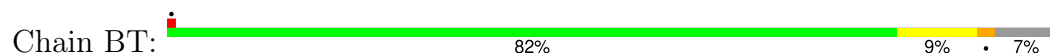
- Molecule 44: 50S ribosomal protein L21



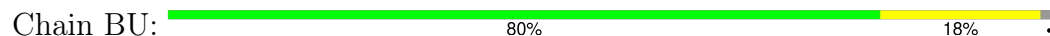
- Molecule 45: 50S ribosomal protein L22



- Molecule 46: 50S ribosomal protein L23



- Molecule 47: 50S ribosomal protein L24



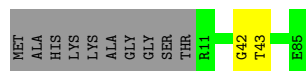
- Molecule 48: 50S ribosomal protein L25





- Molecule 49: 50S ribosomal protein L27

Chain BW: 86% 12%



- Molecule 50: 50S ribosomal protein L28

Chain BX: 86% 13%



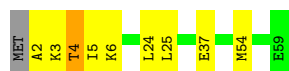
- Molecule 51: 50S ribosomal protein L29

Chain BY: 5% 86% 14%



- Molecule 52: 50S ribosomal protein L30

Chain BZ: 83% 14%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	470397	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52.16	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	28.698	Depositor
Minimum map value	-10.798	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	427.6, 427.6, 427.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 84G, MG, 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	AA	0.27	0/36966	0.31	1/57666 (0.0%)
2	AB	0.30	0/1735	0.48	2/2338 (0.1%)
3	AC	0.19	0/1651	0.31	0/2225
4	AD	0.39	0/1665	0.61	3/2227 (0.1%)
5	AE	0.25	0/1118	0.38	0/1504
6	AF	0.20	0/835	0.34	0/1128
7	AG	0.30	1/1195 (0.1%)	0.35	1/1602 (0.1%)
8	AH	0.31	0/989	0.36	0/1326
9	AI	0.40	0/1034	0.47	0/1375
10	AJ	0.19	0/796	0.34	0/1077
11	AK	0.32	0/893	0.42	0/1205
12	AL	0.57	0/969	0.72	3/1300 (0.2%)
13	AM	0.35	0/892	0.47	0/1193
14	AN	0.19	0/785	0.36	0/1043
15	AO	0.33	0/718	0.30	0/959
16	AP	0.41	0/659	0.47	1/884 (0.1%)
17	AQ	0.45	0/657	0.54	0/881
18	AR	0.22	0/462	0.31	0/621
19	AS	0.37	0/652	0.47	0/877
20	AT	0.58	0/671	0.42	0/888
21	AU	0.20	0/430	0.50	0/570
22	B0	0.50	0/450	0.42	0/599
23	B1	0.41	0/416	0.40	0/554
24	B2	0.32	0/380	0.32	0/498
25	B3	0.28	0/513	0.29	0/676
26	B4	0.26	0/303	0.26	0/397
27	B5	0.17	0/488	0.37	0/649
28	BA	0.32	0/69659	0.30	0/108672
29	BB	0.26	0/2828	0.25	0/4410
30	BC	0.52	0/2121	0.44	0/2852
31	BD	0.43	0/1586	0.48	3/2134 (0.1%)
32	BE	0.26	0/1571	0.29	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BF	0.20	0/1434	0.32	0/1926
34	BG	0.19	0/1343	0.31	0/1816
35	BH	0.20	0/364	0.41	0/490
36	BJ	0.36	0/1152	0.32	0/1551
37	BK	0.26	0/947	0.34	0/1268
38	BL	0.28	0/1054	0.39	0/1403
39	BM	0.26	0/1093	0.31	0/1460
40	BN	0.44	0/973	0.42	0/1301
41	BO	0.36	0/902	0.38	0/1209
42	BP	0.34	0/929	0.35	0/1242
43	BQ	0.30	0/960	0.28	0/1278
44	BR	0.27	0/829	0.37	0/1107
45	BS	0.27	0/864	0.30	0/1156
46	BT	0.32	0/744	0.31	0/994
47	BU	0.24	0/787	0.35	0/1051
48	BV	0.25	0/766	0.26	0/1025
49	BW	0.28	0/576	0.31	0/762
50	BX	0.28	0/635	0.28	0/848
51	BY	0.23	0/510	0.28	0/677
52	BZ	0.53	0/453	0.47	0/605
All	All	0.31	1/153402 (0.0%)	0.33	14/229612 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AG	109	ARG	C-N	-7.08	1.22	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	80	VAL	N-CA-C	-7.82	104.27	113.42
31	BD	151	THR	CA-C-N	-7.62	111.32	119.24
31	BD	151	THR	C-N-CA	-7.62	111.32	119.24
4	AD	112	ALA	CA-C-N	-7.45	110.30	120.28
4	AD	112	ALA	C-N-CA	-7.45	110.30	120.28

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	AA	33015	0	16617	415	0
2	AB	1704	0	1732	38	0
3	AC	1624	0	1696	27	0
4	AD	1643	0	1707	130	0
5	AE	1105	0	1148	32	0
6	AF	817	0	808	15	0
7	AG	1181	0	1238	20	0
8	AH	979	0	1031	10	0
9	AI	1022	0	1070	33	0
10	AJ	786	0	828	26	0
11	AK	877	0	887	17	0
12	AL	955	0	1016	47	0
13	AM	883	0	941	24	0
14	AN	774	0	824	18	0
15	AO	710	0	728	10	0
16	AP	649	0	666	21	0
17	AQ	648	0	691	12	0
18	AR	455	0	478	8	0
19	AS	637	0	665	31	0
20	AT	665	0	714	17	0
21	AU	425	0	449	16	0
22	B0	444	0	458	7	0
23	B1	409	0	440	5	0
24	B2	377	0	418	7	0
25	B3	504	0	572	5	0
26	B4	302	0	340	4	0
27	B5	480	0	478	8	0
28	BA	62195	0	31279	320	0
29	BB	2529	0	1281	12	0
30	BC	2082	0	2154	15	0
31	BD	1565	0	1616	15	0
32	BE	1552	0	1619	13	0
33	BF	1410	0	1444	24	0
34	BG	1323	0	1371	8	0
35	BH	359	0	381	11	0
36	BJ	1129	0	1162	10	0
37	BK	938	0	1012	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BL	1045	0	1117	22	0
39	BM	1074	0	1157	13	0
40	BN	960	0	1000	11	0
41	BO	892	0	923	8	0
42	BP	917	0	962	13	0
43	BQ	947	0	1019	10	0
44	BR	816	0	839	13	0
45	BS	857	0	922	5	0
46	BT	738	0	807	8	0
47	BU	779	0	831	15	0
48	BV	753	0	780	4	0
49	BW	569	0	581	3	0
50	BX	625	0	652	7	0
51	BY	509	0	543	6	0
52	BZ	449	0	488	6	0
53	AA	93	0	0	0	0
53	B0	1	0	0	0	0
53	BA	207	0	0	0	0
53	BB	5	0	0	0	0
53	BC	1	0	0	0	0
53	BN	1	0	0	0	0
53	BQ	1	0	0	0	0
54	AA	76	0	0	3	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
All	All	141469	0	94580	1393	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1393 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:110:THR:HG22	4:AD:113:GLU:H	1.20	0.99
9:AI:65:ILE:HD12	9:AI:79:ILE:HD12	1.46	0.94
1:AA:449:G:H1	1:AA:486:U:H1'	1.34	0.92
7:AG:111:ARG:HD2	7:AG:123:GLU:HG2	1.52	0.91
1:AA:502:A:P	12:AL:113:ALA:HA	2.10	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	
2	AB	216/240 (90%)	189 (88%)	24 (11%)	3 (1%)	9	24
3	AC	204/233 (88%)	183 (90%)	20 (10%)	1 (0%)	25	49
4	AD	203/206 (98%)	175 (86%)	23 (11%)	5 (2%)	4	12
5	AE	148/167 (89%)	125 (84%)	23 (16%)	0	100	100
6	AF	98/135 (73%)	83 (85%)	14 (14%)	1 (1%)	13	33
7	AG	149/179 (83%)	143 (96%)	6 (4%)	0	100	100
8	AH	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	AI	125/130 (96%)	103 (82%)	19 (15%)	3 (2%)	5	13
10	AJ	96/103 (93%)	86 (90%)	6 (6%)	4 (4%)	2	5
11	AK	115/129 (89%)	102 (89%)	13 (11%)	0	100	100
12	AL	121/124 (98%)	103 (85%)	16 (13%)	2 (2%)	7	20
13	AM	112/118 (95%)	99 (88%)	12 (11%)	1 (1%)	14	35
14	AN	92/101 (91%)	79 (86%)	12 (13%)	1 (1%)	12	30
15	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	11	28
16	AP	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	10	26
17	AQ	78/84 (93%)	66 (85%)	12 (15%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
20	AT	83/87 (95%)	77 (93%)	6 (7%)	0	100	100
21	AU	49/71 (69%)	35 (71%)	13 (26%)	1 (2%)	6	16
22	B0	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
23	B1	48/55 (87%)	44 (92%)	4 (8%)	0	100	100
24	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
25	B3	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
26	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	B5	56/70 (80%)	49 (88%)	7 (12%)	0	100	100
30	BC	269/273 (98%)	256 (95%)	11 (4%)	2 (1%)	19	42
31	BD	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
32	BE	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	25	49
33	BF	175/179 (98%)	161 (92%)	14 (8%)	0	100	100
34	BG	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
35	BH	45/149 (30%)	35 (78%)	8 (18%)	2 (4%)	2	4
36	BJ	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
37	BK	120/123 (98%)	108 (90%)	11 (9%)	1 (1%)	16	38
38	BL	141/144 (98%)	123 (87%)	15 (11%)	3 (2%)	5	15
39	BM	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
40	BN	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
41	BO	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
42	BP	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
43	BQ	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
44	BR	101/103 (98%)	86 (85%)	15 (15%)	0	100	100
45	BS	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	14	35
46	BT	91/100 (91%)	86 (94%)	4 (4%)	1 (1%)	12	30
47	BU	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
48	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
49	BW	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
50	BX	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
51	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
52	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
All	All	5432/5912 (92%)	4947 (91%)	450 (8%)	35 (1%)	24	45

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	34	ALA
2	AB	76	ALA
4	AD	153	SER
9	AI	55	VAL
10	AJ	35	GLN

### 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	
2	AB	180/198 (91%)	174 (97%)	6 (3%)	33	62
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	162 (94%)	10 (6%)	17	39
5	AE	113/126 (90%)	113 (100%)	0	100	100
6	AF	87/116 (75%)	87 (100%)	0	100	100
7	AG	124/147 (84%)	121 (98%)	3 (2%)	44	73
8	AH	104/105 (99%)	102 (98%)	2 (2%)	52	79
9	AI	105/107 (98%)	103 (98%)	2 (2%)	52	79
10	AJ	86/90 (96%)	86 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	103/104 (99%)	95 (92%)	8 (8%)	10	26
13	AM	92/96 (96%)	91 (99%)	1 (1%)	70	87
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	75/77 (97%)	73 (97%)	2 (3%)	40	69
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	71 (96%)	3 (4%)	26	54
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	70/79 (89%)	68 (97%)	2 (3%)	37	67
20	AT	65/66 (98%)	63 (97%)	2 (3%)	35	64
21	AU	44/61 (72%)	44 (100%)	0	100	100
22	B0	47/48 (98%)	47 (100%)	0	100	100
23	B1	45/49 (92%)	43 (96%)	2 (4%)	24	51
24	B2	38/38 (100%)	38 (100%)	0	100	100
25	B3	51/52 (98%)	51 (100%)	0	100	100
26	B4	34/34 (100%)	34 (100%)	0	100	100
27	B5	55/62 (89%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BC	216/218 (99%)	215 (100%)	1 (0%)	86	95
31	BD	164/164 (100%)	161 (98%)	3 (2%)	54	80
32	BE	165/165 (100%)	165 (100%)	0	100	100
33	BF	148/150 (99%)	148 (100%)	0	100	100
34	BG	137/138 (99%)	137 (100%)	0	100	100
35	BH	38/114 (33%)	38 (100%)	0	100	100
36	BJ	116/116 (100%)	115 (99%)	1 (1%)	75	90
37	BK	103/104 (99%)	103 (100%)	0	100	100
38	BL	102/103 (99%)	102 (100%)	0	100	100
39	BM	109/109 (100%)	109 (100%)	0	100	100
40	BN	100/103 (97%)	99 (99%)	1 (1%)	73	89
41	BO	86/87 (99%)	84 (98%)	2 (2%)	45	74
42	BP	99/100 (99%)	97 (98%)	2 (2%)	50	78
43	BQ	89/90 (99%)	89 (100%)	0	100	100
44	BR	84/84 (100%)	84 (100%)	0	100	100
45	BS	93/93 (100%)	93 (100%)	0	100	100
46	BT	80/84 (95%)	78 (98%)	2 (2%)	42	72
47	BU	83/85 (98%)	83 (100%)	0	100	100
48	BV	78/78 (100%)	78 (100%)	0	100	100
49	BW	56/63 (89%)	56 (100%)	0	100	100
50	BX	67/68 (98%)	67 (100%)	0	100	100
51	BY	55/55 (100%)	55 (100%)	0	100	100
52	BZ	48/49 (98%)	46 (96%)	2 (4%)	25	53
All	All	4532/4829 (94%)	4475 (99%)	57 (1%)	64	85

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	AL	107	VAL
52	BZ	4	THR
17	AQ	6	ARG
46	BT	4	GLU
41	BO	31	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
43	BQ	44	GLN
43	BQ	72	ASN
50	BX	36	HIS
17	AQ	9	GLN
16	AP	63	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1539 (99%)	244 (15%)	14 (0%)
28	BA	2895/2903 (99%)	408 (14%)	19 (0%)
29	BB	117/120 (97%)	12 (10%)	1 (0%)
All	All	4550/4562 (99%)	664 (14%)	34 (0%)

5 of 664 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	22	G
1	AA	39	G
1	AA	47	C

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	BA	1913	A
28	BA	2109	U
28	BA	2308	G
1	AA	1317	C
1	AA	1201	A

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

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 313 ligands modelled in this entry, 311 are monoatomic - leaving 2 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	$\# Z  > 2$
54	84G	AA	1694	-	39,40,40	1.83	8 (20%)	48,57,57	1.18	5 (10%)
54	84G	AA	1695	-	39,40,40	0.55	1 (2%)	48,57,57	1.05	3 (6%)

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
54	84G	AA	1694	-	-	3/23/76/76	0/3/3/3
54	84G	AA	1695	-	-	3/23/76/76	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	AA	1694	84G	C3-N1	6.55	1.48	1.34
54	AA	1694	84G	C21-C20	-3.85	1.48	1.53
54	AA	1694	84G	O6-C16	3.60	1.51	1.41
54	AA	1694	84G	C11-C12	-3.10	1.45	1.52
54	AA	1694	84G	O1-C3	-3.03	1.17	1.23

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	1694	84G	C-C1-C2	-3.00	108.42	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	1694	84G	C5-C4-N1	-2.74	106.58	110.78
54	AA	1695	84G	C-C1-C2	-2.52	109.07	112.52
54	AA	1695	84G	C4-N1-C3	-2.46	118.97	123.25
54	AA	1694	84G	C4-N1-C3	-2.16	119.50	123.25

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	AA	1694	84G	N3-C10-C9-O3
54	AA	1695	84G	C14-C7-O2-C8
54	AA	1694	84G	O6-C17-C18-O7
54	AA	1694	84G	C19-C17-C18-O7
54	AA	1695	84G	N-C-C1-C2

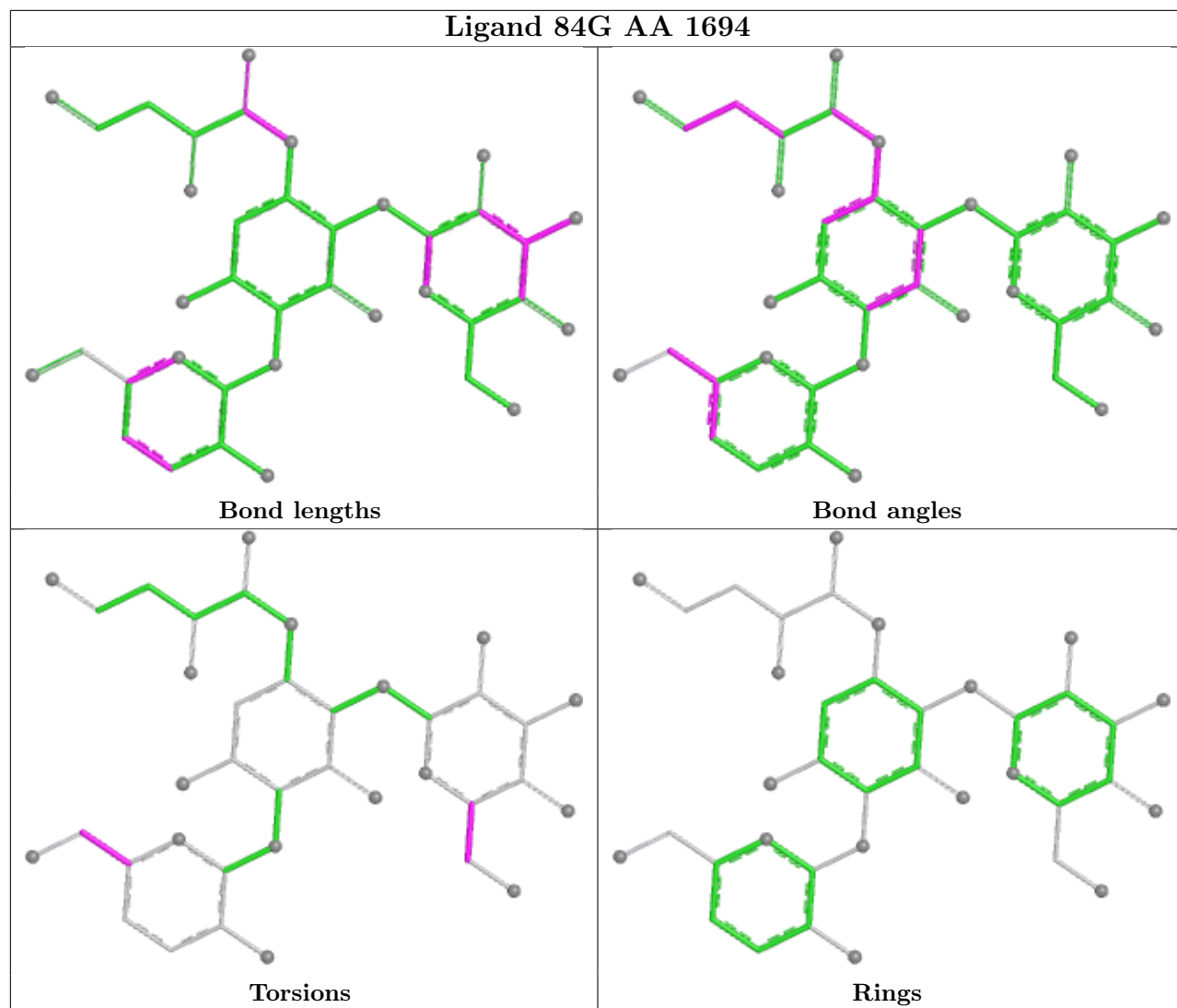
There are no ring outliers.

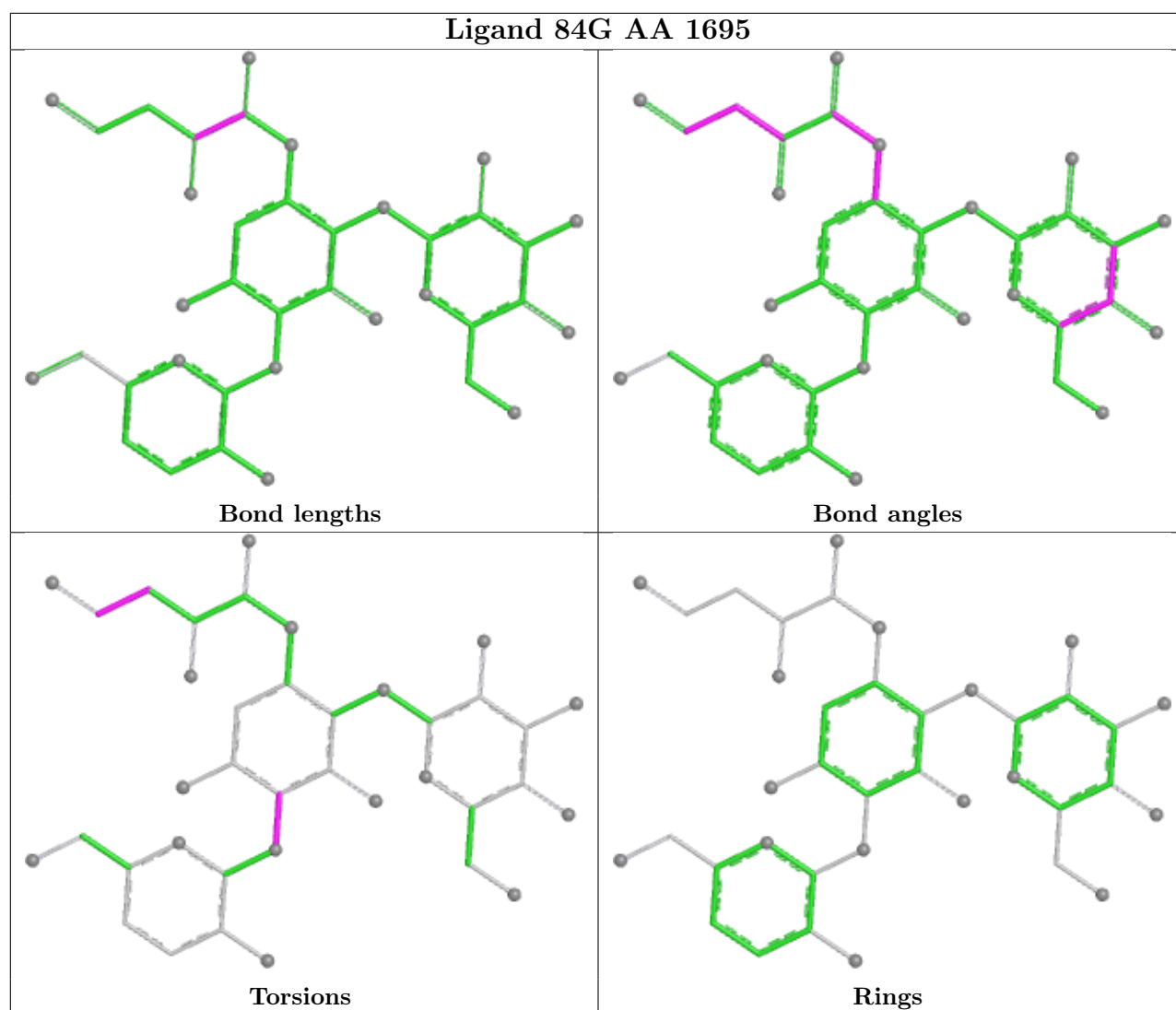
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	AA	1694	84G	3	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.

## Ligand 84G AA 1694





## 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.

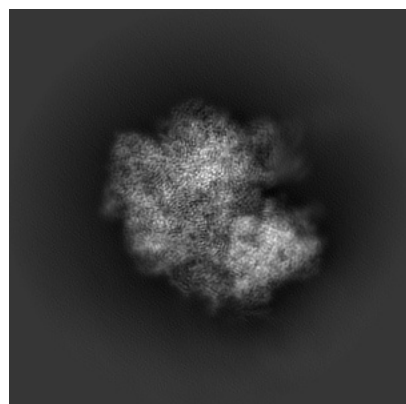
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44193. These allow visual inspection of the internal detail of the map and identification of artifacts.

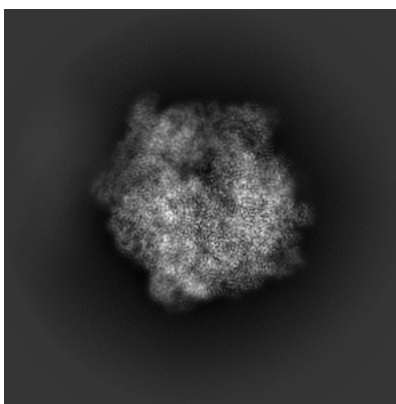
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

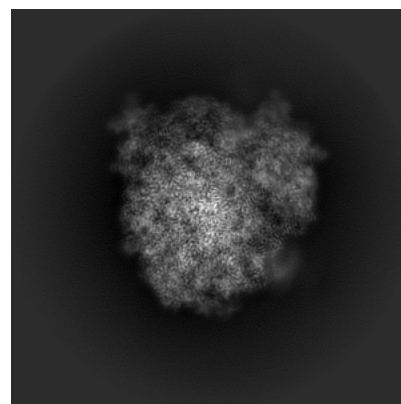
#### 6.1.1 Primary map



X

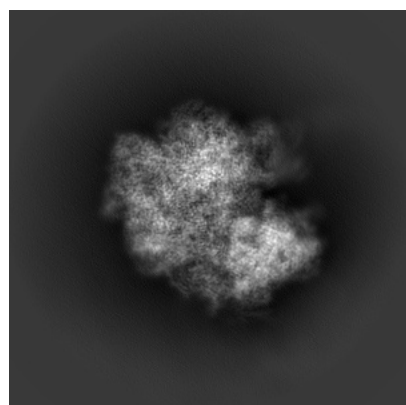


Y

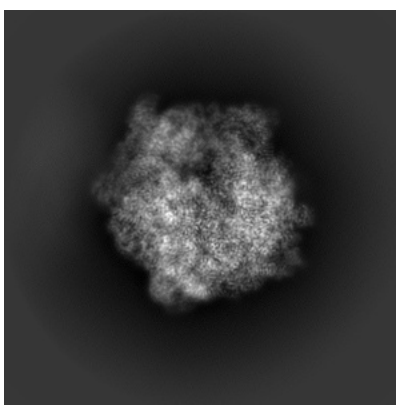


Z

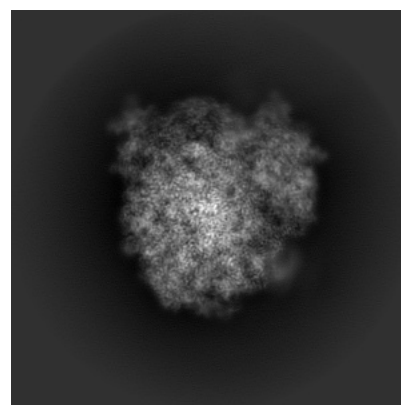
#### 6.1.2 Raw map



X



Y

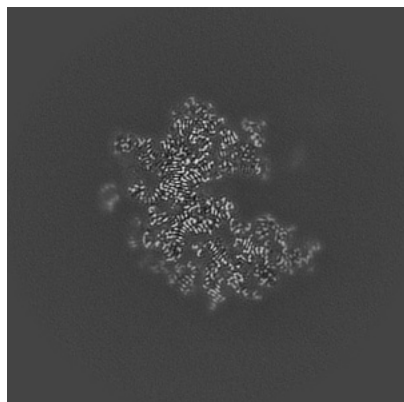


Z

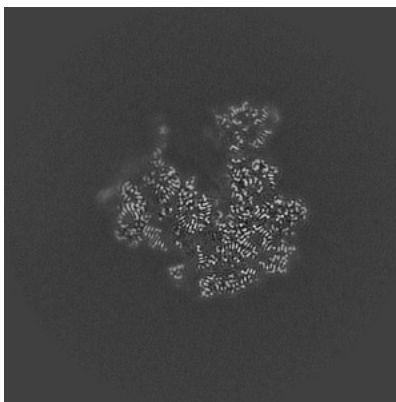
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

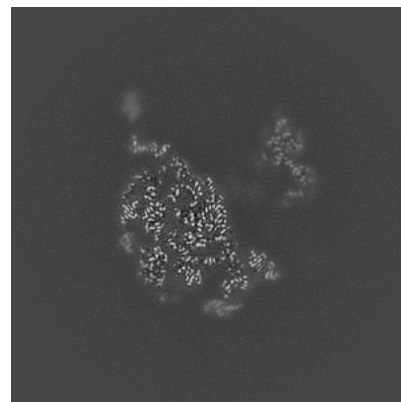
### 6.2.1 Primary map



X Index: 200

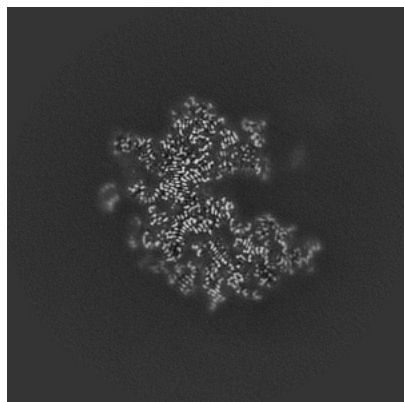


Y Index: 200

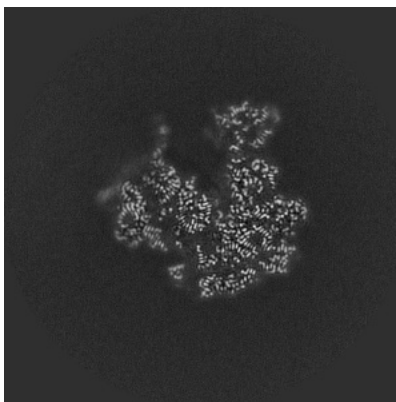


Z Index: 200

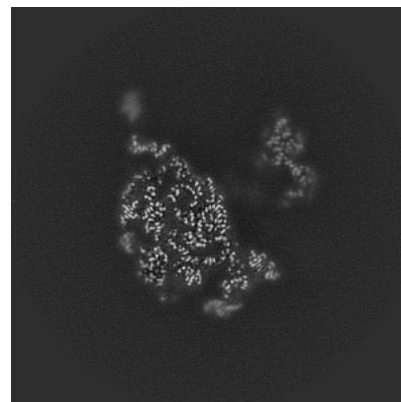
### 6.2.2 Raw map



X Index: 200



Y Index: 200

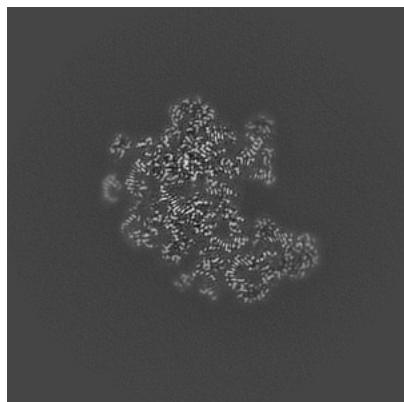


Z Index: 200

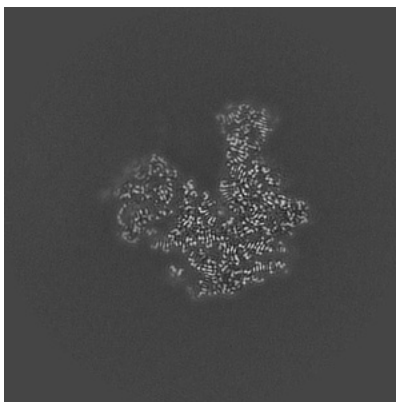
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

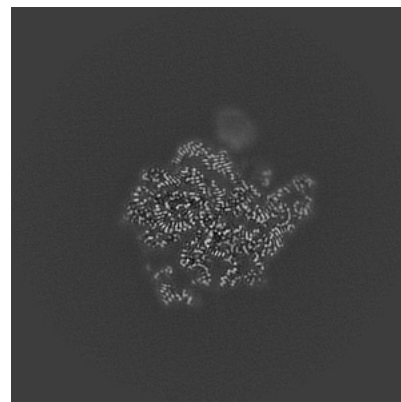
### 6.3.1 Primary map



X Index: 190

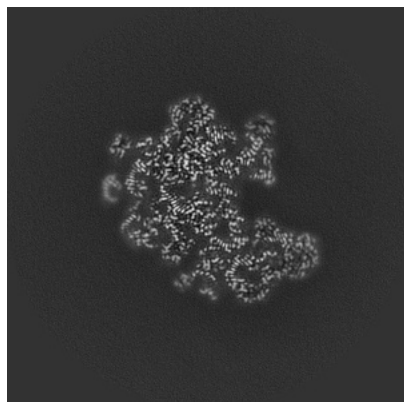


Y Index: 196

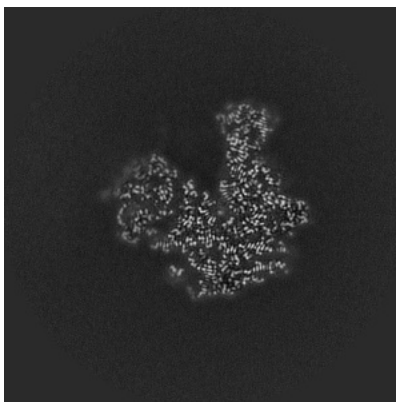


Z Index: 234

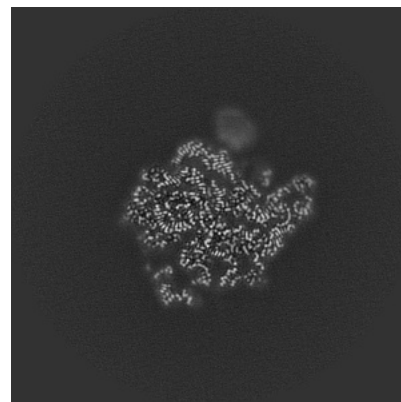
### 6.3.2 Raw map



X Index: 190



Y Index: 196

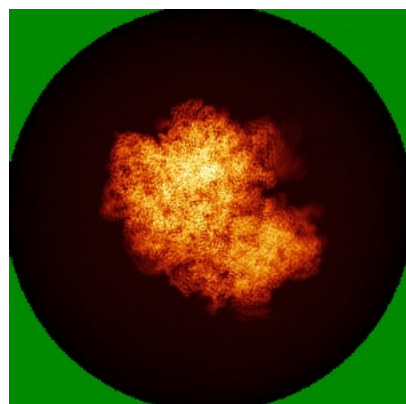


Z Index: 234

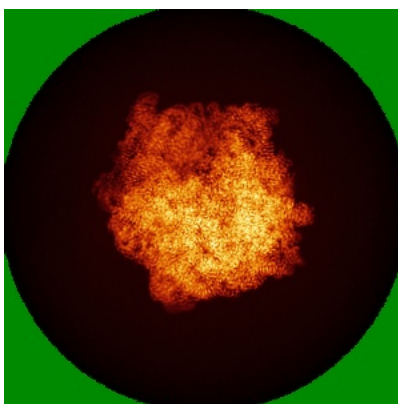
The images above show the largest variance slices of the map in three orthogonal directions.

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

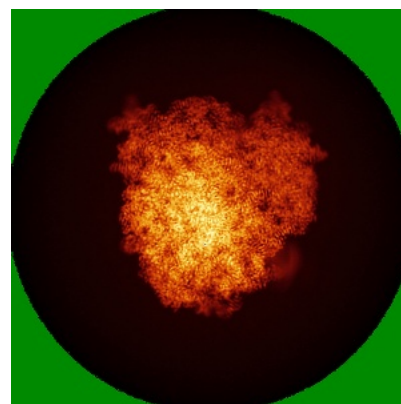
### 6.4.1 Primary map



X



Y

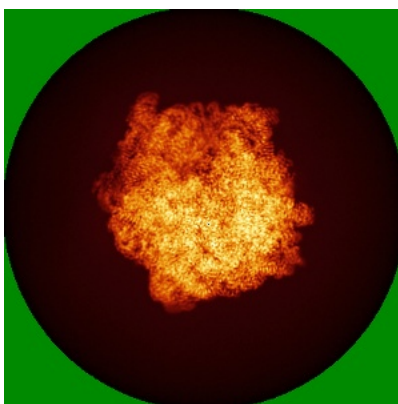


Z

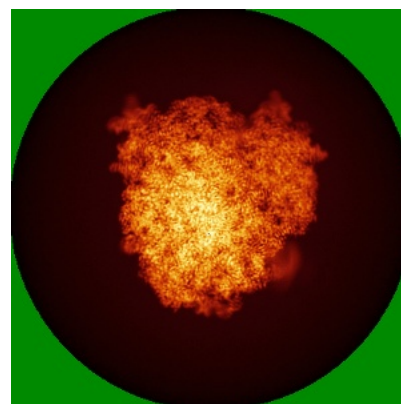
### 6.4.2 Raw map



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.

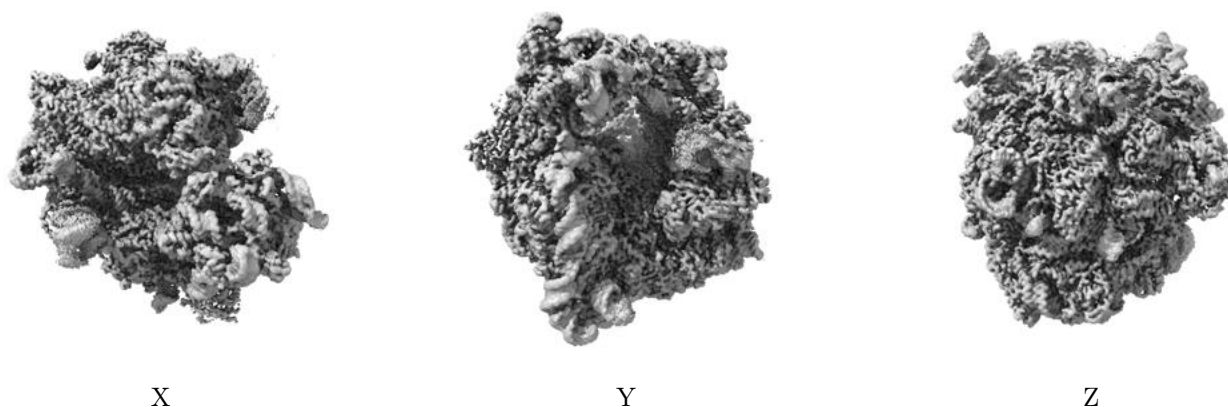
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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.

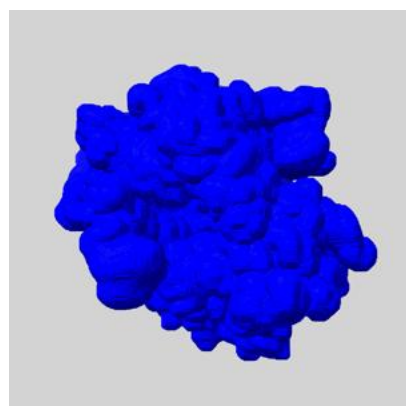
## 6.6 Mask visualisation [i](#)

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

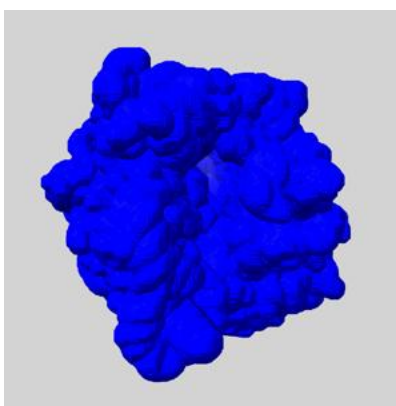
A mask typically either:

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

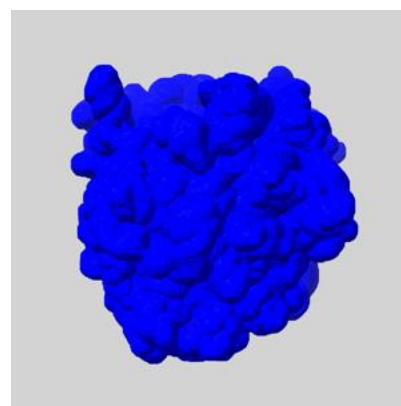
### 6.6.1 emd\_44193\_msk\_1.map [i](#)



X



Y

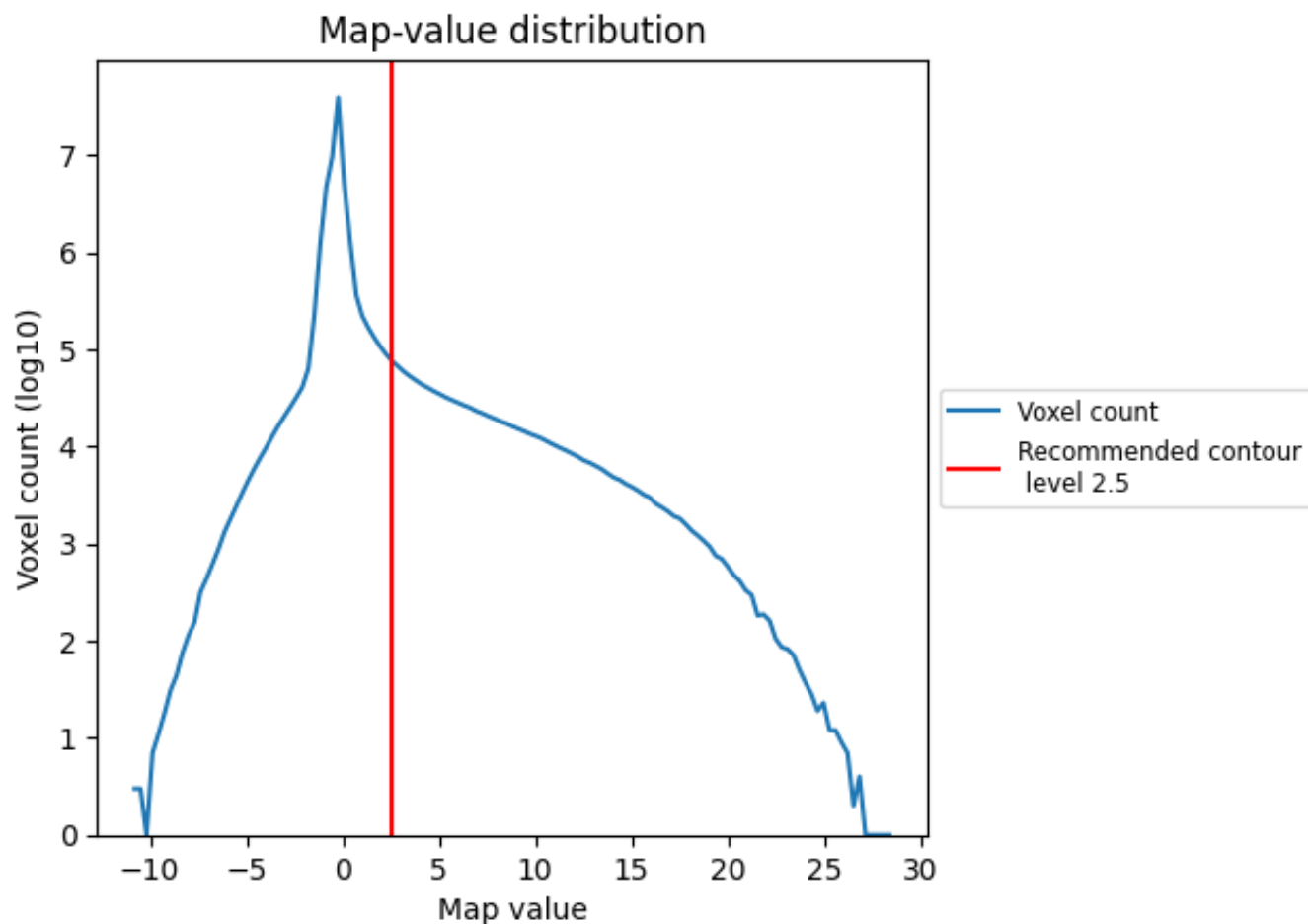


Z

## 7 Map analysis [i](#)

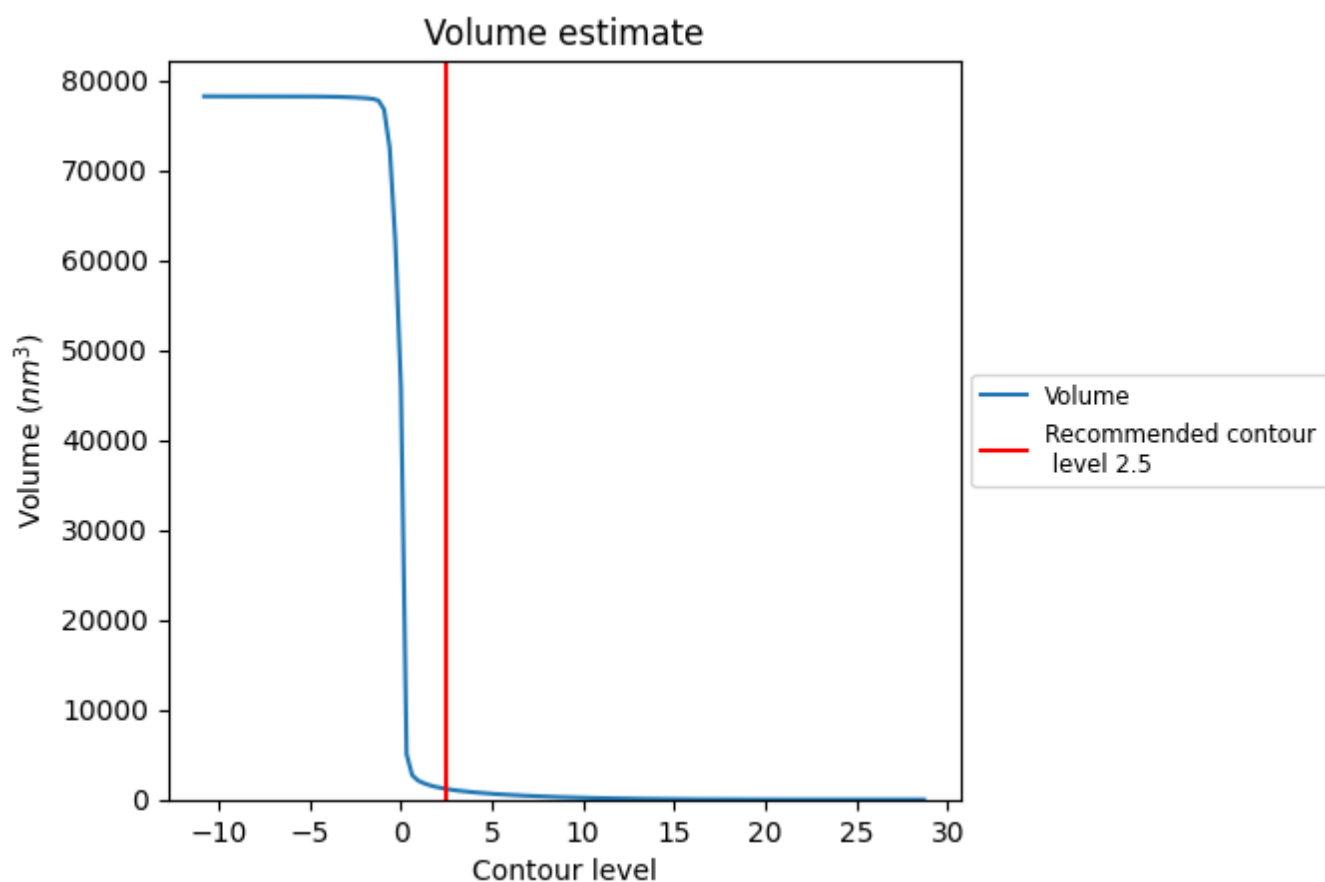
This section contains the results of statistical analysis of the map.

### 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.

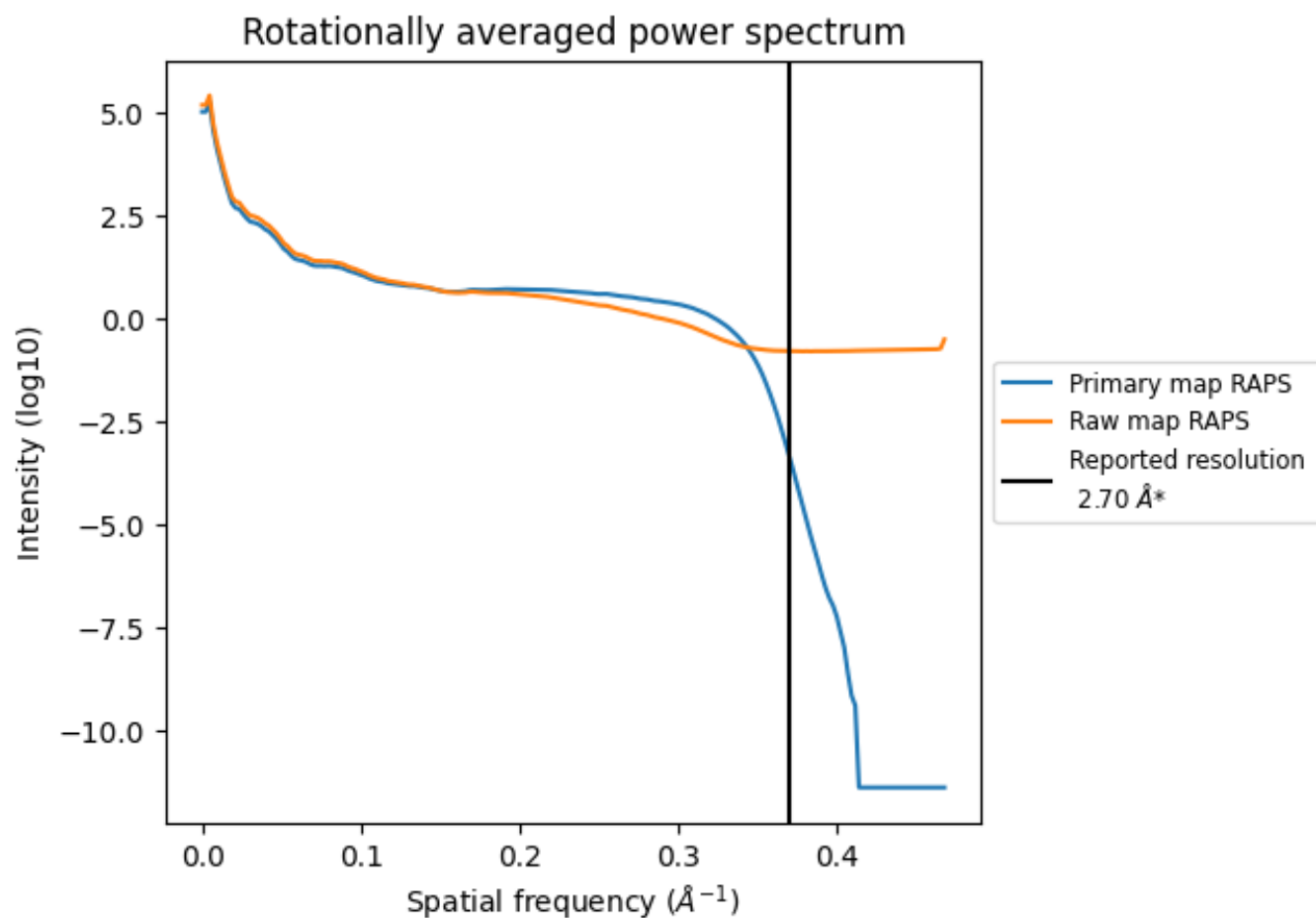
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1174  $\text{nm}^3$ ; this corresponds to an approximate mass of 1060 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 ⓘ

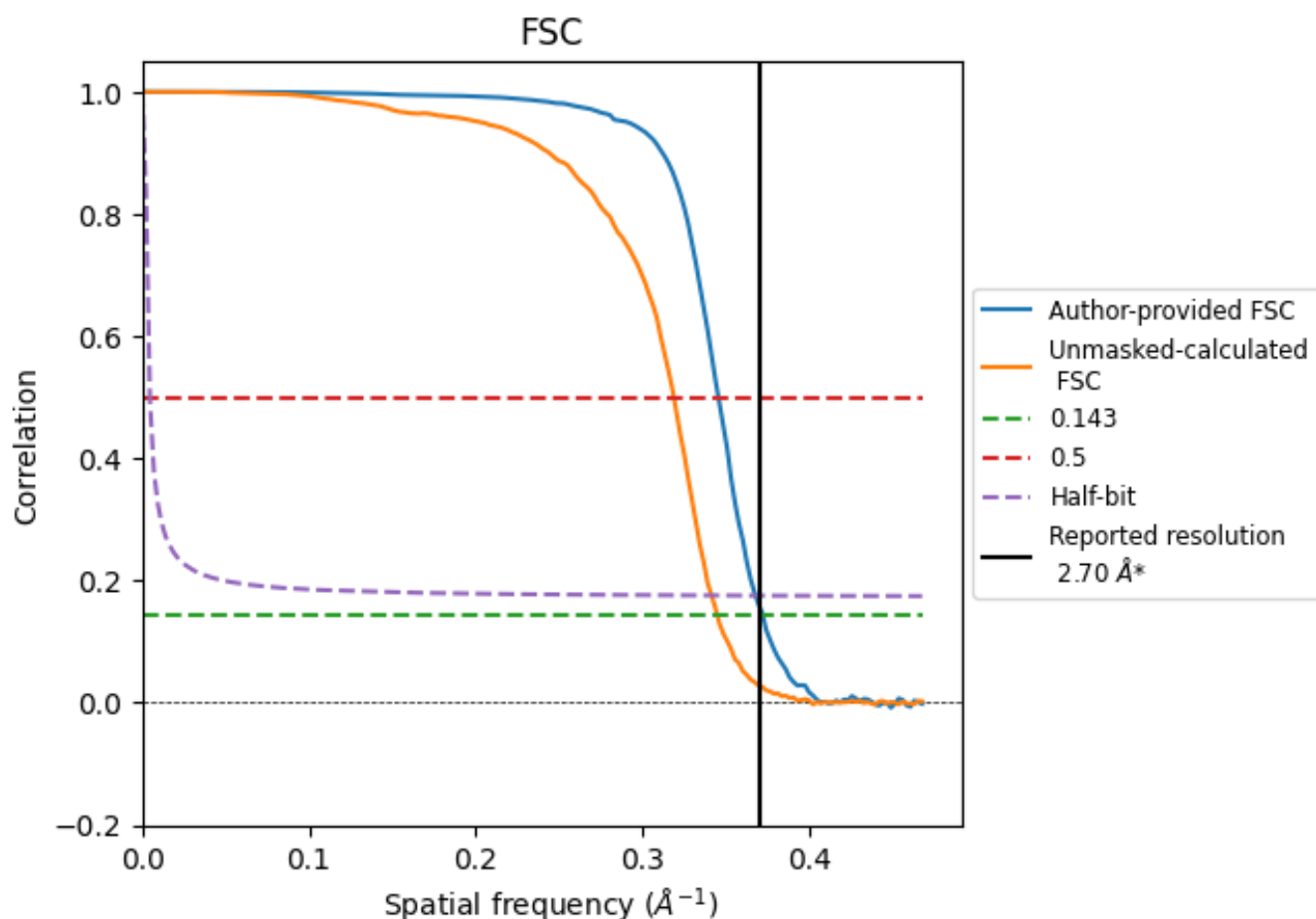


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

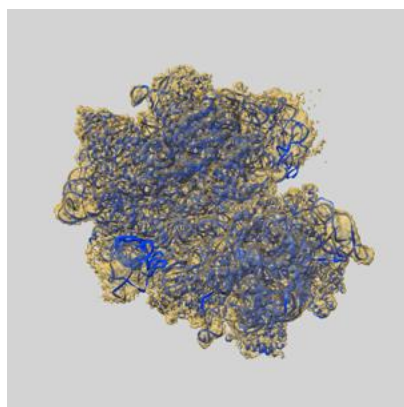
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	2.89	2.72
Unmasked-calculated*	2.90	3.14	2.93

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

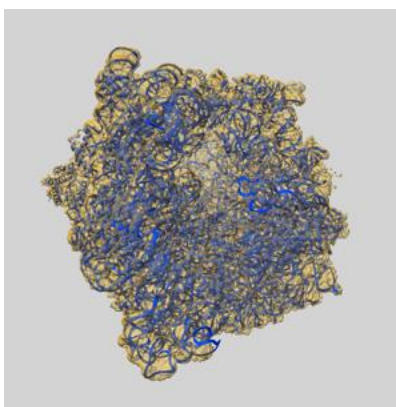
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44193 and PDB model 9B50. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

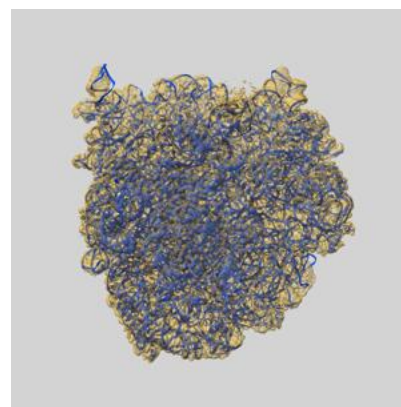
### 9.1 Map-model overlay [i](#)



X



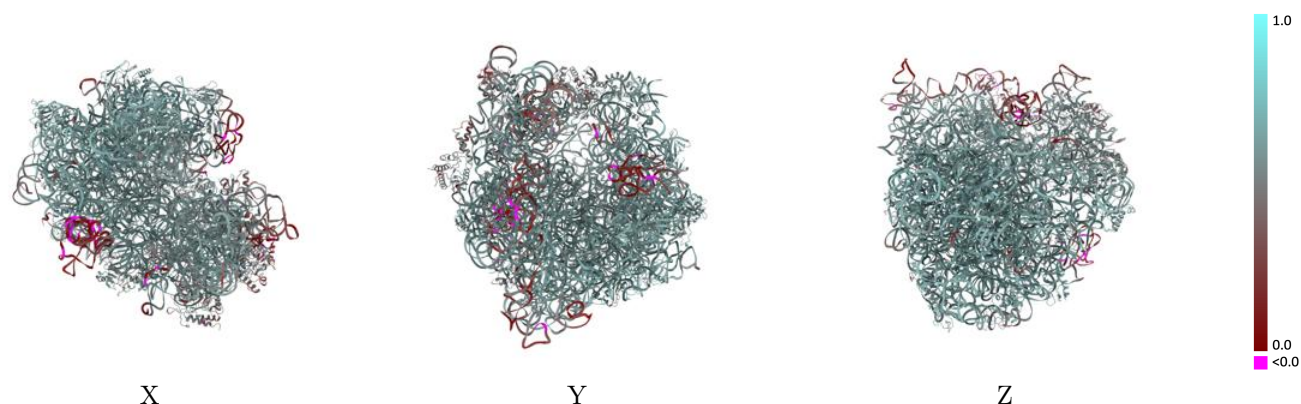
Y



Z

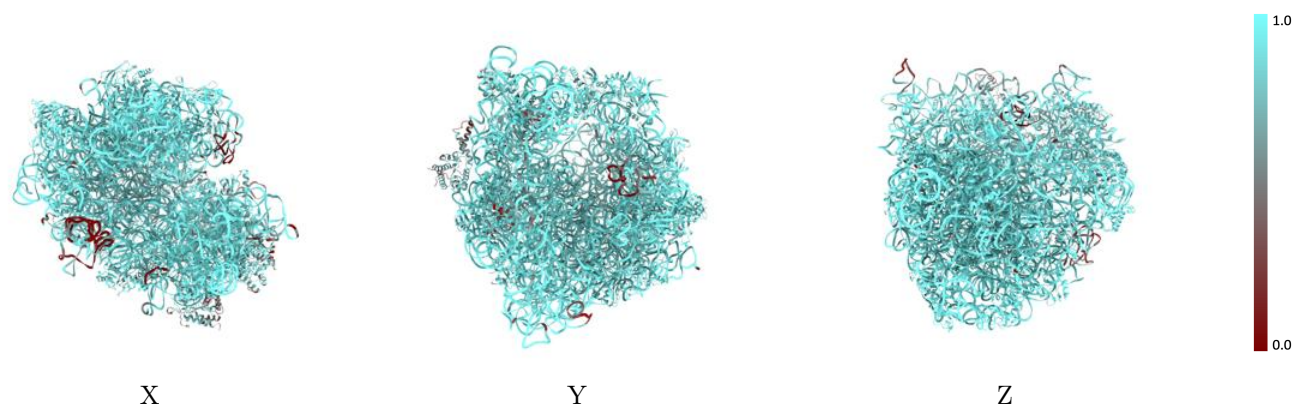
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



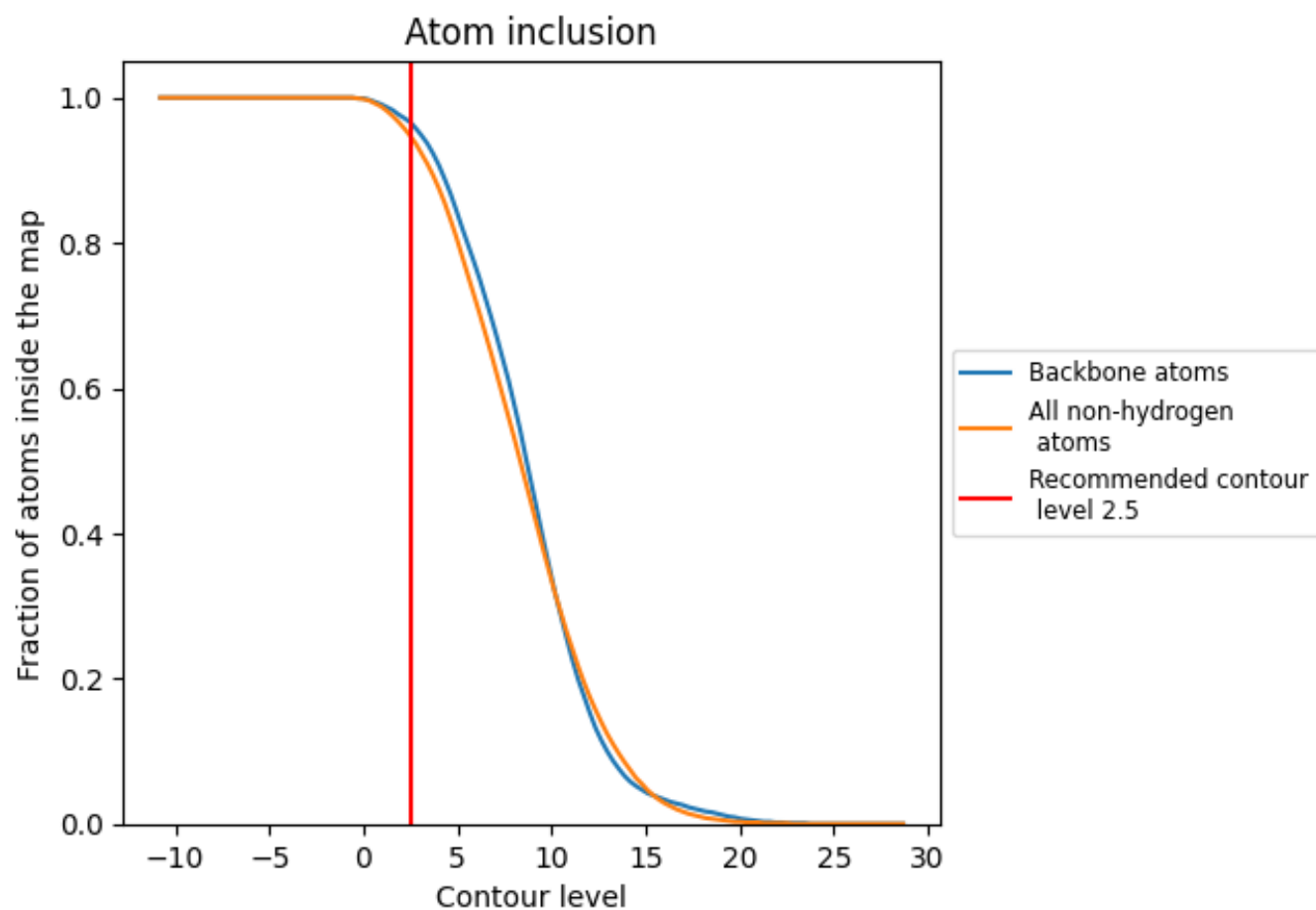
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.5750
AA	 0.9610	 0.5530
AB	 0.6350	 0.4760
AC	 0.8930	 0.5430
AD	 0.7380	 0.3620
AE	 0.9320	 0.5740
AF	 0.9020	 0.5330
AG	 0.8670	 0.5060
AH	 0.9530	 0.6000
AI	 0.8530	 0.4860
AJ	 0.8090	 0.4680
AK	 0.9340	 0.5640
AL	 0.9070	 0.5590
AM	 0.8850	 0.5040
AN	 0.9030	 0.5170
AO	 0.9530	 0.5930
AP	 0.9140	 0.5500
AQ	 0.9180	 0.5550
AR	 0.9540	 0.5690
AS	 0.8790	 0.4950
AT	 0.9340	 0.5710
AU	 0.6450	 0.3900
B0	 0.9530	 0.6180
B1	 0.9400	 0.5950
B2	 0.9720	 0.6390
B3	 0.9860	 0.6410
B4	 0.9690	 0.6200
B5	 0.8180	 0.4930
BA	 0.9630	 0.5930
BB	 0.9950	 0.6040
BC	 0.9790	 0.6320
BD	 0.9690	 0.6280
BE	 0.9550	 0.6050
BF	 0.8970	 0.5420
BG	 0.9110	 0.5600



*Continued on next page...*

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Chain	Atom inclusion	Q-score
BH	 0.7750	 0.4790
BJ	 0.9700	 0.6220
BK	 0.9660	 0.6140
BL	 0.9670	 0.6110
BM	 0.9650	 0.6120
BN	 0.9780	 0.6180
BO	 0.9560	 0.5940
BP	 0.9480	 0.6130
BQ	 0.9890	 0.6370
BR	 0.9320	 0.5960
BS	 0.9560	 0.6160
BT	 0.9330	 0.5900
BU	 0.9470	 0.5790
BV	 0.9290	 0.6020
BW	 0.9680	 0.6260
BX	 0.9670	 0.6240
BY	 0.9090	 0.5640
BZ	 0.9520	 0.6150