



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 11:52 pm GMT

PDB ID : 6I0Y
EMDB ID : EMD-0322
Title : TnaC-stalled ribosome complex with the titin I27 domain folding close to the ribosomal exit tunnel
Authors : Su, T.; Kudva, R.; von Heijne, G.; Beckmann, R.
Deposited on : 2018-10-26
Resolution : 3.20 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:

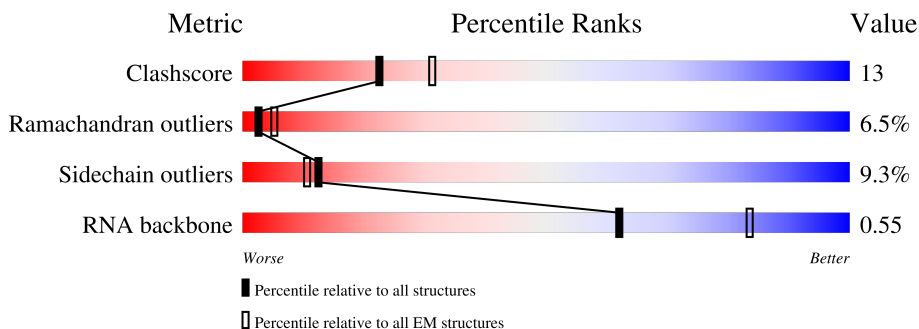
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	h	104	94% (Green)
2	0	57	75% (Green), 19% (Yellow), 5% (Red), 1% (Grey)
3	1	55	56% (Green), 27% (Yellow), 7% (Orange), 9% (Grey), 5% (Red)
4	2	46	76% (Green), 22% (Yellow), 2% (Red), 1% (Grey)
5	3	65	75% (Green), 18% (Yellow), 5% (Orange), 2% (Red), 1% (Grey)
6	4	38	55% (Green), 39% (Yellow), 5% (Orange), 1% (Red), 1% (Grey)
7	5	165	25% (Green), 38% (Yellow), 18% (Orange), 8% (Red), 10% (Grey)



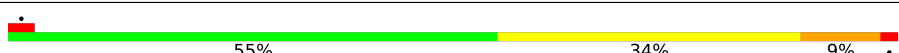

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Mol	Chain	Length	Quality of chain
8	6	121	
9	7	24	
10	8	94	
11	A	2903	
12	B	118	
13	C	273	
14	D	209	
15	E	201	
16	F	177	
17	G	176	
18	H	50	
19	I	141	
20	J	142	
21	K	122	
22	L	143	
23	M	136	
24	N	120	
25	O	116	
26	P	114	
27	Q	117	
28	R	103	
29	S	110	
30	T	93	
31	V	77	
32	W	79	

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Mol	Chain	Length	Quality of chain
33	X	77	 <p>70% 23% 5%</p>
34	Y	63	 <p>8% 60% 38%</p>
35	Z	58	 <p>55% 34% 9%</p>
36	z	89	 <p>64% 63% 34%</p>

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 93619 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L24.

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

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	0	56	444	269	94	80	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	1	50	409	263	75	71	0	0

- Molecule 4 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	46	377	228	90	57	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	3	64	504	323	105	74	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	4	38	302	185	65	48	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 8 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 9 is a protein called Tryptophanase operon leader peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	7	16	Total	C	N	O	0	0
			139	89	26	24		

- Molecule 10 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	8	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 11 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

- Molecule 12 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 13 is a protein called 50S ribosomal protein L2.

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

- Molecule 14 is a protein called 50S ribosomal protein L3.

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

- Molecule 15 is a protein called 50S ribosomal protein L4.

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

- Molecule 16 is a protein called 50S ribosomal protein L5.

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

- Molecule 17 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 18 is a protein called 50S ribosomal protein L9.

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

- Molecule 19 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 20 is a protein called 50S ribosomal protein L13.

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

- Molecule 21 is a protein called 50S ribosomal protein L14.

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

- Molecule 22 is a protein called 50S ribosomal protein L15.

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

- Molecule 23 is a protein called 50S ribosomal protein L16.

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

- Molecule 24 is a protein called 50S ribosomal protein L17.

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

- Molecule 25 is a protein called 50S ribosomal protein L18.

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

- Molecule 26 is a protein called 50S ribosomal protein L19.

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

- Molecule 27 is a protein called 50S ribosomal protein L20.

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

- Molecule 28 is a protein called 50S ribosomal protein L21.

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

- Molecule 29 is a protein called 50S ribosomal protein L22.

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

- Molecule 30 is a protein called 50S ribosomal protein L23.

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

- Molecule 31 is a RNA chain called Proline tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 32 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

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

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

- Molecule 34 is a protein called 50S ribosomal protein L29.

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

- Molecule 35 is a protein called 50S ribosomal protein L30.

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

- Molecule 36 is a protein called Titin.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	89	Total	C	N	O	S	0	0
			688	439	113	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	3	GLU	LYS	conflict	UNP Q8WZ42

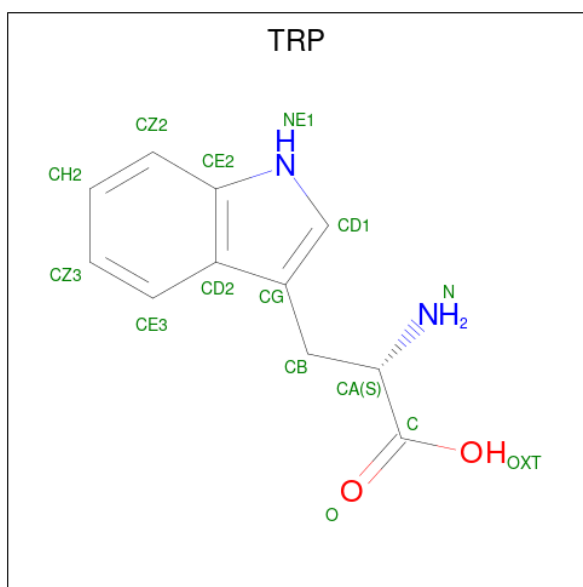
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	4	1	Total	Mg	0
			1	1	
37	A	136	Total	Mg	0
			136	136	
37	B	4	Total	Mg	0
			4	4	
37	C	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	4	1	Total	Zn	0
			1	1	

- Molecule 39 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
39	A	1	15	11	2	2	0

- Molecule 40 is water.

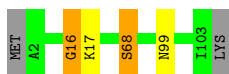
Mol	Chain	Residues	Atoms		AltConf
40	4	1	Total	O	0
			1	1	
40	A	415	Total	O	0
			415	415	
40	B	14	Total	O	0
			14	14	
40	C	2	Total	O	0
			2	2	
40	D	3	Total	O	0
			3	3	
40	E	1	Total	O	0
			1	1	
40	L	3	Total	O	0
			3	3	

3 Residue-property plots [i](#)


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

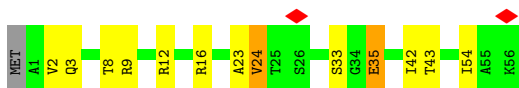
- Molecule 1: 50S ribosomal protein L24

Chain h:  94%



- Molecule 2: 50S ribosomal protein L32

Chain 0:  75% 19%




- Molecule 3: 50S ribosomal protein L33

Chain 1:  5% 56% 27% 7% 9%



- Molecule 4: 50S ribosomal protein L34

Chain 2:  76% 22%

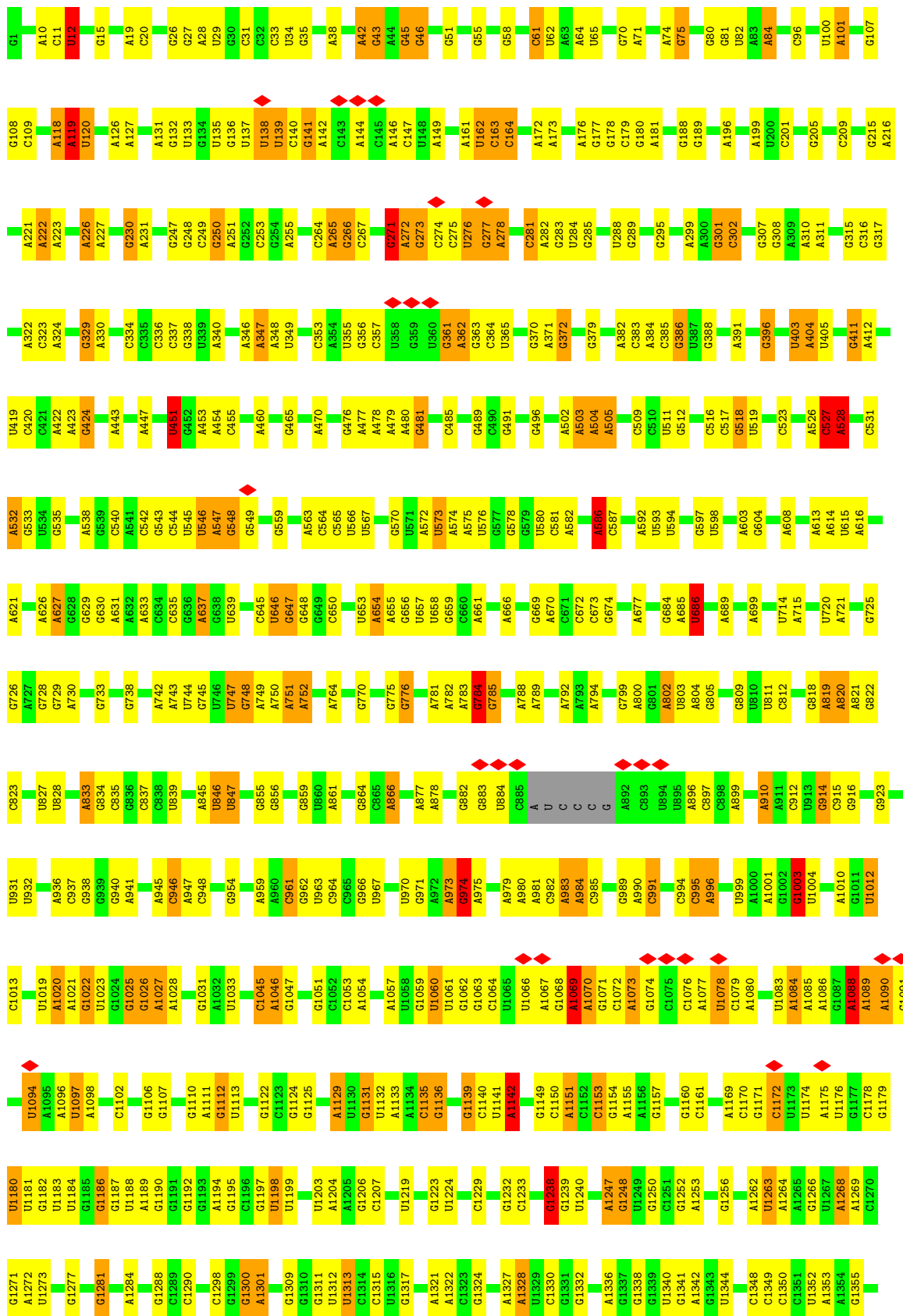


- Molecule 5: 50S ribosomal protein L35

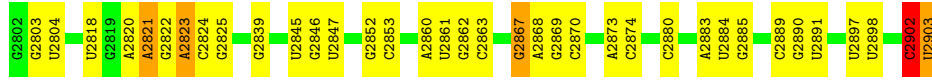
Chain 3:  75% 18% 5%



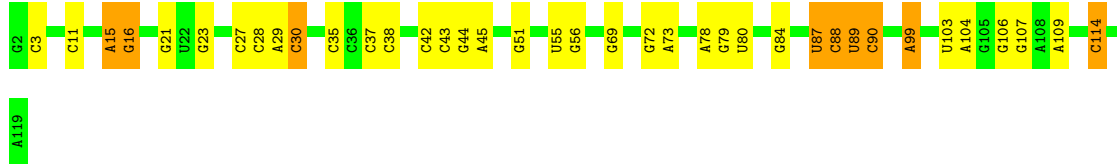
- Molecule 6: 50S ribosomal protein L36



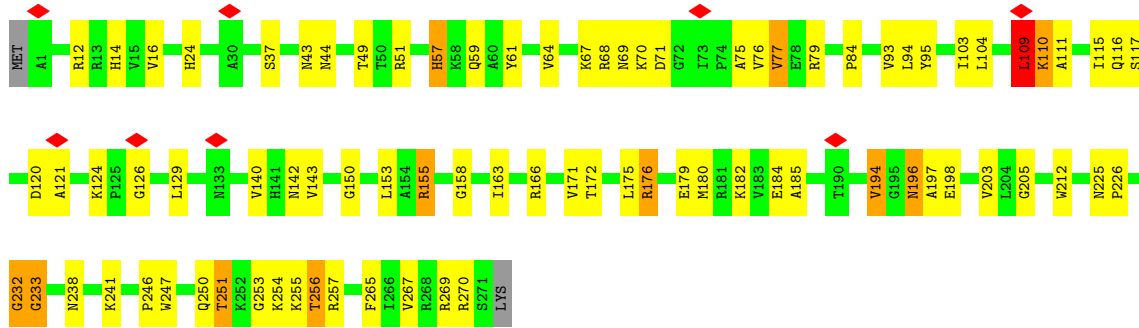
U2609	U2610	U2613	A2614	U2615	C2616	U2617	C2618	C2619	U2629	U2637	U2638	U2642	U2643	U2644	U2645	U2651	U2564	U2555	U2556	U2557	U2558	A2564	A2565	A2566	U2567	U2571	A2572	C2573	U2576	U2579	U2580	C2581	C2582	U2583	U2584	U2585	U2586	U2587	U2688	U2689	U2690	U2698	C2699	U2701	C2702	C2703	C2704	U2707	C2710				
G2325	C2326	A2327	A2328	U2329	C2330	C2331	C2332	U2333	U2334	A2335	A2336	C2337	G2341	C2342	U2343	U2344	C2345	A2346	C2347	U2348	A2352	C2353	C2354	G2355	G2361	G2365	A2366	C2367	C2368	G2383	U2384	C2385	A2386	U2387	C2388	C2389	U2393	G2396	U2402	C2403	U2404	G2405	A2406	U2407	U2408	G2409	G2410	G2415	G2421				
C2422	U2423	A2424	A2425	A2426	C2427	C2428	U2429	A2430	A2435	G2436	C2437	U2438	A2439	C2440	U2441	C2442	C2443	G2446	C2447	C2448	G2455	C2467	A2468	A2469	G2470	A2476	U2477	A2478	U2479	A2482	C2486	U2491	C2498	C2499	U2500	C2501	C2502	U2504	C2505	U2506	C2507	C2508	U2514	U2515	A2516	C2517	A2518						
U2244	A2247	G2250	G2253	U2259	U2262	C2263	A2267	A2268	C2269	U2270	A2271	A2272	A2273	U2274	C2275	G2276	G2277	A2278	G2279	G2282	A2284	C2285	G2286	A2287	C2288	G2289	A2297	U2298	A2298	U2299	C2301	U2302	U2305	C2306	G2307	A2309	C2310	A2311	U2312	C2313	U2314	C2315	U2318	U2319	U2320	U2321	U2322	G2328	U2329	G2330	U2331	A2332	U2334
U2092	G2093	A2094	C2103	C2104	U2105	G2107	A2108	U2109	G2110	U2015	U2016	U2017	G2018	A2019	A2020	C2021	U2022	A2023	A2030	U2031	A2032	A2033	A2037	G2038	U2039	G2040	C2043	C2047	G2048	G2053	A2054	C2055	G2056	G2057	A2060	C2061	A2062	C2063	G2069	A2070	A2071	C2072	C2073	U2074	U2075	C2091	G2157						
U1782	A1783	A1784	A1785	A1786	A1789	C1790	A1791	C1795	U1796	U1798	C1799	C1800	A1801	A1802	A1803	C1804	A1805	A1808	G1811	U1812	G1813	G1814	A1815	C1816	G1817	U1818	A1819	U1820	G1824	G1828	A1829	C1830	G1831	C1832	C1833	C1837	C1838	G1839	C1843	C1844	A1847	A1848	G1857	A1858	C1867	G1869							
C1870	A1871	A1872	A1873	G1884	C1905	G1906	A1907	C1908	C1909	A1913	U1914	U1915	A1918	G1922	U1923	A1927	A1928	G1929	G1930	G1935	A1936	A1937	A1938	U1939	U1943	U1944	U1946	G1950	U1955	U1956	C1957	A1960	U1963	A1966	C1967	G1968	A1969	A1970	U1971	G1972	A1977	A1978	U1979	G1980	G1983								
A1676	A1677	G1681	G1684	C1685	C1686	A1691	U1692	G1703	C1704	A1705	U1714	G1715	A1603	C1604	C1605	C1606	C1607	A1608	A1609	C1611	C1612	G1613	A1614	C1615	A1616	G1622	A1626	G1627	C1638	C1639	G1643	C1644	C1645	C1646	U1647	U1648	G1649	A1652	G1653	A1654	A1655	C1658	G1659	U1662	C1659	U1662	A1669	C1670	G1674	C1675			
U1458	G1459	G1465	U1466	A1469	U1474	G1475	U1476	A1477	G1478	G1479	U1482	U1485	U1486	U1487	A1493	A1494	A1495	A1504	A1508	A1509	C1510	G1514	A1515	U1523	G1524	C1533	U1534	C1535	C1536	G1537	U1542	G1543	A1553	A1558	U1565	A1566	G1567	A1568	A1570	A1571	U1578	G1581	C1582										
A1583	U1584	C1585	A1586	G1587	G1588	A1591	C1592	G1593	U1594	A1603	C1604	C1605	C1606	C1607	A1608	A1609	C1611	C1612	G1613	A1614	C1615	A1616	G1622	A1626	G1627	C1638	C1639	G1643	C1644	C1645	C1646	U1647	U1648	G1649	A1652	G1653	A1654	A1655	C1658	G1659	U1662	C1659	U1662	A1669	C1670	G1674	C1675						



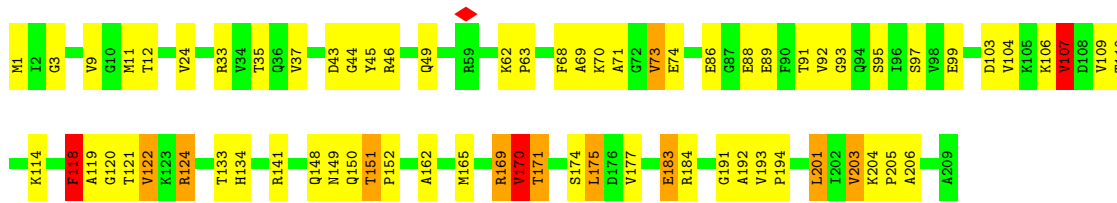
• Molecule 12: 5S ribosomal RNA



• Molecule 13: 50S ribosomal protein L2



• Molecule 14: 50S ribosomal protein L3

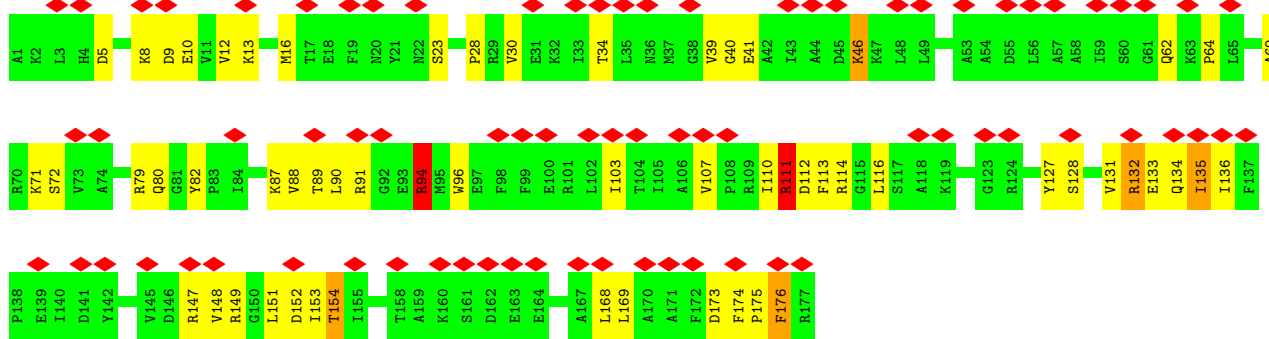
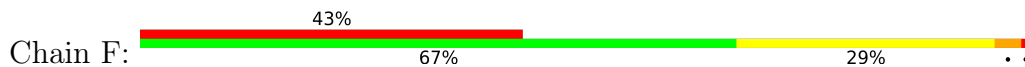


• Molecule 15: 50S ribosomal protein L4

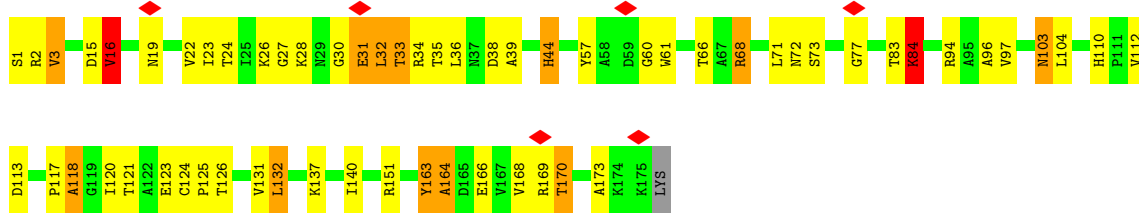




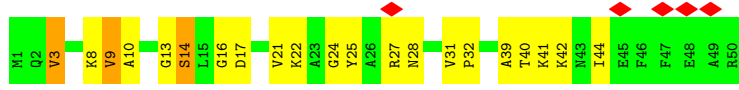
• Molecule 16: 50S ribosomal protein L5



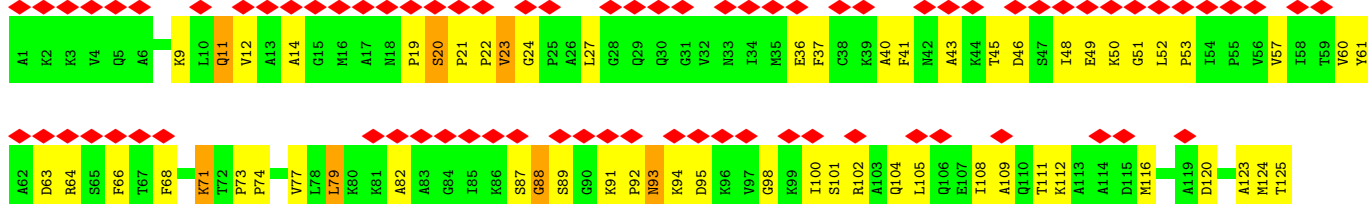
• Molecule 17: 50S ribosomal protein L6

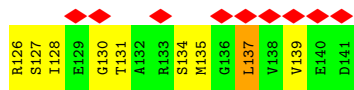


• Molecule 18: 50S ribosomal protein L9

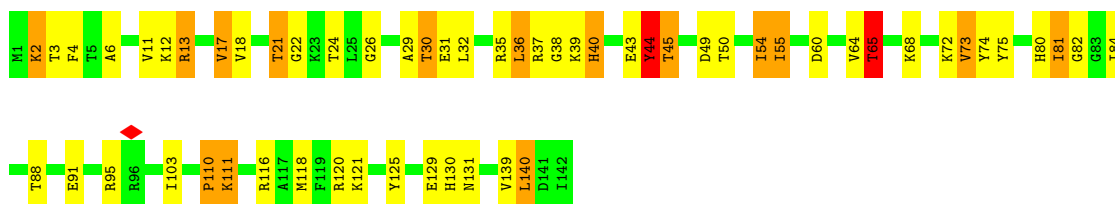


• Molecule 19: 50S ribosomal protein L11

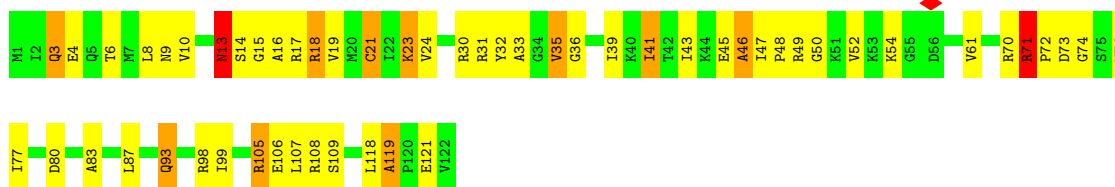




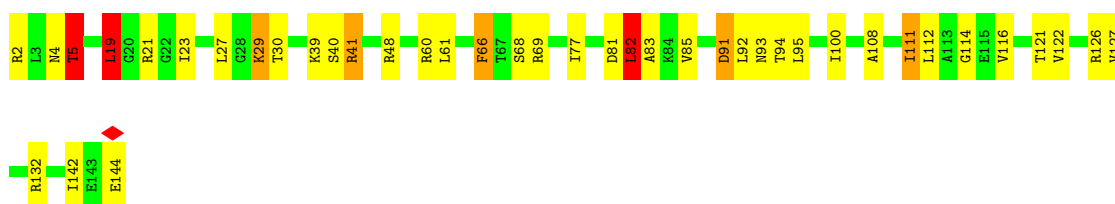
• Molecule 20: 50S ribosomal protein L13



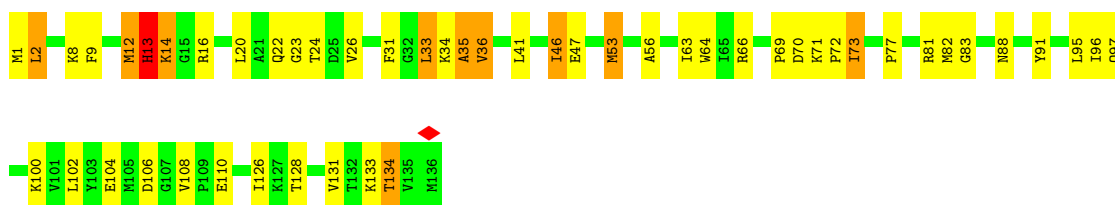
• Molecule 21: 50S ribosomal protein L14



• Molecule 22: 50S ribosomal protein L15

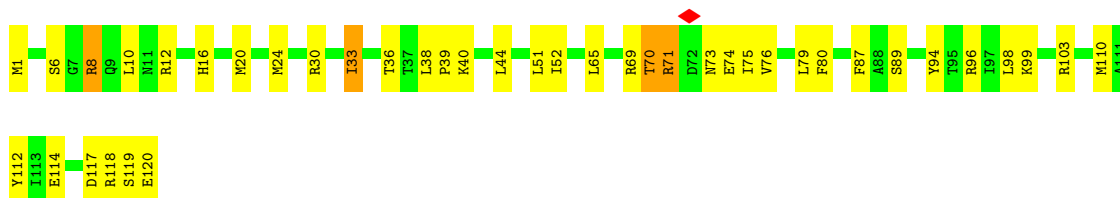


• Molecule 23: 50S ribosomal protein L16



• Molecule 24: 50S ribosomal protein L17





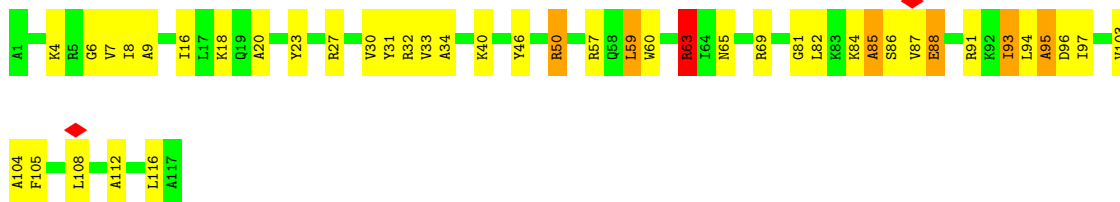
• Molecule 25: 50S ribosomal protein L18



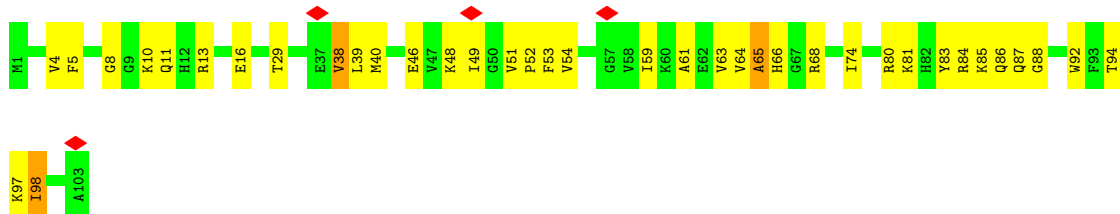
• Molecule 26: 50S ribosomal protein L19



• Molecule 27: 50S ribosomal protein L20

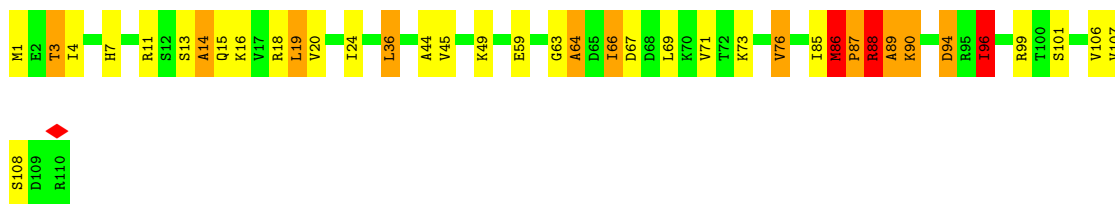


• Molecule 28: 50S ribosomal protein L21



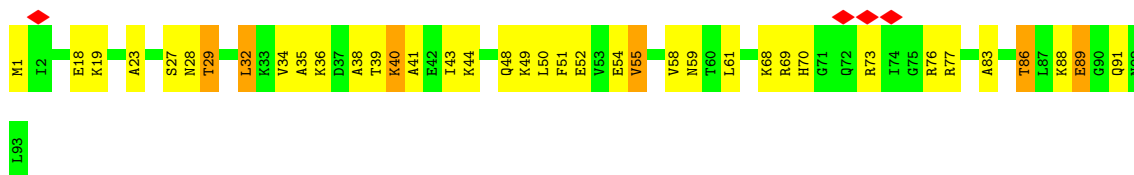
• Molecule 29: 50S ribosomal protein L22

Chain S: 



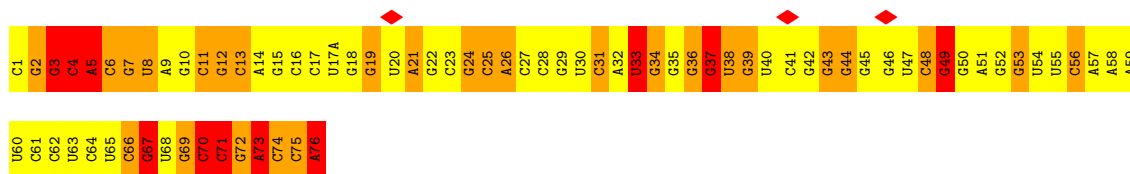
- Molecule 30: 50S ribosomal protein L23

Chain T: 



- Molecule 31: Proline tRNA

Chain V: 



- Molecule 32: 50S ribosomal protein L27

Chain W: 

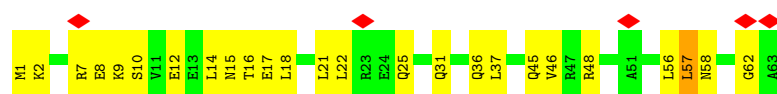


- Molecule 33: 50S ribosomal protein L28

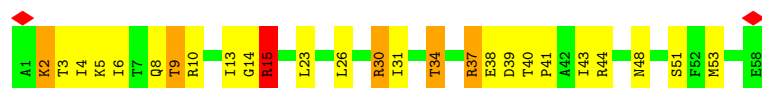
Chain X: 



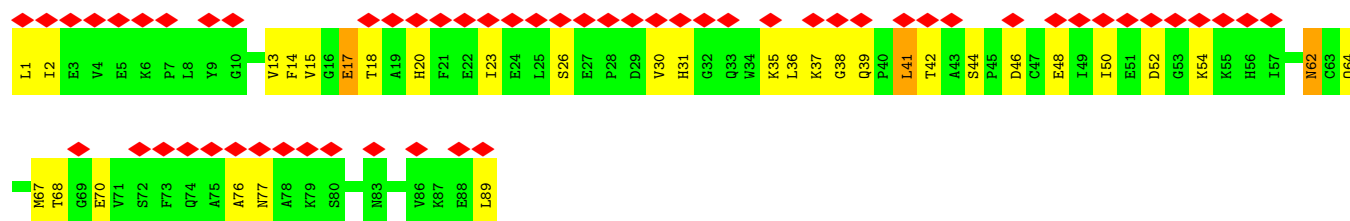
- Molecule 34: 50S ribosomal protein L29



- Molecule 35: 50S ribosomal protein L30



- Molecule 36: Titin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	301510	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 ($e^-/\text{\AA}^2$)	0.926	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.240	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.019	Depositor
Map size (\AA)	394.31998, 394.31998, 394.31998	wwPDB
Map dimensions	372, 372, 372	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	h	0.73	1/787 (0.1%)	0.89	1/1051 (0.1%)
2	0	0.54	0/450	0.70	0/599
3	1	0.53	0/416	0.75	0/554
4	2	0.53	0/380	0.70	0/498
5	3	0.53	0/513	0.75	0/676
6	4	0.59	0/303	0.84	0/397
7	5	0.74	0/1131	1.32	26/1524 (1.7%)
8	6	0.58	0/227	0.65	0/304
9	7	0.52	0/143	0.91	1/193 (0.5%)
10	8	0.48	0/766	0.67	1/1025 (0.1%)
11	A	0.81	19/68626 (0.0%)	1.23	309/107056 (0.3%)
12	B	0.67	0/2828	1.10	3/4410 (0.1%)
13	C	0.54	0/2121	0.80	3/2852 (0.1%)
14	D	0.58	0/1586	0.77	1/2134 (0.0%)
15	E	0.53	0/1571	0.76	2/2113 (0.1%)
16	F	0.50	0/1434	0.71	1/1926 (0.1%)
17	G	0.56	0/1333	0.74	0/1805
18	H	0.53	0/389	0.73	0/523
19	I	0.62	0/1046	0.84	1/1410 (0.1%)
20	J	0.63	1/1152 (0.1%)	0.78	0/1551
21	K	0.65	1/947 (0.1%)	0.77	0/1268
22	L	0.56	0/1054	0.79	2/1403 (0.1%)
23	M	0.61	0/1093	0.77	0/1460
24	N	0.51	0/973	0.69	0/1301
25	O	0.46	0/902	0.70	0/1209
26	P	0.53	0/929	0.78	1/1242 (0.1%)
27	Q	0.62	0/960	0.71	1/1278 (0.1%)
28	R	0.61	1/829 (0.1%)	0.76	0/1107
29	S	0.84	2/864 (0.2%)	1.31	6/1156 (0.5%)
30	T	0.55	0/744	0.85	0/994
31	V	2.38	77/1842 (4.2%)	2.83	255/2870 (8.9%)
32	W	0.69	0/603	1.00	1/797 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	X	0.50	0/635	0.79	1/848 (0.1%)
34	Y	0.46	0/510	0.75	0/677
35	Z	0.54	0/453	0.84	1/605 (0.2%)
36	z	1.05	0/701	1.24	0/946
All	All	0.81	102/101241 (0.1%)	1.19	617/151762 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	5	0	1
13	C	0	1
14	D	0	1
20	J	0	1
21	K	0	1
29	S	0	3
31	V	0	13
All	All	0	21

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	39	G	N9-C4	15.37	1.50	1.38
31	V	69	G	C6-N1	13.06	1.48	1.39
31	V	5	A	C6-N1	12.86	1.44	1.35
31	V	39	G	C2-N3	12.30	1.42	1.32
31	V	39	G	N1-C2	11.24	1.46	1.37

The worst 5 of 617 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	86	MET	C-N-CD	-30.06	54.47	120.60
31	V	73	A	N1-C6-N6	22.82	132.29	118.60
31	V	69	G	N1-C6-O6	19.95	131.87	119.90
11	A	1073	A	N1-C6-N6	-19.92	106.65	118.60
31	V	69	G	C5-C6-O6	-19.63	116.82	128.60

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	5	130	PRO	Peptide
13	C	233	GLY	Peptide
14	D	9	VAL	Peptide
20	J	110	PRO	Peptide
21	K	71	ARG	Peptide

5.2 Too-close contacts [i](#)

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	h	779	0	829	0	0
2	0	444	0	461	17	0
3	1	409	0	440	16	0
4	2	377	0	418	6	0
5	3	504	0	574	11	0
6	4	302	0	340	16	0
7	5	1117	0	1155	124	0
8	6	227	0	237	6	0
9	7	139	0	134	12	0
10	8	753	0	780	11	0
11	A	61274	0	30816	819	0
12	B	2529	0	1281	20	0
13	C	2082	0	2157	53	0
14	D	1565	0	1616	49	0
15	E	1552	0	1619	36	0
16	F	1410	0	1445	44	0
17	G	1313	0	1361	36	0
18	H	384	0	405	13	0
19	I	1032	0	1088	53	0
20	J	1129	0	1162	51	0
21	K	938	0	1012	42	0
22	L	1045	0	1117	35	0
23	M	1074	0	1157	28	0
24	N	960	0	1000	30	0
25	O	892	0	923	21	0
26	P	917	0	965	42	0
27	Q	947	0	1022	49	0
28	R	816	0	839	34	0
29	S	857	0	922	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	T	738	0	807	34	0
31	V	1649	0	833	53	0
32	W	596	0	610	81	0
33	X	625	0	655	18	0
34	Y	509	0	543	13	0
35	Z	449	0	491	17	0
36	z	688	0	691	0	0
37	4	1	0	0	0	0
37	A	136	0	0	0	0
37	B	4	0	0	0	0
37	C	1	0	0	0	0
37	E	1	0	0	0	0
38	4	1	0	0	0	0
39	A	15	0	9	3	0
40	4	1	0	0	0	0
40	A	415	0	0	77	0
40	B	14	0	0	1	0
40	C	2	0	0	0	0
40	D	3	0	0	0	0
40	E	1	0	0	0	0
40	L	3	0	0	0	0
All	All	93619	0	61914	1673	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 13.

The worst 5 of 1673 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)
16:F:79:ARG:NH2	31:V:56:C:O2	1.62	1.30
11:A:2062:A:H2'	11:A:2063:C:C6	1.70	1.27
11:A:2062:A:H2'	11:A:2063:C:C5	1.71	1.23
11:A:1923:U:H5''	31:V:24:G:O2'	1.04	1.18
9:7:24:PRO:HB2	31:V:76:A:O3'	1.40	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	100/104 (96%)	92 (92%)	6 (6%)	2 (2%)	7	38
2	0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	7
3	1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1	10
4	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
5	3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4	26
6	4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	5
7	5	146/165 (88%)	77 (53%)	41 (28%)	28 (19%)	0	0
8	6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	3	23
9	7	14/24 (58%)	13 (93%)	0	1 (7%)	1	8
10	8	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
13	C	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2	14
14	D	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	9
15	E	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	2	16
16	F	175/177 (99%)	141 (81%)	30 (17%)	4 (2%)	6	34
17	G	173/176 (98%)	126 (73%)	30 (17%)	17 (10%)	0	3
18	H	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	0	3
19	I	139/141 (99%)	97 (70%)	33 (24%)	9 (6%)	1	10
20	J	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1	10
21	K	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	1	5
22	L	141/143 (99%)	104 (74%)	32 (23%)	5 (4%)	3	24
23	M	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	5
24	N	118/120 (98%)	101 (86%)	16 (14%)	1 (1%)	19	58
25	O	114/116 (98%)	95 (83%)	18 (16%)	1 (1%)	17	56
26	P	112/114 (98%)	86 (77%)	17 (15%)	9 (8%)	1	6
27	Q	115/117 (98%)	99 (86%)	12 (10%)	4 (4%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	R	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4	28
29	S	108/110 (98%)	91 (84%)	10 (9%)	7 (6%)	1	10
30	T	91/93 (98%)	57 (63%)	24 (26%)	10 (11%)	0	2
32	W	77/79 (98%)	39 (51%)	21 (27%)	17 (22%)	0	0
33	X	75/77 (97%)	64 (85%)	8 (11%)	3 (4%)	3	21
34	Y	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	9
35	Z	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	3	23
36	z	87/89 (98%)	60 (69%)	14 (16%)	13 (15%)	0	1
All	All	3484/3678 (95%)	2699 (78%)	558 (16%)	227 (6%)	2	10

5 of 227 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	0	23	ALA
5	3	22	LYS
6	4	8	LYS
7	5	27	VAL
7	5	48	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h	83/85 (98%)	81 (98%)	2 (2%)	49	77
2	0	47/48 (98%)	46 (98%)	1 (2%)	53	79
3	1	45/49 (92%)	42 (93%)	3 (7%)	16	50
4	2	38/38 (100%)	35 (92%)	3 (8%)	12	43
5	3	51/52 (98%)	46 (90%)	5 (10%)	8	31
6	4	34/34 (100%)	31 (91%)	3 (9%)	10	36
7	5	112/123 (91%)	93 (83%)	19 (17%)	2	10
8	6	26/85 (31%)	22 (85%)	4 (15%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	7	16/24 (67%)	12 (75%)	4 (25%)	0	2
10	8	78/78 (100%)	75 (96%)	3 (4%)	33	67
13	C	216/218 (99%)	202 (94%)	14 (6%)	17	51
14	D	164/164 (100%)	151 (92%)	13 (8%)	12	43
15	E	165/165 (100%)	146 (88%)	19 (12%)	5	24
16	F	148/148 (100%)	138 (93%)	10 (7%)	16	49
17	G	136/137 (99%)	122 (90%)	14 (10%)	7	29
18	H	40/40 (100%)	39 (98%)	1 (2%)	47	77
19	I	109/109 (100%)	105 (96%)	4 (4%)	34	68
20	J	116/116 (100%)	100 (86%)	16 (14%)	3	16
21	K	103/103 (100%)	92 (89%)	11 (11%)	6	27
22	L	102/102 (100%)	95 (93%)	7 (7%)	15	49
23	M	109/109 (100%)	93 (85%)	16 (15%)	3	14
24	N	100/100 (100%)	93 (93%)	7 (7%)	15	48
25	O	86/86 (100%)	78 (91%)	8 (9%)	9	33
26	P	99/99 (100%)	91 (92%)	8 (8%)	11	42
27	Q	89/89 (100%)	81 (91%)	8 (9%)	9	34
28	R	84/84 (100%)	78 (93%)	6 (7%)	14	47
29	S	93/93 (100%)	83 (89%)	10 (11%)	6	27
30	T	80/80 (100%)	78 (98%)	2 (2%)	47	77
32	W	59/59 (100%)	53 (90%)	6 (10%)	7	29
33	X	67/67 (100%)	61 (91%)	6 (9%)	9	34
34	Y	55/55 (100%)	52 (94%)	3 (6%)	21	57
35	Z	48/48 (100%)	40 (83%)	8 (17%)	2	10
36	z	75/75 (100%)	52 (69%)	23 (31%)	0	0
All	All	2873/2962 (97%)	2606 (91%)	267 (9%)	12	33

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	X	34	SER
35	Z	15	ARG
36	z	52	ASP

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Mol	Chain	Res	Type
16	F	46	LYS
16	F	16	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
36	z	39	GLN
36	z	31	HIS
34	Y	38	GLN
16	F	26	GLN
34	Y	41	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	2850/2903 (98%)	457 (16%)	40 (1%)
12	B	117/118 (99%)	17 (14%)	0
31	V	76/77 (98%)	15 (19%)	0
All	All	3043/3098 (98%)	489 (16%)	40 (1%)

5 of 489 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	10	A
11	A	12	U
11	A	15	G
11	A	34	U
11	A	35	G

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1847	A
11	A	2326	C
11	A	1870	C
11	A	2142	A
11	A	2756	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 145 ligands modelled in this entry, 144 are monoatomic - leaving 1 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
39	TRP	A	3001	-	14,16,16	0.94	0	16,22,22	0.94	0

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
39	TRP	A	3001	-	-	6/7/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	A	3001	TRP	OXT-C-CA-N
39	A	3001	TRP	OXT-C-CA-CB
39	A	3001	TRP	O-C-CA-CB
39	A	3001	TRP	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
39	A	3001	TRP	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	A	3001	TRP	3	0

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.

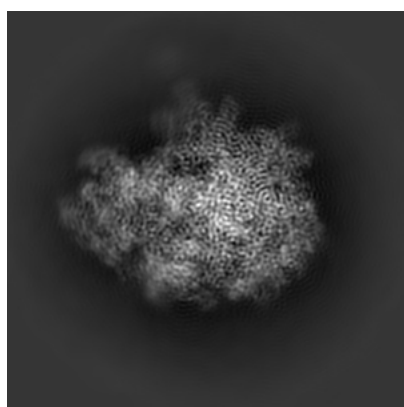
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0322. These allow visual inspection of the internal detail of the map and identification of artifacts.

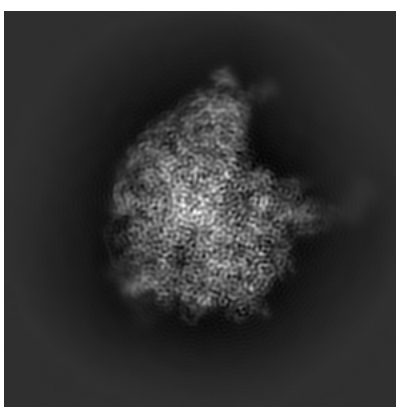
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

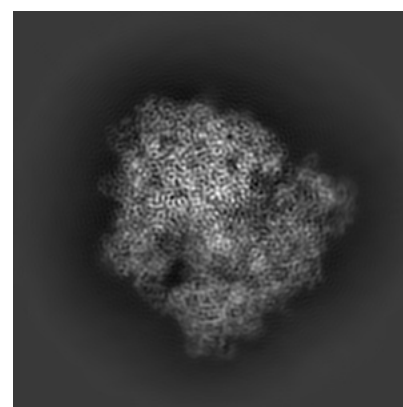
6.1.1 Primary map



X



Y

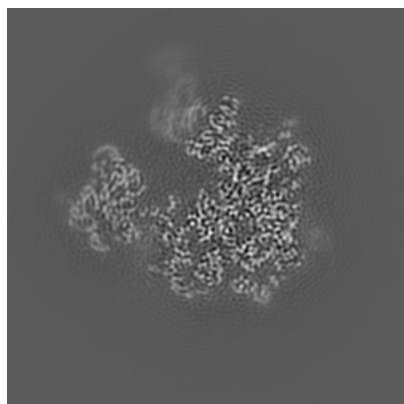


Z

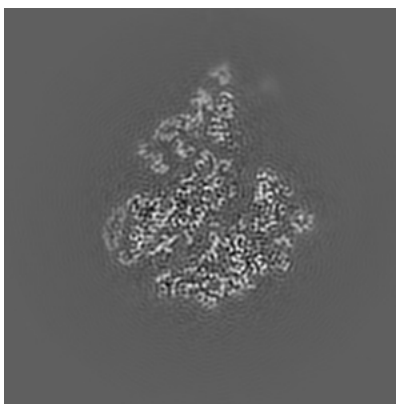
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

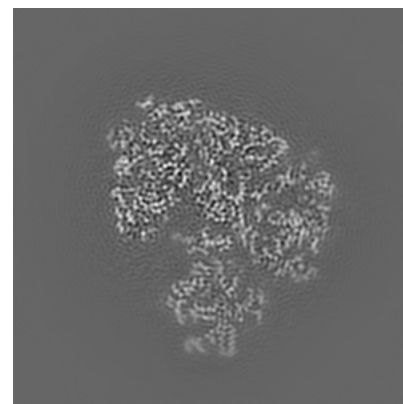
6.2.1 Primary map



X Index: 186



Y Index: 186

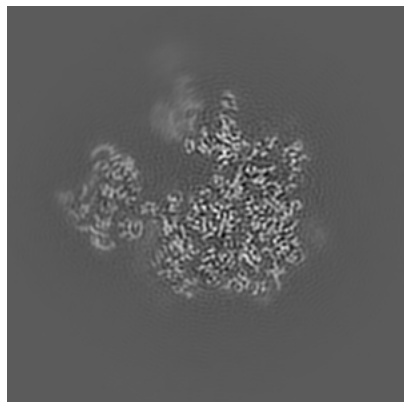


Z Index: 186

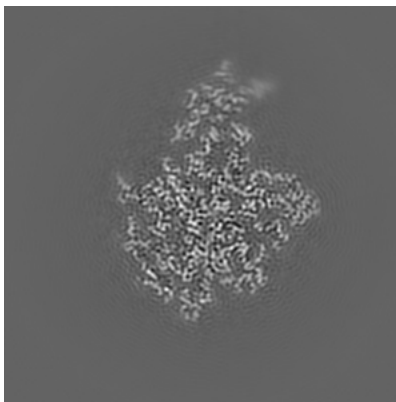
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

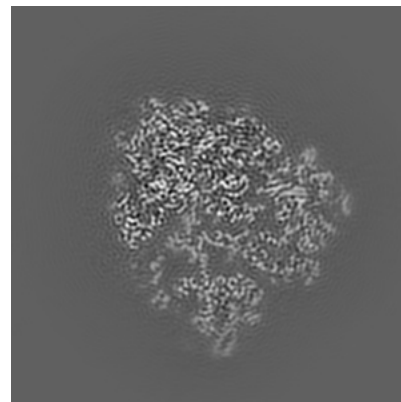
6.3.1 Primary map



X Index: 190



Y Index: 204

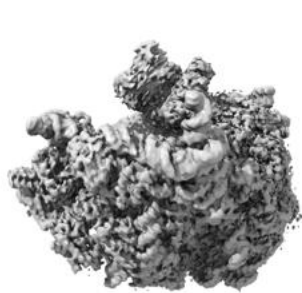


Z Index: 194

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

6.4 Orthogonal surface views [i](#)

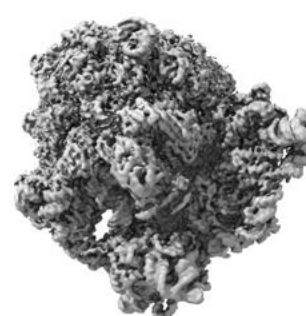
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

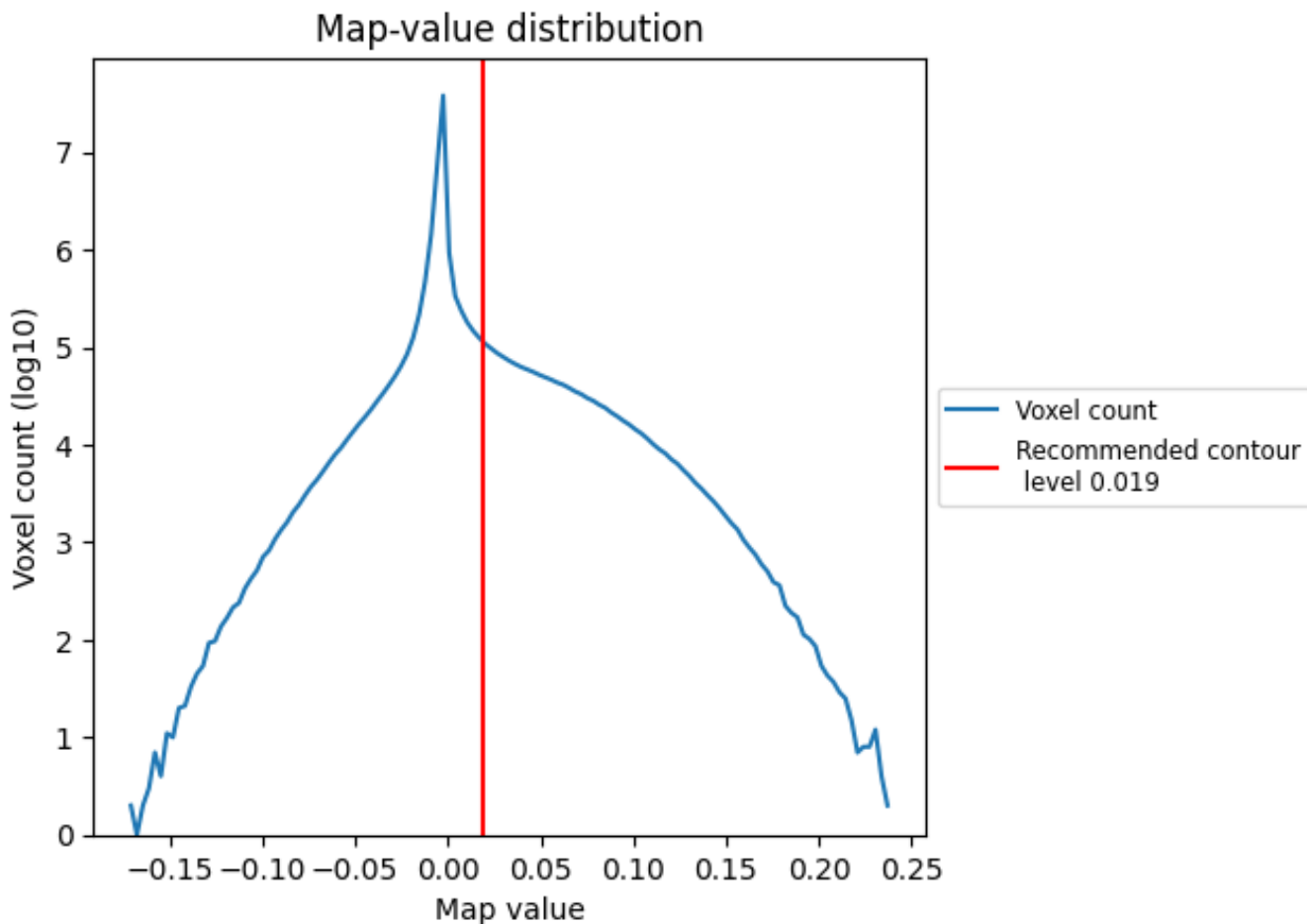
6.5 Mask visualisation

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

7 Map analysis [i](#)

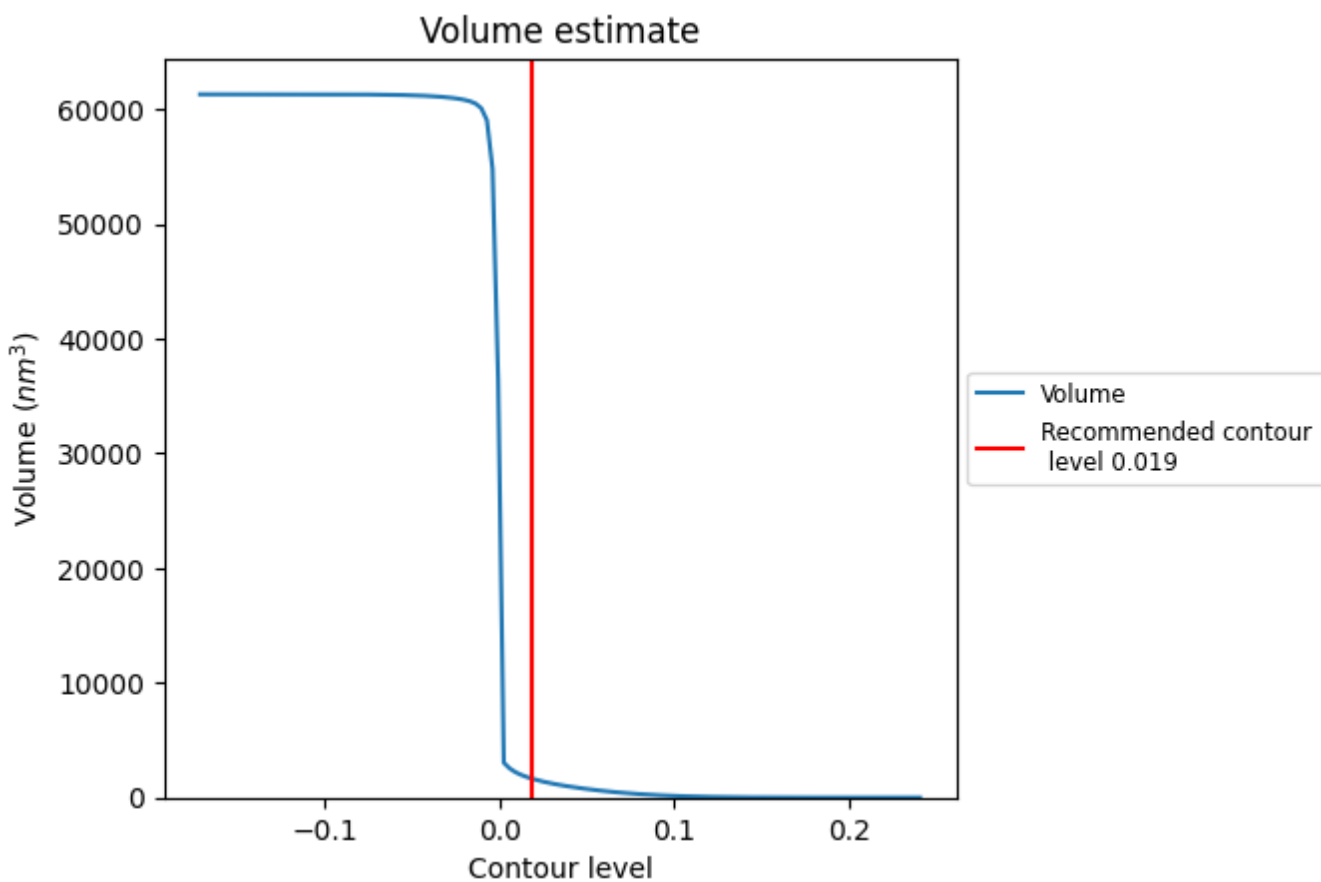
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

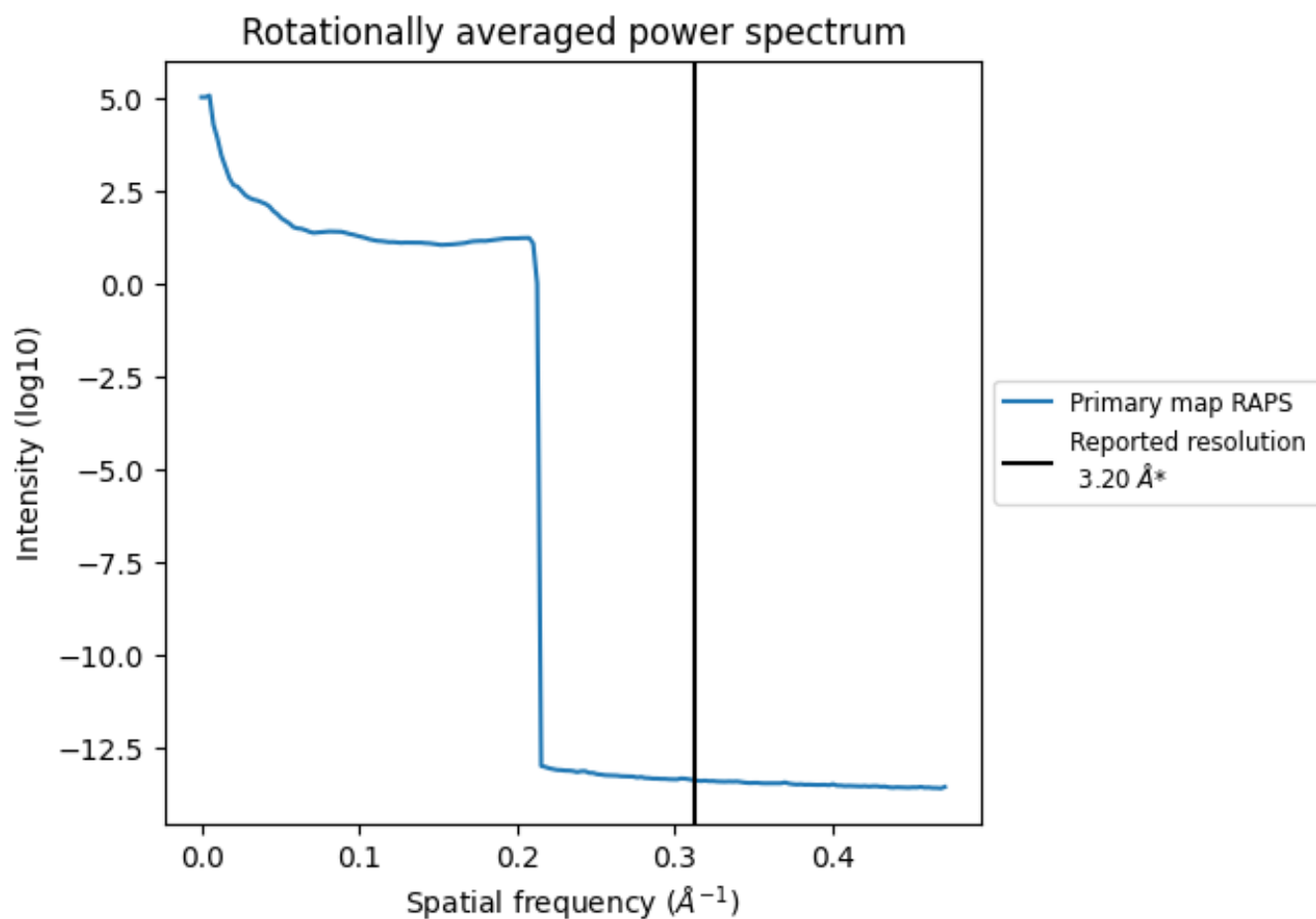
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1634 nm³; this corresponds to an approximate mass of 1476 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](#)

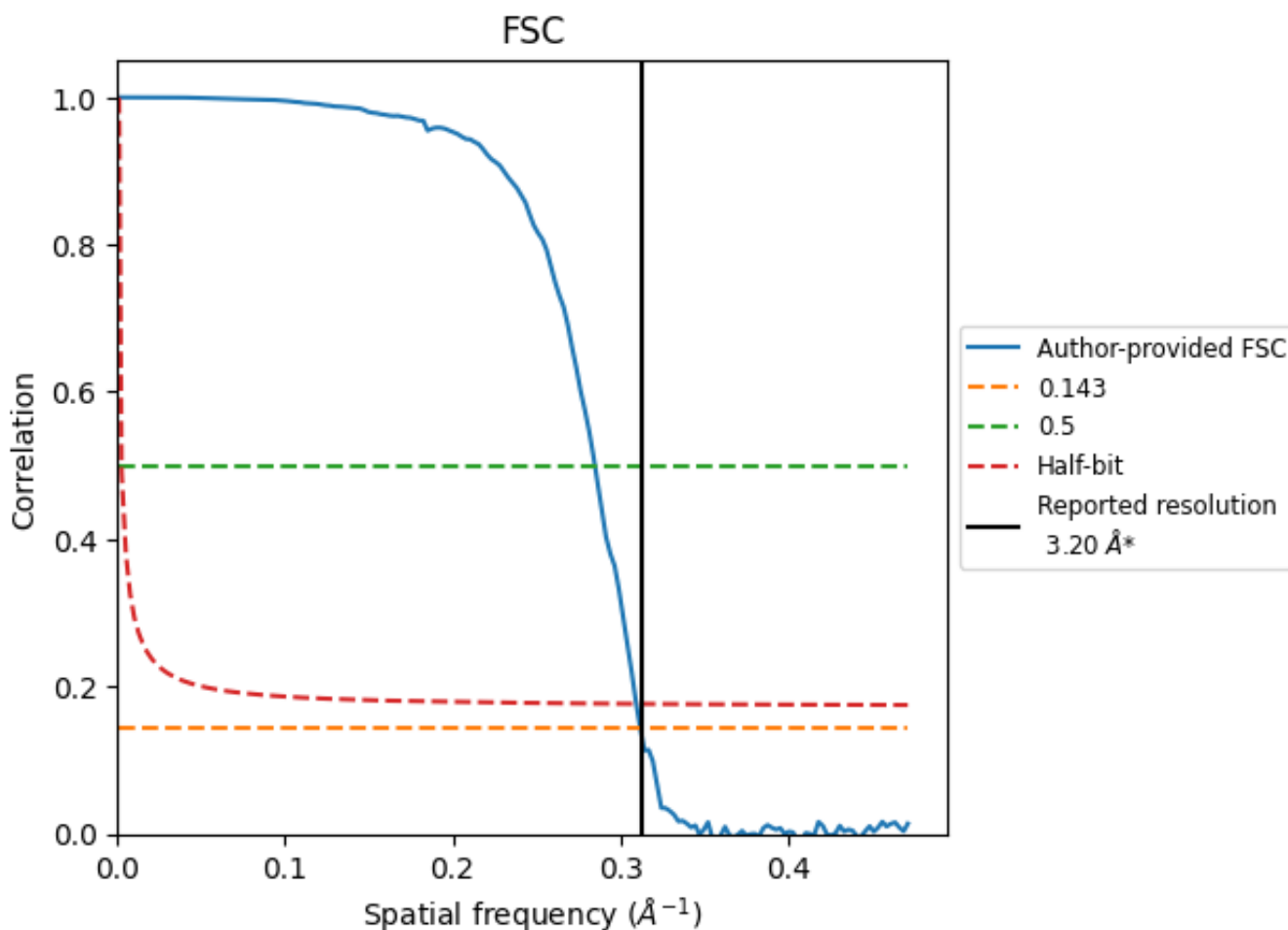


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

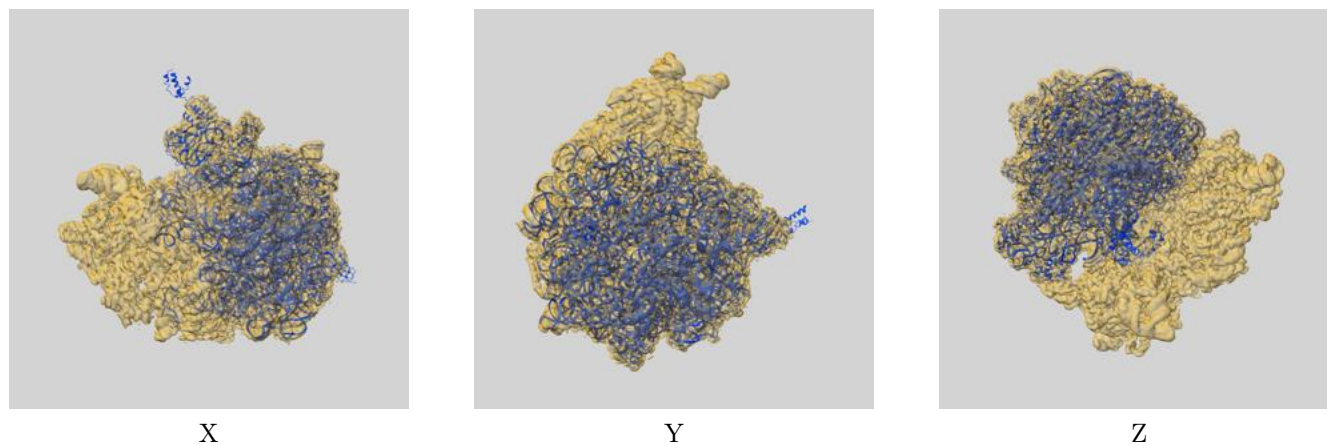
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.51	3.23
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

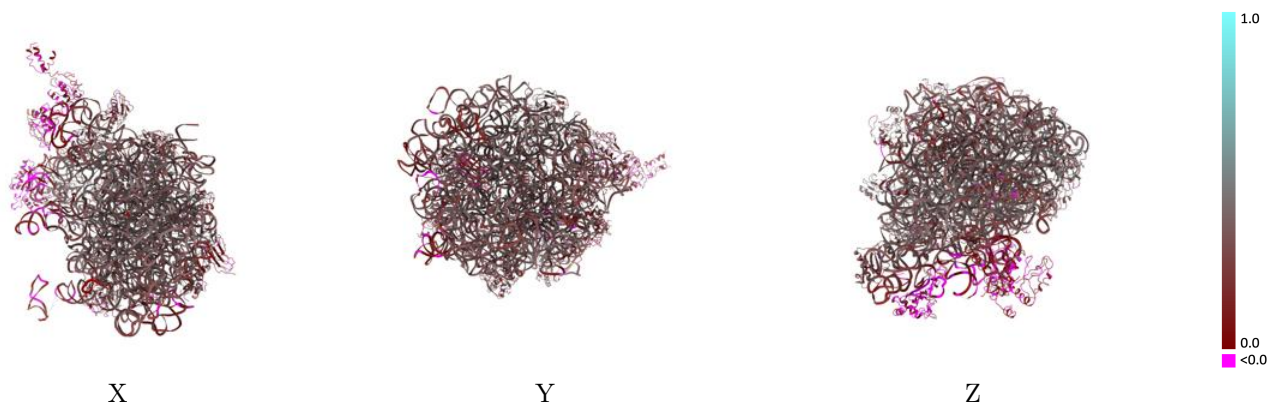
This section contains information regarding the fit between EMDB map EMD-0322 and PDB model 6I0Y. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



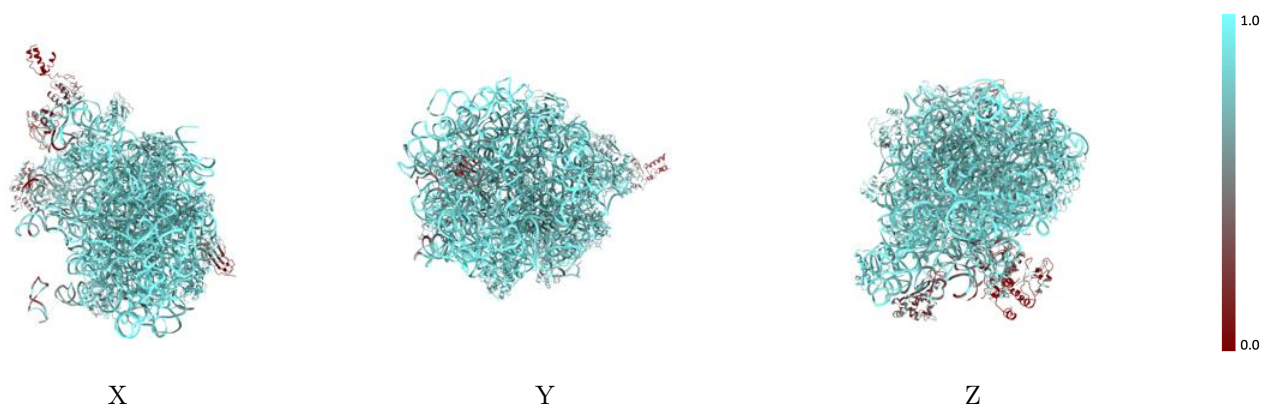
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



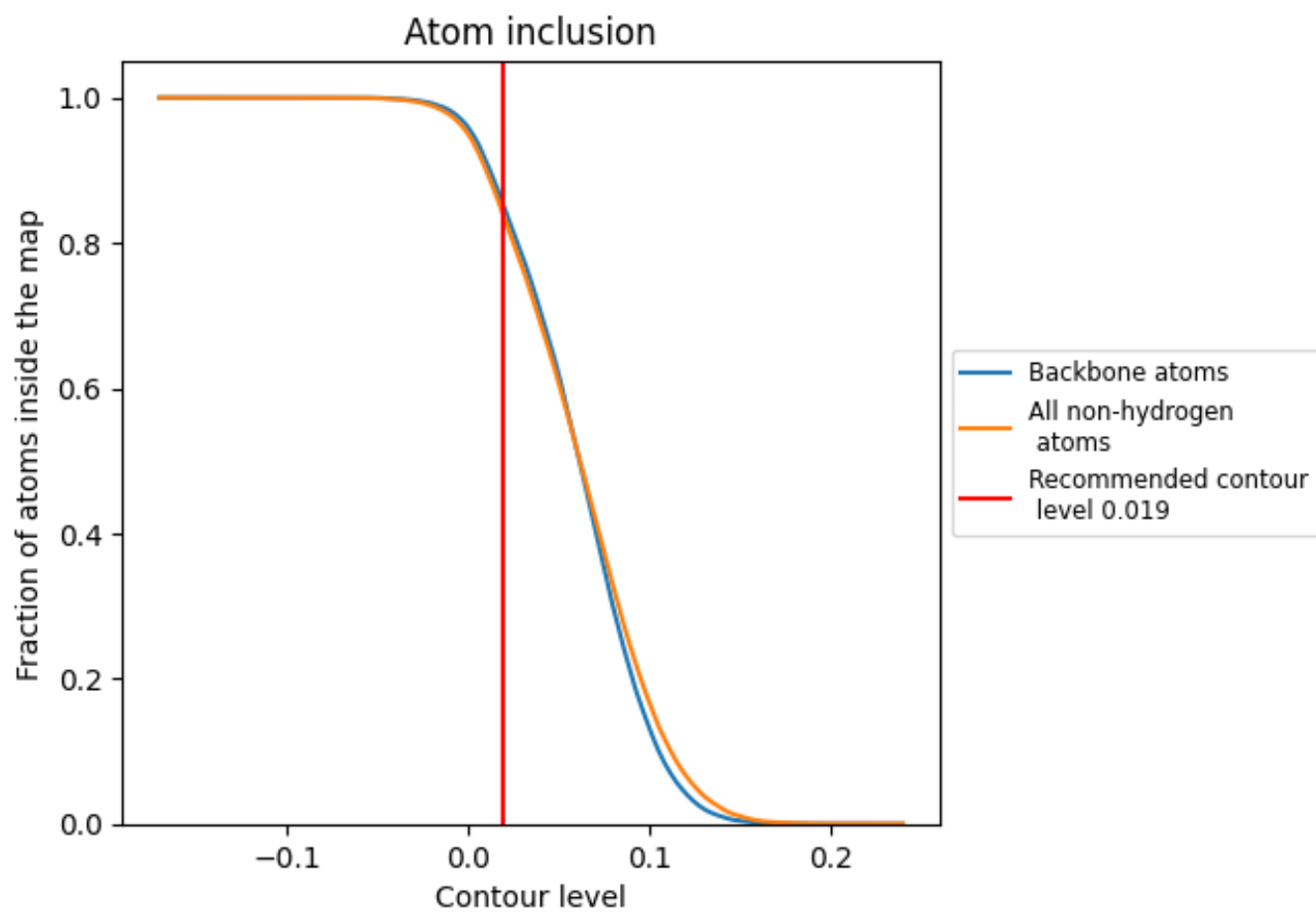
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8408	 0.3050
0	 0.8154	 0.3330
1	 0.8155	 0.3060
2	 0.8282	 0.3250
3	 0.8656	 0.3850
4	 0.8129	 0.3330
5	 0.3821	 0.0800
6	 0.0000	 0.0630
7	 0.7206	 0.2810
8	 0.7967	 0.3240
A	 0.8934	 0.3250
B	 0.8796	 0.2830
C	 0.7868	 0.2870
D	 0.8257	 0.3490
E	 0.7922	 0.3250
F	 0.4676	 -0.0220
G	 0.7863	 0.2640
H	 0.6887	 0.2060
I	 0.3160	 0.0540
J	 0.8045	 0.3010
K	 0.8007	 0.3460
L	 0.8258	 0.3420
M	 0.8167	 0.3460
N	 0.8590	 0.3490
O	 0.8262	 0.3090
P	 0.7962	 0.3310
Q	 0.7952	 0.2860
R	 0.8030	 0.3110
S	 0.8038	 0.3410
T	 0.7673	 0.3200
V	 0.7107	 0.1310
W	 0.7690	 0.2990
X	 0.8403	 0.3390
Y	 0.7887	 0.2610
Z	 0.7918	 0.3030



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Chain	Atom inclusion	Q-score
h	 0.7992	 0.3170
z	 0.3017	 0.1300