wwPDB EM Validation Summary Report (i)

Dec 12, 2022 – 05:48 am GMT

PDB ID	:	6XZ7
EMDB ID	:	EMD-10655
Title	:	E. coli 50S ribosomal subunit in complex with dirithromycin, fMet-Phe-tRNA(Phe) and deacylated tRNA(iMet).
Authors	:	Pichkur, E.B.; Polikanov, Y.S.; Myasnikov, A.G.; Konevega, A.L.
Deposited on	:	2020-02-03
Resolution	:	2.10 Å(reported)
Based on initial model	:	4YBB

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 (i) 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 (1)) were used in the production of this report:

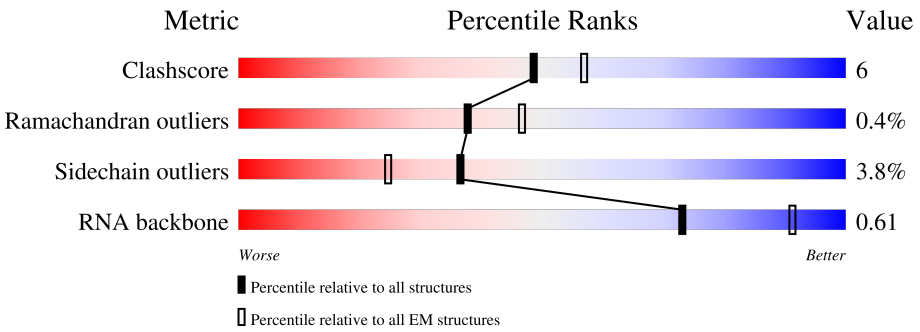
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.10 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2897	7%, 76%, 21%, •
2	B	120	•, 80%, 18%, •
3	C	271	85%, 15%
4	D	209	89%, 11%
5	E	201	•, 88%, 11%, •
6	F	177	40%, 54%, 40%, 6%, •
7	G	176	19%, 70%, 26%, •

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Mol	Chain	Length	Quality of chain
8	H	135	100%, 68%, 29%
9	I	134	100%, 77%, 21%
10	J	142	87%, 12%
11	K	123	85%, 15%
12	L	144	87%, 13%
13	M	136	88%, 11%
14	N	125	6%, 93%, 6%
15	O	117	80%, 19%
16	P	114	84%, 15%
17	Q	117	97%
18	R	103	90%, 7%
19	S	110	92%, 7%
20	T	93	85%, 14%
21	U	102	5%, 86%, 13%
22	V	94	81%, 18%
23	W	76	87%, 13%
24	X	77	88%, 12%
25	Y	62	6%, 89%, 11%
26	Z	58	90%, 9%
27	a	56	98%
28	b	51	98%
29	c	46	96%
30	d	64	94%, 6%
31	e	38	97%
32	f	76	70%, 24%, 55%, 21%

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Mol	Chain	Length	Quality of chain
33	g	76	62% 22% 47% 30%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 94915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2897	62252	27778	11454	20121	2899	3	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2083	1288	423	365	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	209	1566	980	288	294	4	1	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	177	1411	899	249	257	6	0	0

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

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

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	135	1023	649	179	192	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	85	VAL	SER	conflict	UNP P0A7J3
H	86	THR	MET	conflict	UNP P0A7J3

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	134	979	619	169	185	6	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	144	1053	654	207	190	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	136	1075	686	205	178	6	1	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	117	900	557	179	163	1	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	93	739	466	139	132	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	102	780	492	146	142	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	76	580	359	117	103	1	1	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	62	501	308	98	94	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 32 is a RNA chain called Deacylated tRNAi(Met).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
32	f	76	1625	725	294	529	76	1	0	0

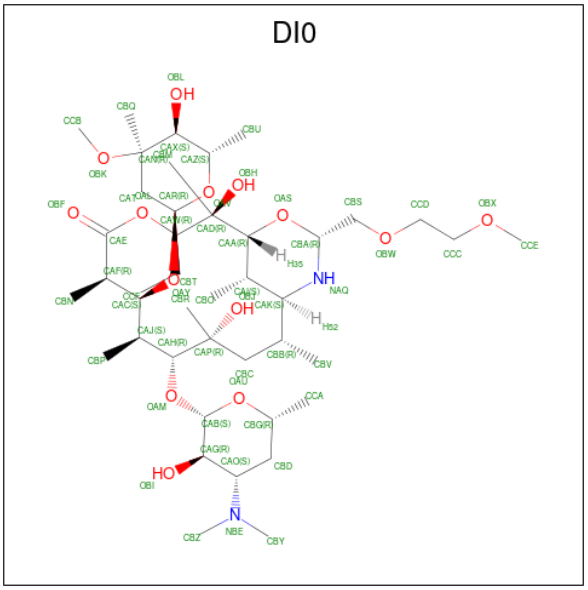
- Molecule 33 is a RNA chain called fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
33	g	76	1667	760	297	534	75	1	0	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	A	174	174	174	0
			Total	Mg	
34	B	3	3	3	0
			Total	Mg	
34	U	1	1	1	0

- Molecule 35 is Dirithromycin (three-letter code: DI0) (formula: $C_{42}H_{78}N_2O_{14}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
35	A	1	58	42	2	14	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	A	498	498	498	0
			Total	O	
36	B	9	9	9	0
			Total	O	
36	C	7	7	7	0
			Total	O	
36	D	1	1	1	0
			Total	O	
36	E	1	1	1	0

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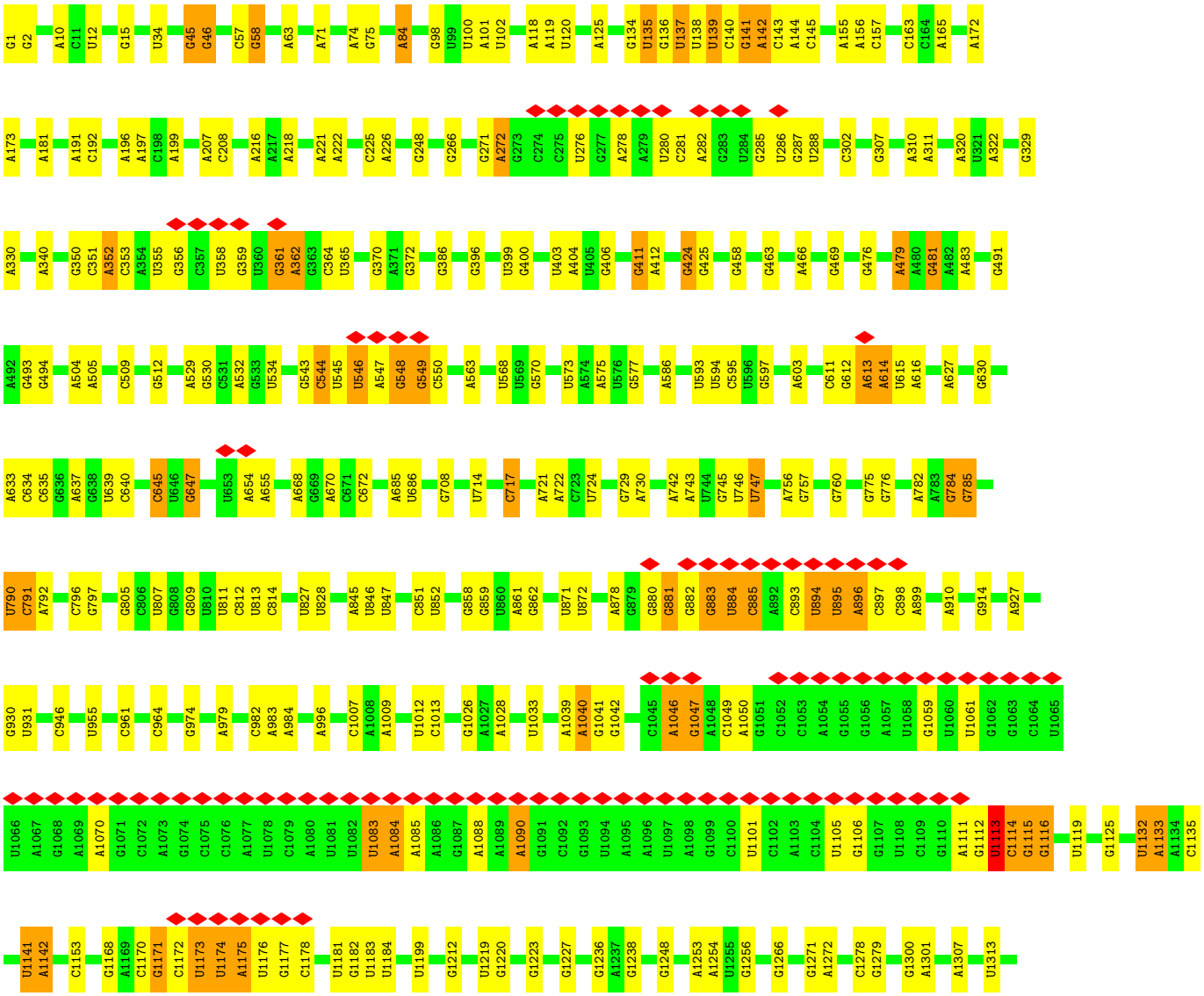
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	L	6	6	6	0
			Total	O	
36	N	1	1	1	0
			Total	O	
36	T	1	1	1	0
			Total	O	
36	d	4	4	4	0

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: 23S rRNA

Chain A:



G1324 U1329 C1345 U1352 C1357 G1358 A1365 C1370 G1371 G1377 A1378 U1379 A1383 A1384 A1385 U1394 A1395 U1396 U1405 U1406 C1414 U1415 G1416 C1417 A1420 G1421 C1428 G1429 G1430 A1431 A1434 G1435 G1441 U1442 G1450 C1451 G1452 G1459 G1475 U1476 A1477 G1478

G1482 A1490 C1493 A1494 A1495 A1496 U1497 U1506 C1507 A1508 A1509 G1510 U1513 G1514 A1515 G1524 G1527 A1528 G1529 C1533 U1534 A1535 C1536 G1537 A1544 U1563 C1564 C1565 A1566 A1569 U1578 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 A1603 C1606 C1607 A1608

A1618 U1621 U1647 U1648 G1649 A1650 G1651 G1659 G1674 C1675 A1676 G1715 C1728 U1729 C1730 U1736 G1737 G1738 G1743 A1744 A1745 A1746 U1747 C1764 A1773 C1774 U1775 G1776 A1791 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1808 A1809 A1810 G1811 C1816 G1826 A1829

G1835 A1847 A1848 C1868 G1869 C1870 A1871 A1872 G1873 C1874 G1875 C1881 U1882 A1899 G1906 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 G1929 G1930 U1931 A1932 G1933 A1936 U1939 U1955 A1960 C1961 C1962 C1967 G1968 A1969 A1970 U1971 G1972 U1991 G1992 U1993 C1997 C2000

C2006 G2010 U2011 G2012 C2023 A2030 A2031 G2032 A2033 C2043 A2052 C2055 G2056 A2060 G2061 A2062 G2069 G2093 A2097 U2098 U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127

G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2186 U2187

U2188 U2189 G2190 A2191 U2192 G2193 U2194 U2195 A2198 G2204 A2211 A2225 U2233 G2234 G2238 G2239 U2243 U2244 G2251 A2268 A2273 A2274 G2279 C2283 A2287 A2288 U2291 U2292 A2297 A2298 U2299 G2304 U2305 G2308 U2312 C2313 A2314 G2315 G2316 U2321 A2322

G2323 U2324 G2325 C2326 A2327 A2328 U2329 G2330 A2333 U2334 A2335 A2336 C2339 A2340 G2345 A2346 C2347 C2350 G2375 A2376 A2377 A2378 G2379 C2380 G2383 U2384 C2385 G2389 U2390 U2402 A2406 A2425 A2435 U2441 G2445 A2448 U2449 U2457 A2469 A2476 U2477 A2478

G2481 A2482 C2483 G2484 G2485 C2486 U2491 C2498 G2502 A2503 U2504 G2505 U2514 C2515 A2516 C2517 A2518 G2525 G2529 G2532 G2535 G2536 U2537 C2538 A2542 A2547 U2552 A2566 G2567 G2576 C2579 U2580 C2591 G2592 G2595 A2598 A2602 G2603 U2604 U2605 U2609

U2613 A2614 U2615 U2629 C2646 G2663 C2683 G2688 U2689 U2690 U2698 C2699 G2714 C2715 C2716 U2720 A2726 A2727 U2728 G2729 G2732 A2733 G2744 A2748 G2751 C2752 A2757 A2765 A2778 C2788 C2789 C2793 C2794 C2795 U2796 U2797 U2798 A2799 A2800 G2808

A2809 U2818 G2819 A2820 A2821 G2822 U2832 A2835 U2845 G2848 U2849 G2857 A2860 U2861 G2867 A2873 A2879 C2880 U2884 G2885 A2886 G2890 U2891 U2898 A2899 A2900 C2901 C2902 U2903

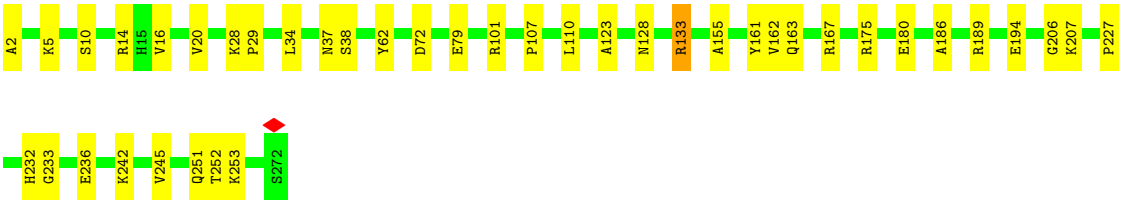
- Molecule 2: 5S rRNA

Chain B:

U1 C2 G9 G24 C31 C35 U40 G41 C42 C43 G44 U48 C49 A50 G51 A52 A53 G56 A66 A78 G79 U89 C90 G107 A108 A109 C118 A119 U120

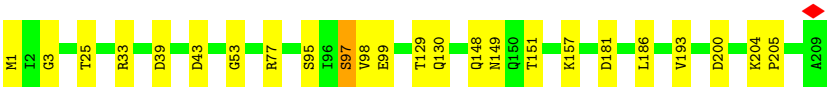
- Molecule 3: 50S ribosomal protein L2

Chain C:



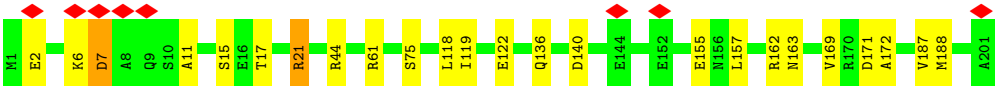
- Molecule 4: 50S ribosomal protein L3

Chain D:



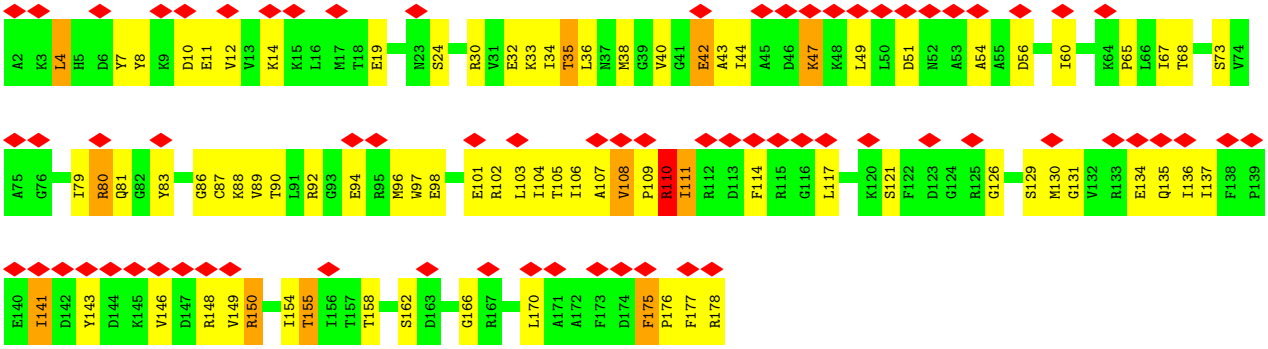
- Molecule 5: 50S ribosomal protein L4

Chain E:



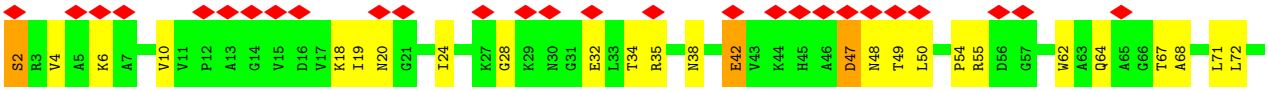
- Molecule 6: 50S ribosomal protein L5

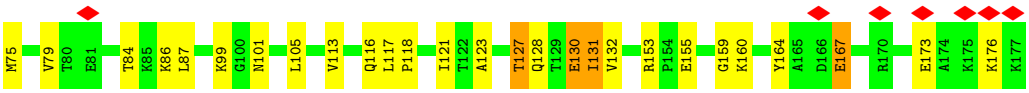
Chain F:



- Molecule 7: 50S ribosomal protein L6

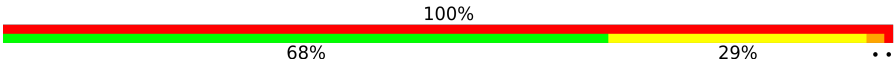
Chain G:

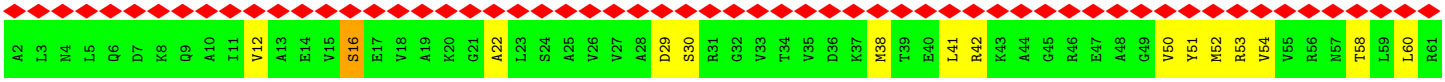


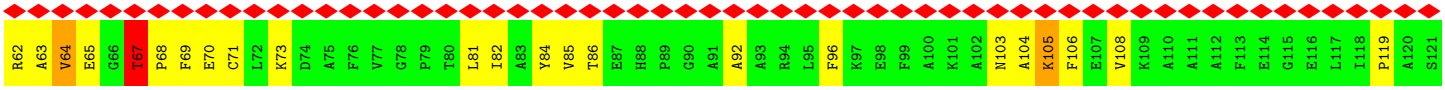


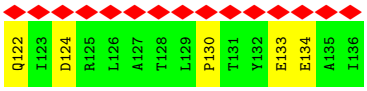
- Molecule 8: 50S ribosomal protein L10

Chain H:



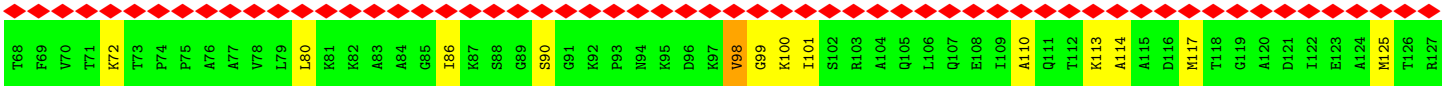


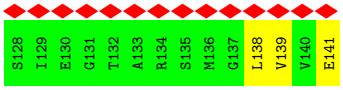




- Molecule 9: 50S ribosomal protein L11

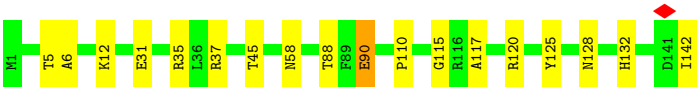
Chain I:





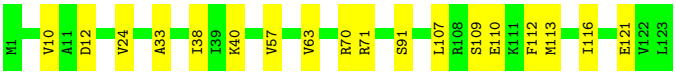
- Molecule 10: 50S ribosomal protein L13

Chain J:



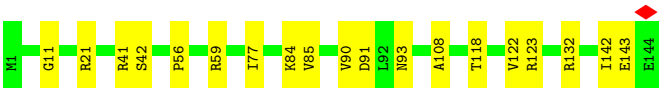
- Molecule 11: 50S ribosomal protein L14

Chain K:



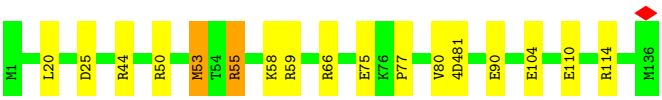
- Molecule 12: 50S ribosomal protein L15

Chain L: 87% 13%



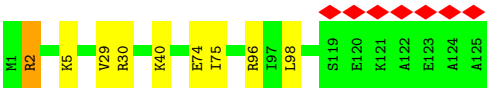
• Molecule 13: 50S ribosomal protein L16

Chain M: 88% 11%



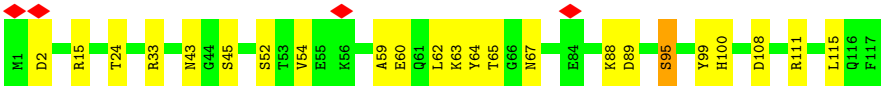
• Molecule 14: 50S ribosomal protein L17

Chain N: 6% 93% 6%



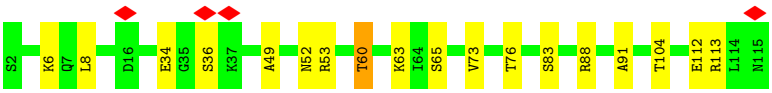
• Molecule 15: 50S ribosomal protein L18

Chain O: 80% 19%



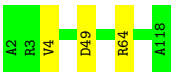
• Molecule 16: 50S ribosomal protein L19

Chain P: 84% 15%



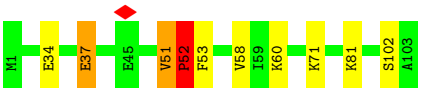
• Molecule 17: 50S ribosomal protein L20

Chain Q: 97%



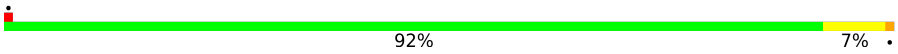
• Molecule 18: 50S ribosomal protein L21

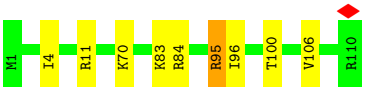
Chain R: 90% 7%



- Molecule 19: 50S ribosomal protein L22

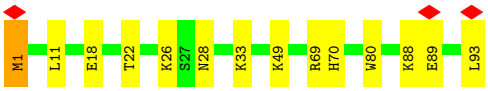
Chain S:





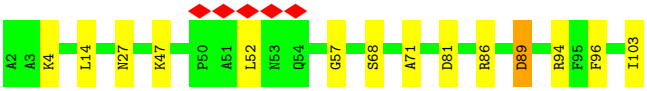
- Molecule 20: 50S ribosomal protein L23

Chain T:



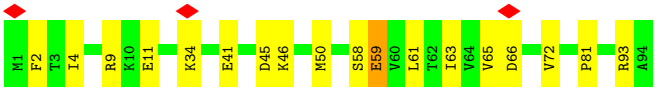
- Molecule 21: 50S ribosomal protein L24

Chain U:



- Molecule 22: 50S ribosomal protein L25

Chain V:

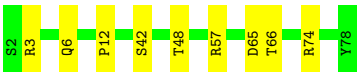


- Molecule 23: 50S ribosomal protein L27

Chain W:

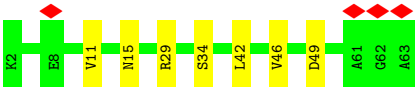
- Molecule 24: 50S ribosomal protein L28

Chain X:



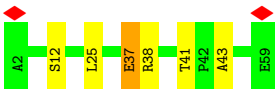
- Molecule 25: 50S ribosomal protein L29

Chain Y:

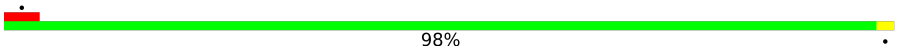


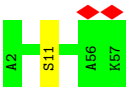
• Molecule 26: 50S ribosomal protein L30

Chain Z:

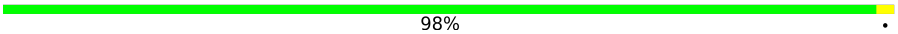


• Molecule 27: 50S ribosomal protein L32

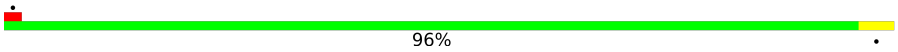
Chain a: 

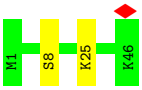


• Molecule 28: 50S ribosomal protein L33

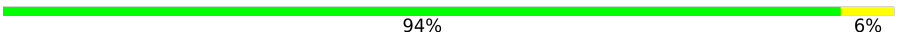
Chain b: 

• Molecule 29: 50S ribosomal protein L34

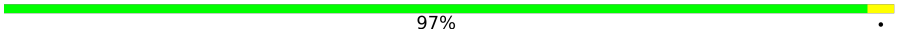
Chain c: 



• Molecule 30: 50S ribosomal protein L35

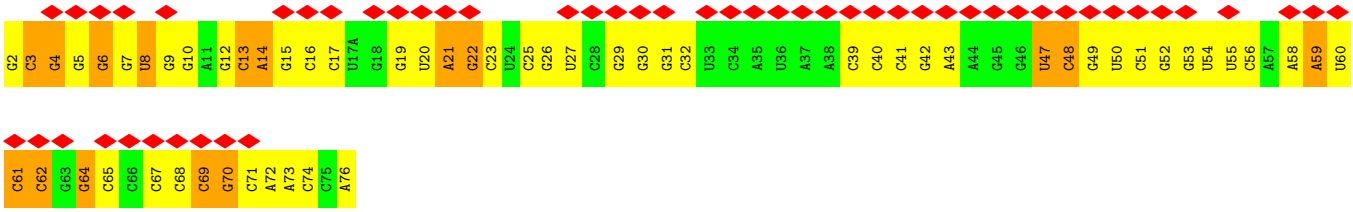
Chain d: 

• Molecule 31: 50S ribosomal protein L36

Chain e: 

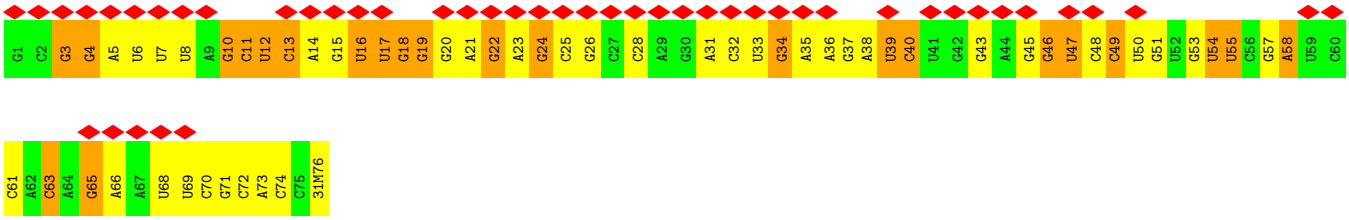
• Molecule 32: Deacylated tRNAi(Met)

Chain f: 70% 24% 55% 21%



- Molecule 33: fMet-Phe-tRNA(Phe)

Chain g: 62% 22% 47% 30%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	401905	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.709	Depositor
Minimum map value	-1.212	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DI0, PSU, OMG, 2MA, MEQ, G7M, 2MG, 4D4, MG, M2G, 4SU, 6MZ, H2U, 1MA, OMU, 1MG, 31M, YYG, 7MG, 5MC, 3TD, OMC, 5MU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.72	1/69172 (0.0%)	0.74	7/107908 (0.0%)
2	B	0.56	0/2872	0.71	0/4478
3	C	0.37	0/2122	0.46	0/2852
4	D	0.36	0/1576	0.46	0/2119
5	E	0.34	0/1571	0.44	0/2113
6	F	0.29	0/1435	0.45	0/1926
7	G	0.30	0/1343	0.46	0/1816
8	H	0.42	0/1037	0.56	0/1402
9	I	0.47	0/993	0.64	0/1341
10	J	0.37	0/1152	0.43	0/1551
11	K	0.36	0/955	0.47	0/1279
12	L	0.34	0/1062	0.47	0/1413
13	M	0.36	0/1081	0.45	0/1443
14	N	0.35	0/1006	0.44	0/1345
15	O	0.31	0/910	0.44	0/1219
16	P	0.36	0/929	0.45	0/1242
17	Q	0.40	0/960	0.38	0/1278
18	R	0.41	0/829	0.54	1/1107 (0.1%)
19	S	0.36	0/864	0.45	0/1156
20	T	0.32	0/745	0.42	0/994
21	U	0.33	0/788	0.48	1/1051 (0.1%)
22	V	0.33	0/766	0.42	0/1025
23	W	0.37	0/587	0.44	0/776
24	X	0.37	0/635	0.46	0/848
25	Y	0.27	0/502	0.37	0/667
26	Z	0.31	0/453	0.44	0/605
27	a	0.35	0/450	0.45	0/599
28	b	0.32	0/421	0.44	0/561
29	c	0.34	0/380	0.43	0/498
30	d	0.38	0/513	0.46	0/676
31	e	0.35	0/303	0.44	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	f	0.80	4/1725 (0.2%)	1.72	77/2689 (2.9%)
33	g	0.68	1/1458 (0.1%)	1.38	33/2272 (1.5%)
All	All	0.64	6/101595 (0.0%)	0.73	119/152646 (0.1%)

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
18	R	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	59	A	O3'-P	-6.50	1.53	1.61
32	f	39	C	O3'-P	-6.25	1.53	1.61
32	f	12	G	O3'-P	-6.06	1.53	1.61
32	f	25	C	O3'-P	-6.00	1.53	1.61
1	A	1774	C	O3'-P	-5.19	1.54	1.61

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	62	C	N1-C1'-C2'	-11.72	98.76	114.00
32	f	30	G	N9-C1'-C2'	-10.75	100.03	114.00
33	g	13	C	C4'-C3'-O3'	9.83	132.66	113.00
33	g	13	C	N1-C1'-C2'	-9.76	101.27	112.00
33	g	24	G	N9-C1'-C2'	-9.75	101.28	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	51	VAL	Mainchain

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	A	62252	0	31324	392	0
2	B	2569	0	1301	13	0
3	C	2083	0	2154	22	0
4	D	1566	0	1617	14	0
5	E	1552	0	1619	13	0
6	F	1411	0	1444	95	0
7	G	1323	0	1371	31	0
8	H	1023	0	1052	36	0
9	I	979	0	1028	30	0
10	J	1129	0	1162	10	0
11	K	946	0	1023	10	0
12	L	1053	0	1129	12	0
13	M	1075	0	1155	10	0
14	N	993	0	1034	6	0
15	O	900	0	935	18	0
16	P	917	0	962	10	0
17	Q	947	0	1019	3	0
18	R	816	0	839	7	0
19	S	857	0	922	5	0
20	T	739	0	807	14	0
21	U	780	0	830	7	0
22	V	753	0	780	11	0
23	W	580	0	593	5	0
24	X	625	0	652	4	0
25	Y	501	0	531	3	0
26	Z	449	0	487	3	0
27	a	444	0	458	0	0
28	b	414	0	442	0	0
29	c	377	0	418	0	0
30	d	504	0	572	0	0
31	e	302	0	343	0	0
32	f	1625	0	829	0	0
33	g	1667	0	880	0	0
34	A	174	0	0	0	0
34	B	3	0	0	0	0
34	U	1	0	0	0	0
35	A	58	0	0	1	0
36	A	498	0	0	13	0
36	B	9	0	0	0	0
36	C	7	0	0	1	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	L	6	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	d	4	0	0	0	0
All	All	94915	0	61712	730	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 730 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)
1:A:883:G:N2	1:A:894:U:O2	1.56	1.37
1:A:1:G:N2	1:A:2902:C:O2	1.64	1.30
9:I:98:VAL:O	9:I:138:LEU:HD23	1.22	1.25
1:A:1:G:N1	1:A:2902:C:N3	1.92	1.17
1:A:1050:A:N3	1:A:2751:G:C2	2.13	1.17

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
3	C	269/271 (99%)	265 (98%)	4 (2%)	0	100 100
4	D	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	29 26
5	E	199/201 (99%)	197 (99%)	2 (1%)	0	100 100
6	F	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	25 21
7	G	174/176 (99%)	168 (97%)	5 (3%)	1 (1%)	25 21
8	H	133/135 (98%)	109 (82%)	18 (14%)	6 (4%)	2 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	4	1
10	J	140/142 (99%)	140 (100%)	0	0	100	100
11	K	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
12	L	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
13	M	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
14	N	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
15	O	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
16	P	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
17	Q	115/117 (98%)	115 (100%)	0	0	100	100
18	R	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	15	11
19	S	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	T	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
21	U	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
22	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	W	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
24	X	75/77 (97%)	75 (100%)	0	0	100	100
25	Y	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	Z	56/58 (97%)	56 (100%)	0	0	100	100
27	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
28	b	49/51 (96%)	49 (100%)	0	0	100	100
29	c	44/46 (96%)	44 (100%)	0	0	100	100
30	d	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	e	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3291/3351 (98%)	3184 (97%)	93 (3%)	14 (0%)	38	32

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	104	ALA
8	H	106	PHE
9	I	15	ALA
9	I	19	ASN
18	R	52	PRO

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	
3	C	216/216 (100%)	213 (99%)	3 (1%)	67	73
4	D	163/163 (100%)	160 (98%)	3 (2%)	59	65
5	E	165/165 (100%)	158 (96%)	7 (4%)	30	30
6	F	148/148 (100%)	127 (86%)	21 (14%)	3	1
7	G	137/137 (100%)	125 (91%)	12 (9%)	10	6
8	H	103/103 (100%)	97 (94%)	6 (6%)	20	17
9	I	104/104 (100%)	102 (98%)	2 (2%)	57	63
10	J	116/116 (100%)	112 (97%)	4 (3%)	37	39
11	K	104/104 (100%)	102 (98%)	2 (2%)	57	63
12	L	103/103 (100%)	101 (98%)	2 (2%)	57	63
13	M	108/108 (100%)	104 (96%)	4 (4%)	34	35
14	N	102/102 (100%)	101 (99%)	1 (1%)	76	82
15	O	87/87 (100%)	85 (98%)	2 (2%)	50	55
16	P	99/99 (100%)	93 (94%)	6 (6%)	18	16
17	Q	89/89 (100%)	89 (100%)	0	100	100
18	R	84/84 (100%)	82 (98%)	2 (2%)	49	53
19	S	93/93 (100%)	91 (98%)	2 (2%)	52	57
20	T	80/80 (100%)	77 (96%)	3 (4%)	33	34
21	U	83/83 (100%)	79 (95%)	4 (5%)	25	24
22	V	78/78 (100%)	76 (97%)	2 (3%)	46	50
23	W	57/58 (98%)	56 (98%)	1 (2%)	59	65
24	X	67/67 (100%)	65 (97%)	2 (3%)	41	44
25	Y	54/54 (100%)	52 (96%)	2 (4%)	34	35
26	Z	48/48 (100%)	46 (96%)	2 (4%)	30	30
27	a	47/47 (100%)	46 (98%)	1 (2%)	53	59
28	b	45/46 (98%)	44 (98%)	1 (2%)	52	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	c	38/38 (100%)	36 (95%)	2 (5%)	22	20
30	d	51/51 (100%)	47 (92%)	4 (8%)	12	9
31	e	34/34 (100%)	33 (97%)	1 (3%)	42	46
All	All	2703/2705 (100%)	2599 (96%)	104 (4%)	36	34

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	142	ILE
16	P	60	THR
30	d	15	LYS
11	K	109	SER
13	M	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
21	U	46	GLN
29	c	29	GLN
25	Y	58	ASN
15	O	100	HIS
21	U	27	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2888/2897 (99%)	382 (13%)	16 (0%)
2	B	119/120 (99%)	7 (5%)	0
32	f	75/76 (98%)	31 (41%)	0
33	g	74/76 (97%)	48 (64%)	0
All	All	3156/3169 (99%)	468 (14%)	16 (0%)

5 of 468 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	15	G
1	A	34	U
1	A	45	G

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Mol	Chain	Res	Type
1	A	46	G

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2193	G
1	A	2158	A
1	A	1535	A
1	A	2130	U
1	A	1494	A

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

45 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
33	5MU	g	54	33	19,22,23	1.54	3 (15%)	28,32,35	2.42	7 (25%)
33	1MA	g	58	33	16,25,26	1.65	5 (31%)	18,37,40	2.30	5 (27%)
1	PSU	A	2457	1	18,21,22	2.46	8 (44%)	22,30,33	1.90	4 (18%)
1	PSU	A	955	1	18,21,22	2.44	8 (44%)	22,30,33	1.85	4 (18%)
1	5MC	A	1962	1	18,22,23	2.01	6 (33%)	26,32,35	1.16	2 (7%)
33	H2U	g	17	33	18,21,22	1.01	2 (11%)	21,30,33	3.29	5 (23%)
33	M2G	g	26	33	20,27,28	1.57	3 (15%)	22,40,43	1.06	2 (9%)
33	5MC	g	40	33	18,22,23	1.27	1 (5%)	26,32,35	2.12	10 (38%)
1	2MA	A	2503	1,34	17,25,26	1.59	3 (17%)	17,37,40	1.04	2 (11%)
33	H2U	g	16	33	18,21,22	0.99	2 (11%)	21,30,33	1.90	2 (9%)
1	5MU	A	1939	1	19,22,23	2.67	7 (36%)	28,32,35	3.95	10 (35%)
33	7MG	g	46	33	22,26,27	2.13	4 (18%)	29,39,42	3.15	10 (34%)
1	H2U	A	2449	1	18,21,22	4.07	5 (27%)	21,30,33	5.20	7 (33%)
33	31M	g	76	1	38,44,45	4.34	18 (47%)	38,61,64	2.23	13 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	PSU	A	1917	1	18,21,22	2.32	8 (44%)	22,30,33	1.82	4 (18%)
1	5MU	A	747	1	19,22,23	2.58	7 (36%)	28,32,35	3.81	11 (39%)
1	OMG	A	2251	32,1	18,26,27	2.46	5 (27%)	19,38,41	1.15	3 (15%)
33	OMC	g	32	33	19,22,23	1.39	3 (15%)	26,31,34	2.13	2 (7%)
32	5MU	f	54	32	19,22,23	1.65	3 (15%)	28,32,35	2.93	11 (39%)
1	PSU	A	2504	1	18,21,22	2.39	8 (44%)	22,30,33	1.89	4 (18%)
1	PSU	A	2604	1	18,21,22	2.40	8 (44%)	22,30,33	1.87	4 (18%)
1	6MZ	A	2030	1	18,25,26	1.98	1 (5%)	16,36,39	2.59	4 (25%)
13	4D4	M	81	13	9,11,12	2.03	2 (22%)	8,13,15	2.10	4 (50%)
1	PSU	A	2580	1	18,21,22	2.47	10 (55%)	22,30,33	1.90	5 (22%)
32	5MC	f	32	32	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)
1	2MG	A	1835	1	18,26,27	3.37	7 (38%)	16,38,41	1.35	3 (18%)
32	PSU	f	55	32	18,21,22	1.31	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	A	1911	1	18,21,22	2.32	8 (44%)	22,30,33	1.84	4 (18%)
33	2MG	g	10	33	18,26,27	1.53	3 (16%)	16,38,41	1.64	4 (25%)
33	PSU	g	39	33	18,21,22	1.84	5 (27%)	22,30,33	2.49	7 (31%)
1	G7M	A	2069	1	20,26,27	2.24	5 (25%)	17,39,42	0.71	0
33	YYG	g	37	33	31,42,43	2.16	7 (22%)	33,62,65	2.03	10 (30%)
4	MEQ	D	150[A]	4	8,9,10	0.95	0	5,10,12	0.66	0
33	OMG	g	34	33	18,26,27	1.57	3 (16%)	19,38,41	1.52	4 (21%)
1	OMU	A	2552	1	19,22,23	2.68	7 (36%)	26,31,34	1.86	6 (23%)
33	PSU	g	55	33	18,21,22	2.22	6 (33%)	22,30,33	2.47	8 (36%)
1	3TD	A	1915	1	18,22,23	6.42	12 (66%)	22,32,35	1.93	4 (18%)
32	4SU	f	8	32	18,21,22	3.20	5 (27%)	26,30,33	3.64	10 (38%)
1	2MG	A	2445	1	18,26,27	3.39	7 (38%)	16,38,41	1.30	3 (18%)
33	5MC	g	49	33	18,22,23	1.07	2 (11%)	26,32,35	1.72	4 (15%)
1	PSU	A	2605	1	18,21,22	2.39	8 (44%)	22,30,33	1.87	4 (18%)
1	1MG	A	745	1	18,26,27	2.80	4 (22%)	19,39,42	1.28	3 (15%)
1	OMC	A	2498	1,34	19,22,23	1.90	6 (31%)	26,31,34	0.96	1 (3%)
1	PSU	A	746	1,34	18,21,22	2.37	9 (50%)	22,30,33	1.80	4 (18%)
1	6MZ	A	1618	1	18,25,26	1.98	1 (5%)	16,36,39	2.19	4 (25%)

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
33	5MU	g	54	33	-	2/7/25/26	0/2/2/2
33	1MA	g	58	33	-	2/3/25/26	0/3/3/3
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
33	H2U	g	17	33	-	5/7/38/39	0/2/2/2
33	M2G	g	26	33	-	0/7/29/30	0/3/3/3
33	5MC	g	40	33	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	1,34	-	1/3/25/26	0/3/3/3
33	H2U	g	16	33	-	3/7/38/39	0/2/2/2
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
33	7MG	g	46	33	-	3/7/37/38	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
33	31M	g	76	1	-	6/27/49/50	0/4/4/4
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	A	747	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	32,1	-	1/5/27/28	0/3/3/3
33	OMC	g	32	33	-	0/9/27/28	0/2/2/2
32	5MU	f	54	32	-	1/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	2/5/27/28	0/3/3/3
13	4D4	M	81	13	-	3/11/12/14	-
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
32	5MC	f	32	32	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
32	PSU	f	55	32	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
33	2MG	g	10	33	-	0/5/27/28	0/3/3/3
33	PSU	g	39	33	-	3/7/25/26	0/2/2/2
1	G7M	A	2069	1	-	1/3/25/26	0/3/3/3
33	YYG	g	37	33	-	16/20/42/43	0/3/4/4
4	MEQ	D	150[A]	4	-	4/8/9/11	-
33	OMG	g	34	33	-	3/5/27/28	0/3/3/3
1	OMU	A	2552	1	-	0/9/27/28	0/2/2/2
33	PSU	g	55	33	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	0/7/25/26	0/2/2/2
32	4SU	f	8	32	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	5MC	g	49	33	-	3/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	OMC	A	2498	1,34	-	0/9/27/28	0/2/2/2
1	PSU	A	746	1,34	-	2/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3

The worst 5 of 239 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	C2'-C1'	-18.07	1.30	1.53
33	g	76	31M	C2'-C1'	-16.92	1.28	1.53
1	A	1915	3TD	O4'-C1'	14.21	1.63	1.43
33	g	76	31M	O4'-C1'	12.06	1.57	1.41
1	A	2449	H2U	O4-C4	10.10	1.43	1.23

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2449	H2U	C4-N3-C2	-15.23	113.16	125.79
33	g	17	H2U	C4-N3-C2	-13.77	114.37	125.79
1	A	2449	H2U	O2-C2-N1	-11.49	108.68	123.11
33	g	46	7MG	N9-C4-N3	10.82	141.66	125.47
32	f	8	4SU	C4-N3-C2	-10.44	117.20	127.34

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	150[A]	MEQ	N-CA-CB-CG
13	M	81	4D4	NE-CD-CG-CB
1	A	746	PSU	C2'-C1'-C5-C4
1	A	2251	OMG	C1'-C2'-O2'-CM2
33	g	17	H2U	O4'-C1'-N1-C6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1939	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2251	OMG	1	0
1	A	2604	PSU	1	0
1	A	2030	6MZ	2	0
1	A	1915	3TD	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 179 ligands modelled in this entry, 178 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	$\#\|Z\| > 2$
35	DI0	A	3175	-	58,61,61	1.62	11 (18%)	77,92,92	1.65	20 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DI0	A	3175	-	-	10/70/121/121	0/3/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3175	DI0	CAF-CAE	-5.60	1.39	1.51
35	A	3175	DI0	OBI-CAG	-4.12	1.33	1.43
35	A	3175	DI0	OAU-CBG	-3.41	1.38	1.44
35	A	3175	DI0	OAY-CAC	-3.13	1.35	1.43
35	A	3175	DI0	CBC-CBB	2.86	1.58	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	3175	DI0	OAL-CAW-CBT	4.88	116.70	107.40
35	A	3175	DI0	CBT-CAW-CAD	-4.69	106.31	115.20
35	A	3175	DI0	OBK-CAN-CAX	4.22	110.07	103.81
35	A	3175	DI0	CAP-CAH-CAJ	-3.35	109.30	114.05
35	A	3175	DI0	CBR-CAP-CBC	-2.75	106.45	111.09

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	3175	DI0	NAQ-CBA-CBS-OBW
35	A	3175	DI0	NAQ-CAK-CBB-CBC
35	A	3175	DI0	CAJ-CAH-CAP-OBJ
35	A	3175	DI0	OBX-CCC-CCD-OBW
35	A	3175	DI0	OAL-CAW-CBT-CCF

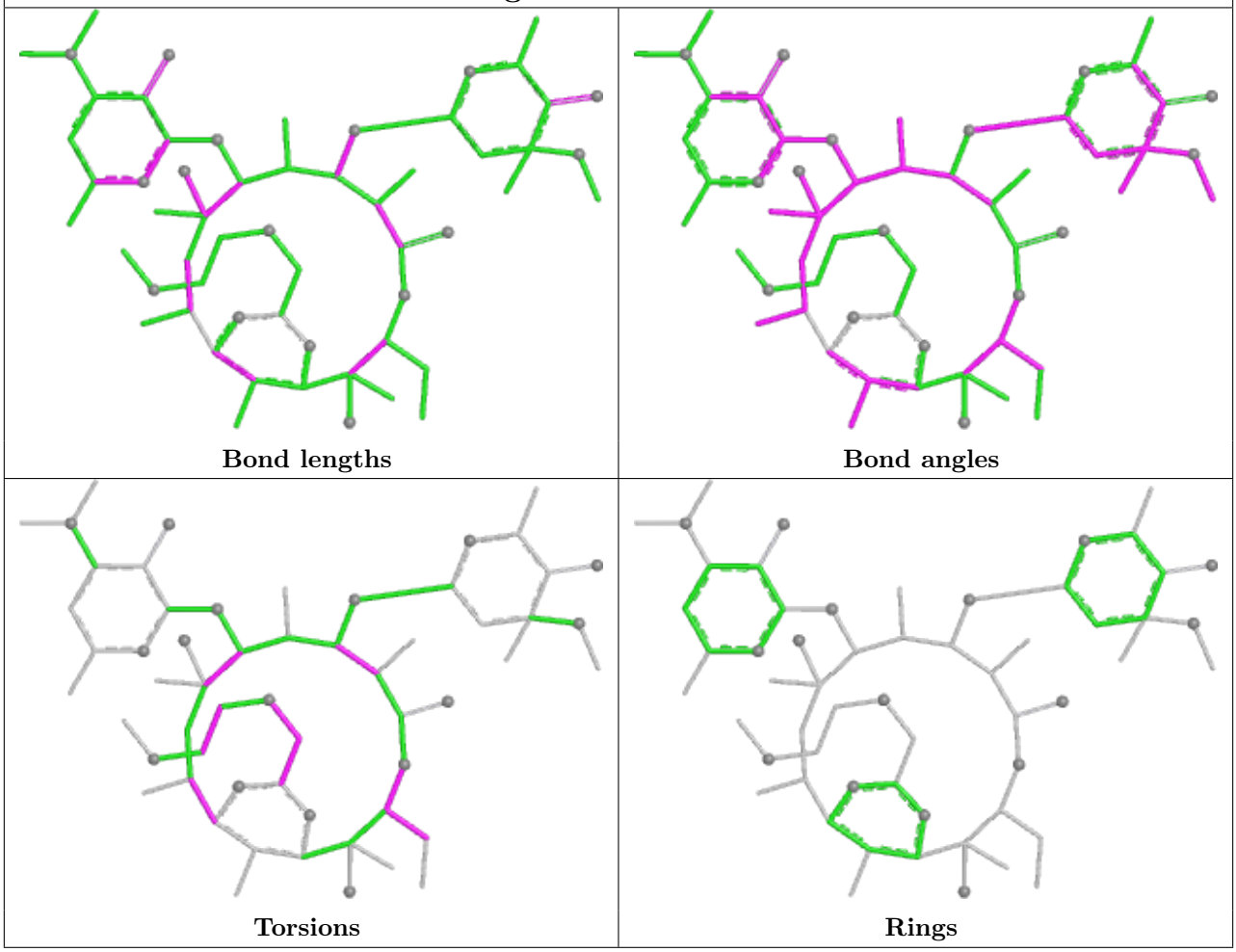
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	3175	DI0	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 DI0 A 3175



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
33	g	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	885:C	O3'	892:A	P	11.25
1	A	1915:3TD	O3'	1916:A	P	1.31

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	g	75:C	O3'	76:31M	P	1.09

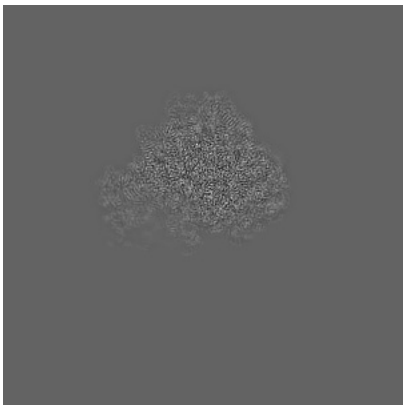
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10655. These allow visual inspection of the internal detail of the map and identification of artifacts.

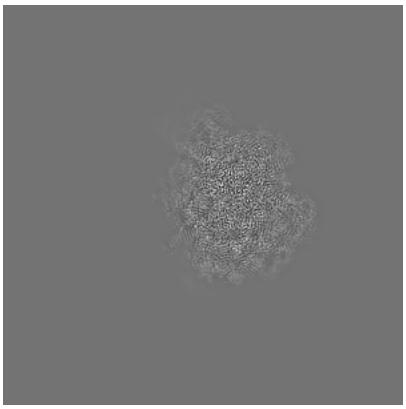
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

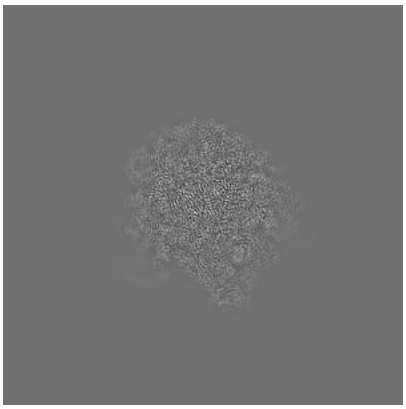
6.1.1 Primary map



X

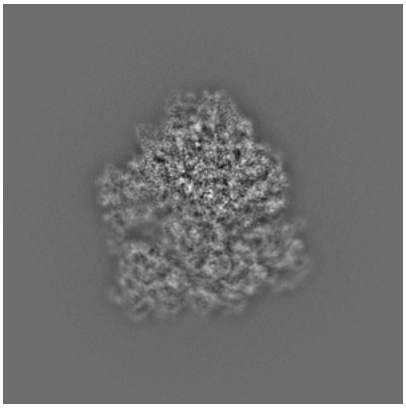


Y

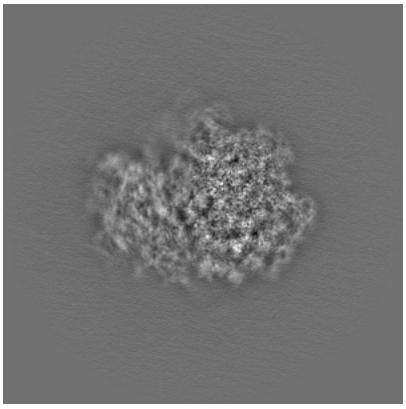


Z

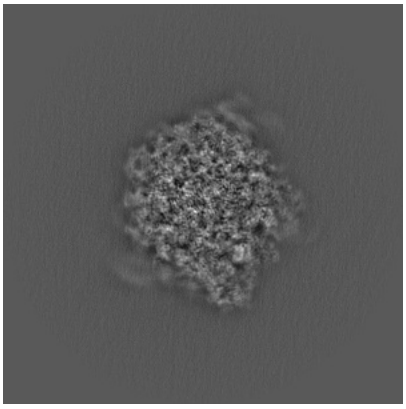
6.1.2 Raw map



X



Y



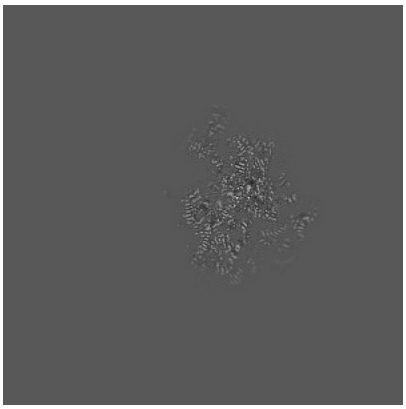
Z

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

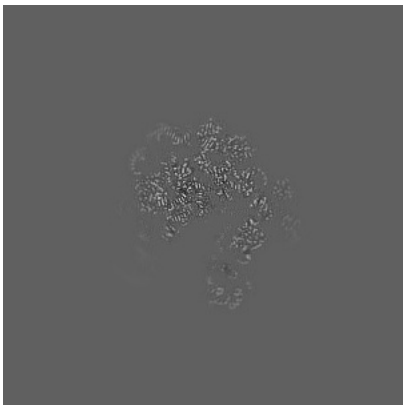
6.2 Central slices (i)

6.2.1 Primary map

X Index: 256

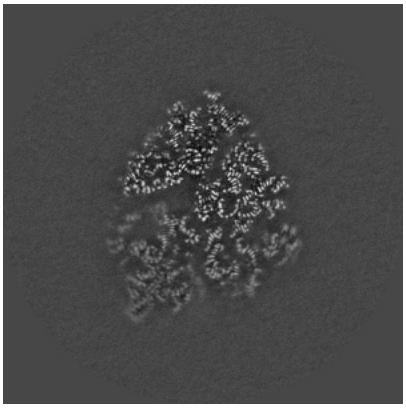


Y Index: 256

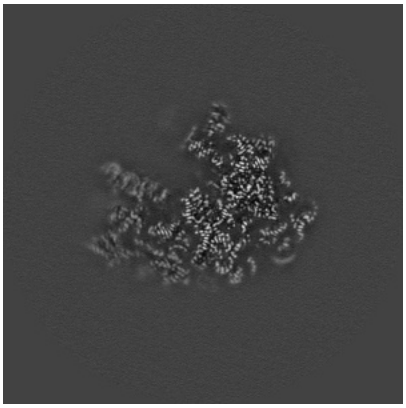


Z Index: 256

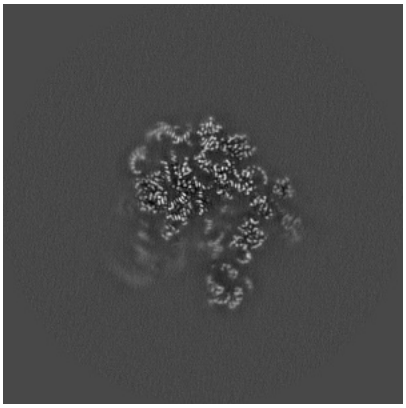
6.2.2 Raw map



X Index: 256



Y Index: 256



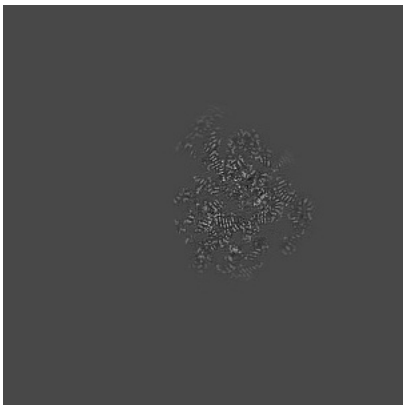
Z Index: 256

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

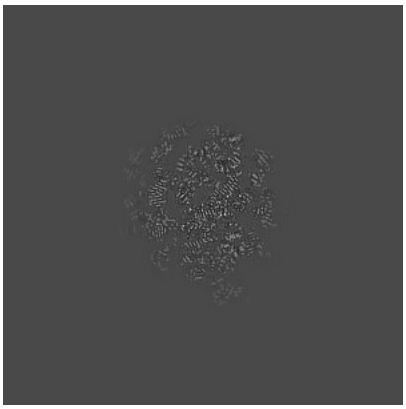
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 274

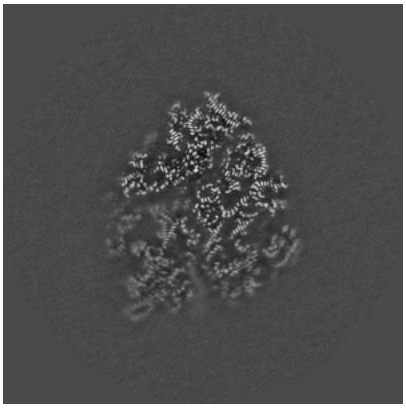


Y Index: 267

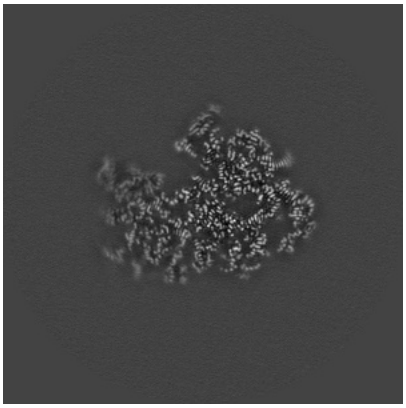


Z Index: 297

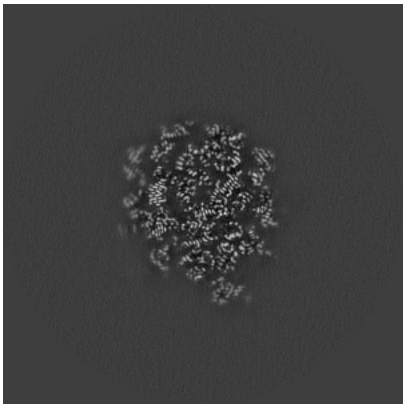
6.3.2 Raw map



X Index: 259



Y Index: 271



Z Index: 297

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 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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.

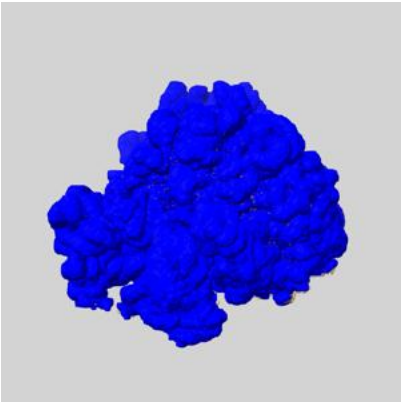
6.5 Mask visualisation (i)

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

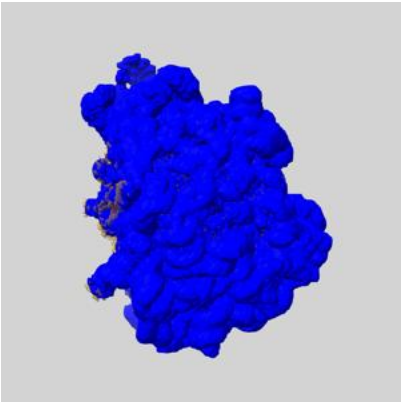
A mask typically either:

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

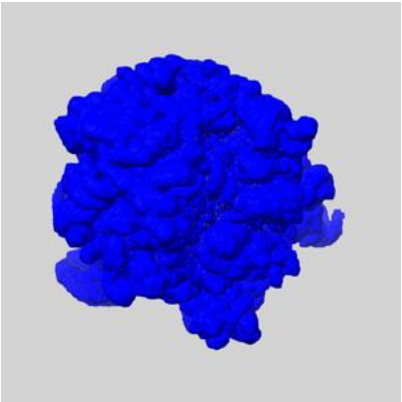
6.5.1 emd_10655_msk_1.map (i)



X



Y

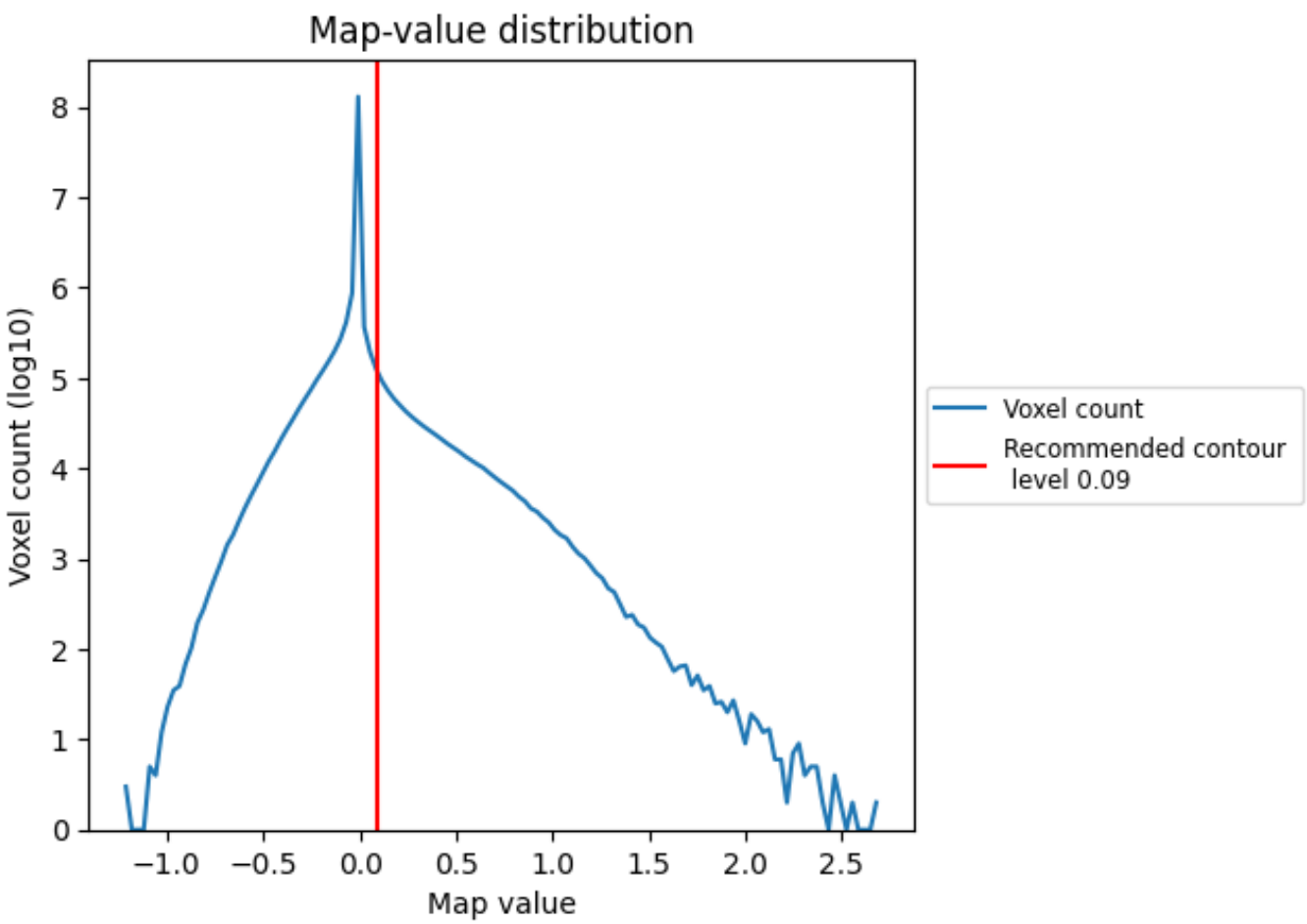


Z

7 Map analysis (i)

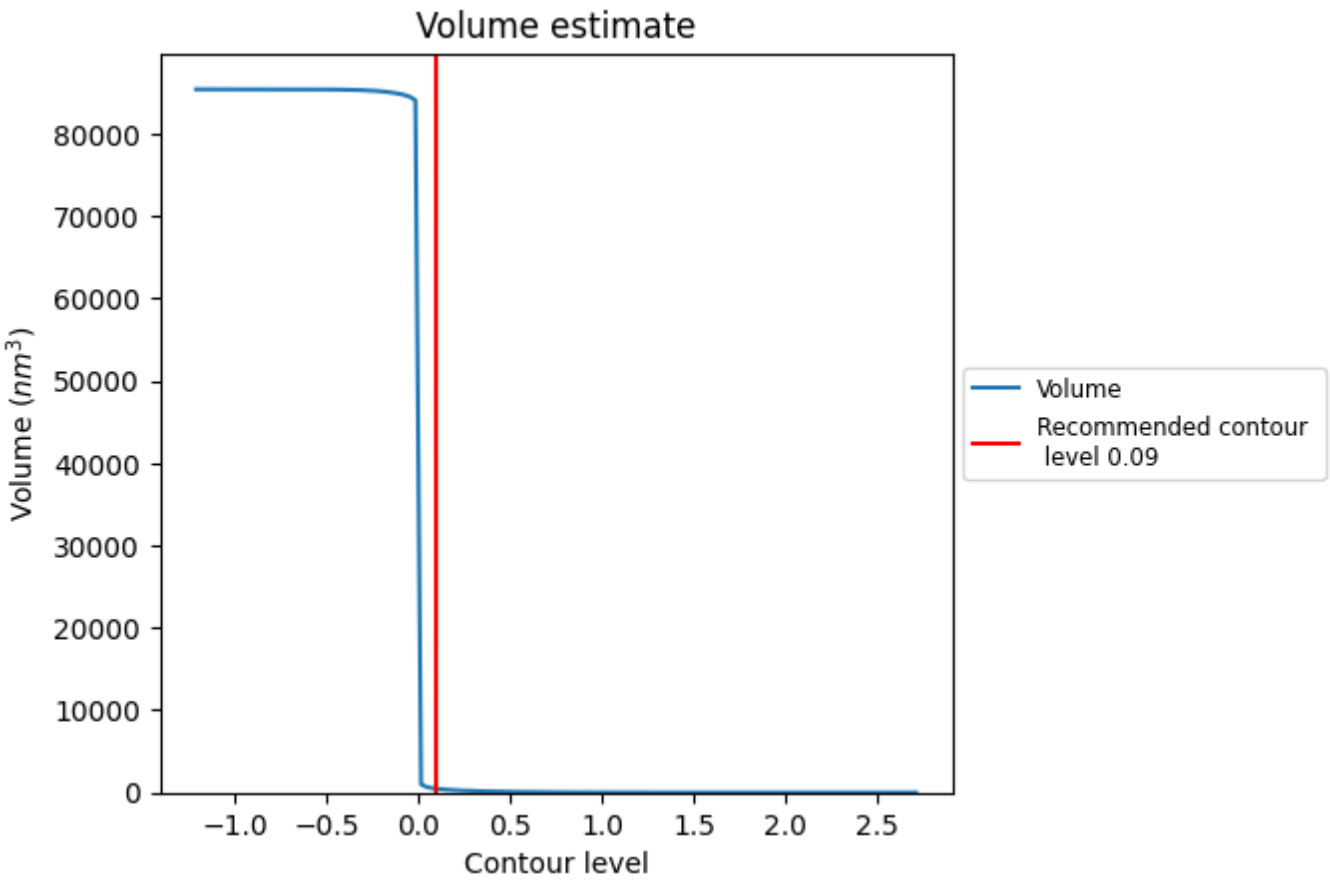
This section contains the results of statistical analysis of the map.

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.

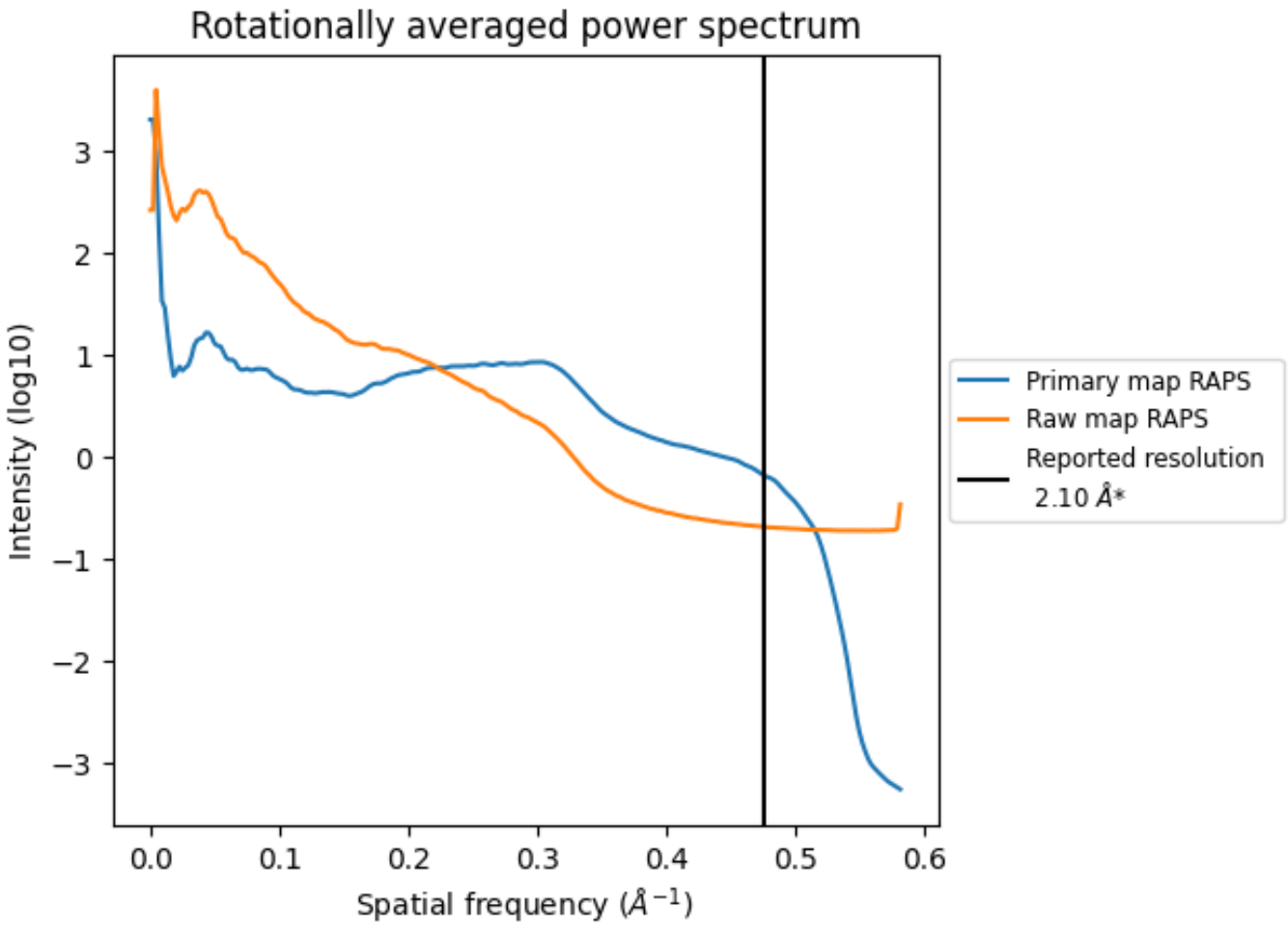
7.2 Volume estimate (i)



The volume at the recommended contour level is 487 nm^3; this corresponds to an approximate mass of 440 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)

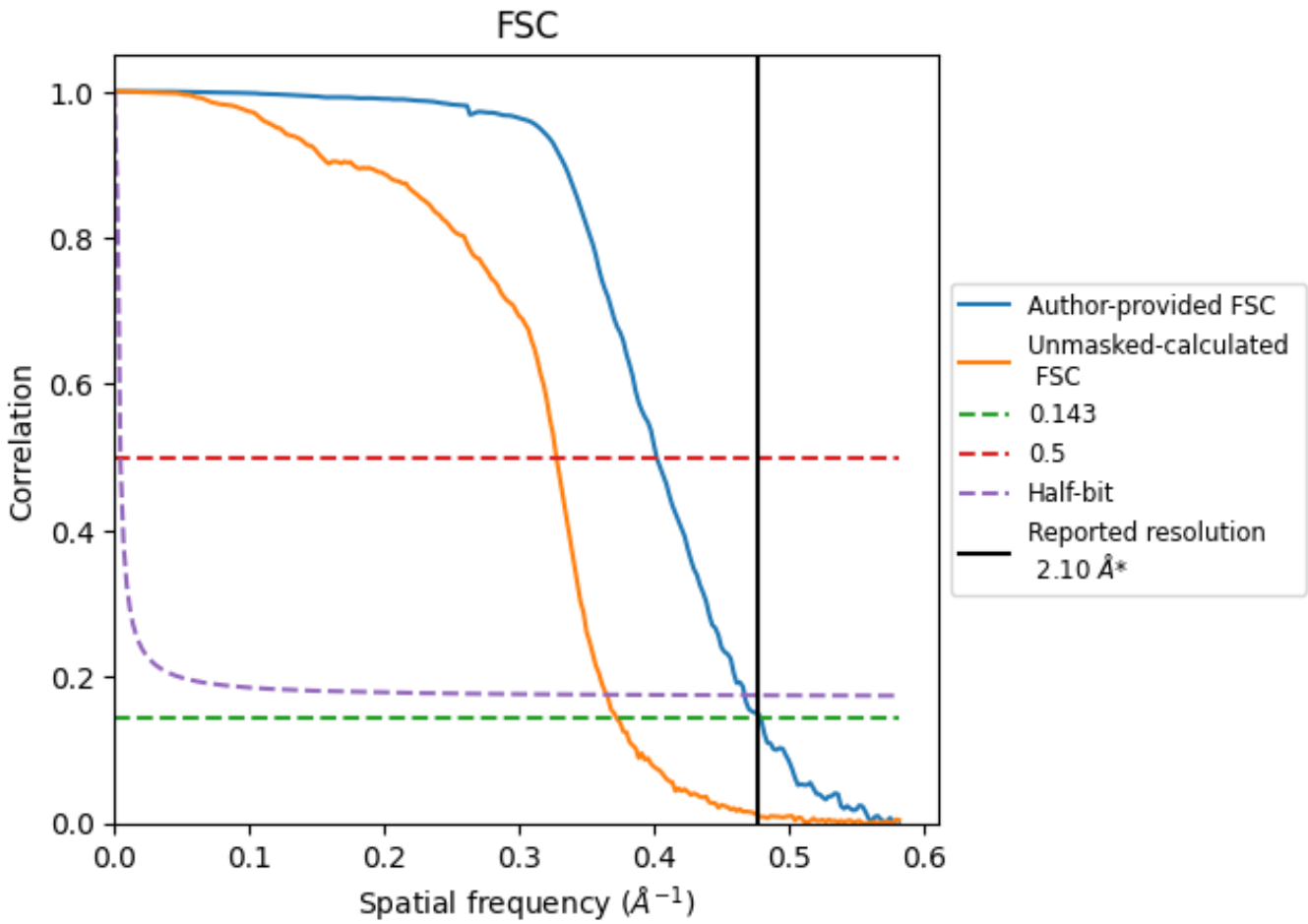


*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8.2 Resolution estimates (i)

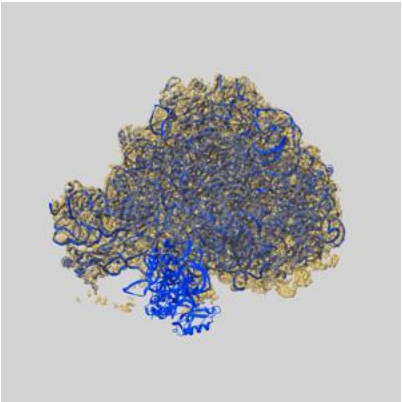
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.09	2.49	2.14
Unmasked-calculated*	2.69	3.05	2.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.69 differs from the reported value 2.1 by more than 10 %

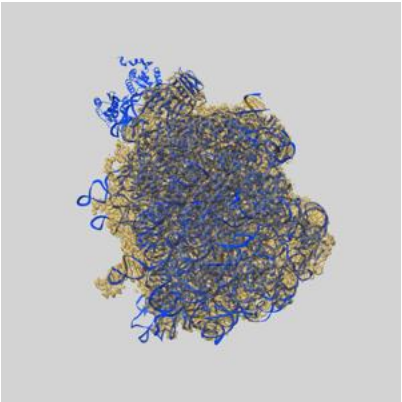
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10655 and PDB model 6XZ7. Per-residue inclusion information can be found in section 3 on page 12.

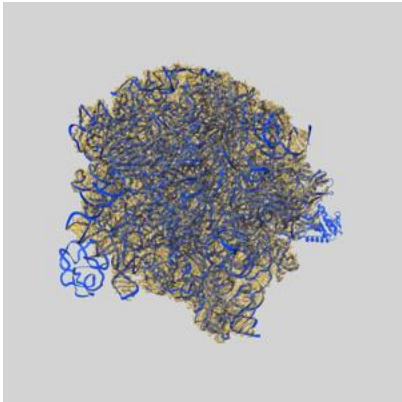
9.1 Map-model overlay (i)



X



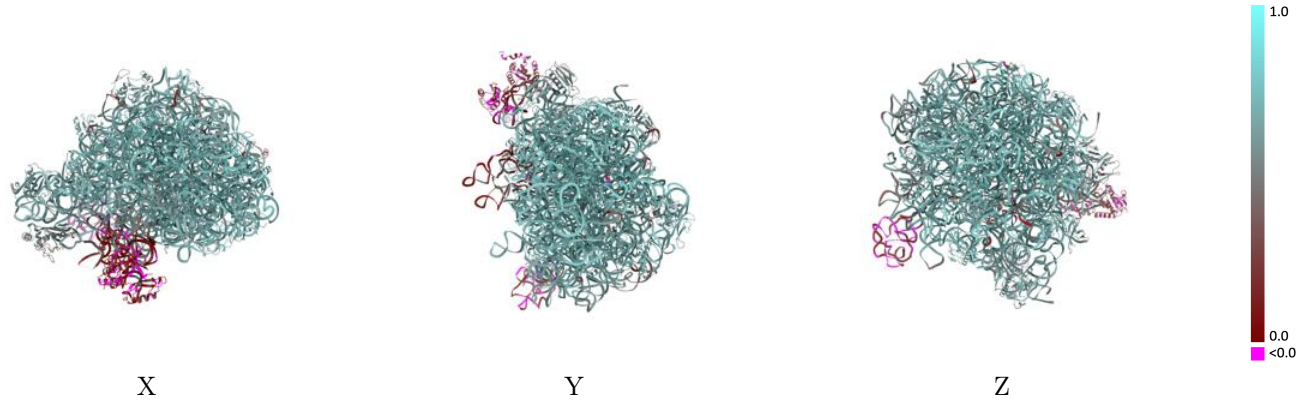
Y



Z

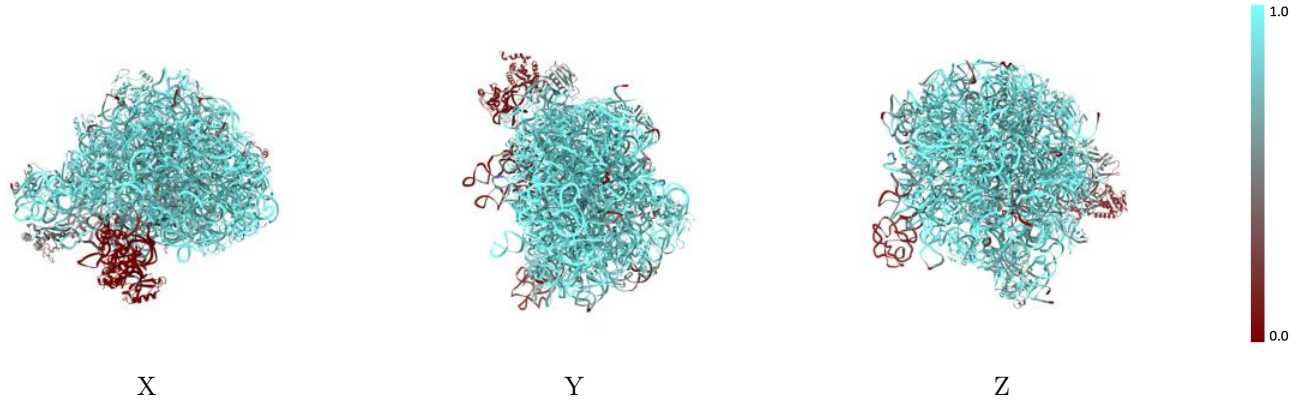
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



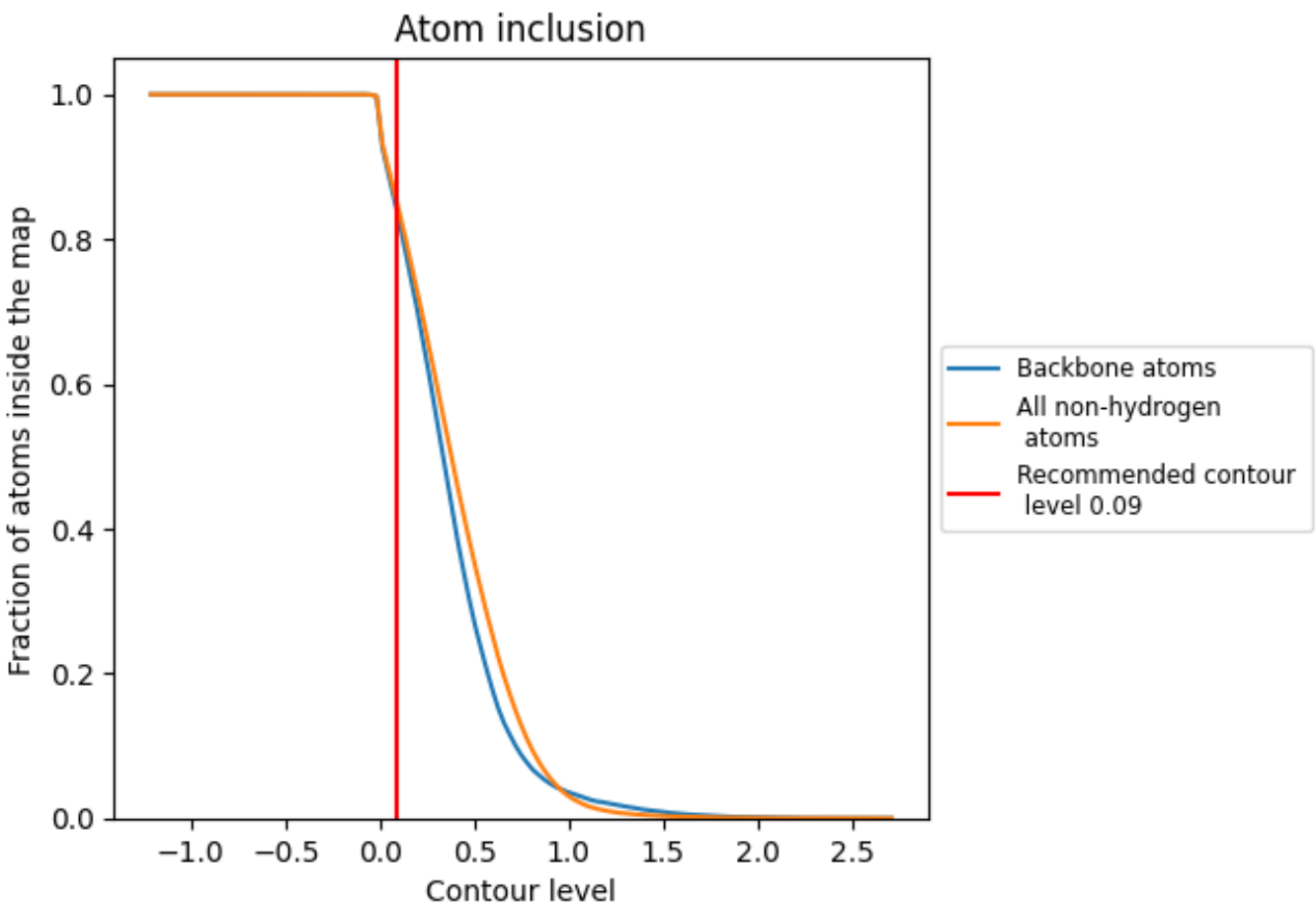
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8517	0.6430
A	0.9028	0.6720
B	0.9086	0.6460
C	0.9499	0.7170
D	0.9344	0.7080
E	0.8783	0.6770
F	0.4672	0.4930
G	0.6222	0.5550
H	0.0000	0.1280
I	0.0000	0.0590
J	0.9373	0.7070
K	0.9338	0.7020
L	0.9277	0.6990
M	0.9406	0.7050
N	0.9257	0.7040
O	0.8060	0.6160
P	0.8930	0.6750
Q	0.9659	0.7490
R	0.8821	0.6700
S	0.9222	0.7070
T	0.8728	0.6540
U	0.8440	0.6310
V	0.8442	0.6340
W	0.9220	0.6990
X	0.9351	0.6880
Y	0.7975	0.6110
Z	0.8970	0.6860
a	0.9182	0.7040
b	0.8448	0.6480
c	0.9577	0.7370
d	0.9776	0.7360
e	0.9486	0.6900
f	0.2320	0.2270
g	0.2573	0.2550