wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 05:04 pm GMT

PDB ID	:	7BL5
EMDB ID	:	EMD-12218
Title	:	pre-50S-ObgE particle
Authors	:	Hilal, T.; Nikolay, R.; Spahn, C.M.T.; Schmidt, S.
Deposited on	:	2021-01-18
Resolution	:	3.30 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 (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:

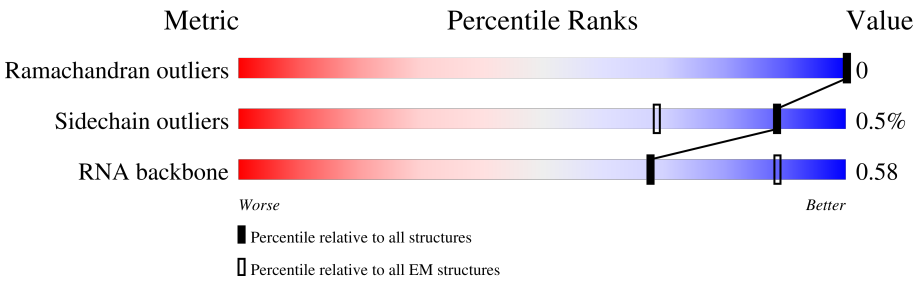
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	273	9%, 99%, .
2	D	209	9%, 100%
3	E	201	19%, 99%, .
4	G	177	44%, 97%, .
5	J	142	10%, 99%, .
6	L	144	22%, 99%, .
7	N	127	., 94%, 6%
8	O	117	45%, 99%, .

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Mol	Chain	Length	Quality of chain
9	Q	118	8% 99%
10	R	103	9% 100%
11	S	110	9% 100%
12	T	100	14% 93% 7%
13	U	104	13% 98%
14	V	94	40% 100%
15	W	85	15% 89% 11%
16	X	78	10% 97%
17	Y	63	25% 100%
18	Z	59	7% 98%
19	0	57	14% 98%
20	1	55	53% 91% 9%
21	2	46	11% 98%
22	B	120	16% 84% 15%
23	I	142	97% 98%
24	K	123	8% 99%
25	P	115	15% 98%
26	6	105	41% 97%
27	7	326	78% 96%
28	8	183	43% 85% 14%
29	9	390	43% 86% 13%
30	M	136	93% 100%
31	A	2919	8% 83% 17%
32	H	149	81% 99%
33	e	165	79% 79% 21%

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Mol	Chain	Length	Quality of chain
34	F	179	75% 98%
35	b	70	61% 67% 33%

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 98927 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 L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	171	1281	806	235	238	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L13.

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

- Molecule 6 is a protein called 50S ribosomal protein L15.

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

- Molecule 7 is a protein called 50S ribosomal protein L17.

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

- Molecule 8 is a protein called 50S ribosomal protein L18.

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

- Molecule 9 is a protein called 50S ribosomal protein L20.

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

- Molecule 10 is a protein called 50S ribosomal protein L21.

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

- Molecule 11 is a protein called 50S ribosomal protein L22.

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

- Molecule 12 is a protein called 50S ribosomal protein L23.

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

- Molecule 13 is a protein called 50S ribosomal protein L24.

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

- Molecule 14 is a protein called 50S ribosomal protein L25.

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

- Molecule 15 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	W	76	575	356	117	101	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L28.

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

- Molecule 17 is a protein called 50S ribosomal protein L29.

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

- Molecule 18 is a protein called 50S ribosomal protein L30.

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

- Molecule 19 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	0	56	444	269	94	80	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	1	50	409	263	75	71	0	0

- Molecule 21 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	2	46	377	228	90	57	2	0	0

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	B	119	2548	1135	466	829	118	0	0

- Molecule 23 is a protein called 50S ribosomal protein L11.

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

- Molecule 24 is a protein called 50S ribosomal protein L14.

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

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	P	113	911	571	178	161	1	0	0

- Molecule 26 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	6	102	780	485	133	157	5	0	0

- Molecule 27 is a protein called Ribosomal large subunit pseudouridine synthase D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	7	317	2533	1593	471	457	12	0	0

- Molecule 28 is a protein called UPF0307 protein YjgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	8	157	1281	792	251	237	1	0	0

- Molecule 29 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	9	338	2582	1626	453	490	13	0	0

- Molecule 30 is a protein called 50S ribosomal protein L16.

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	A	2913	62534	27897	11506	20218	2913	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	H	149	1110	699	197	213	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	131	988	625	175	183	5	0	0

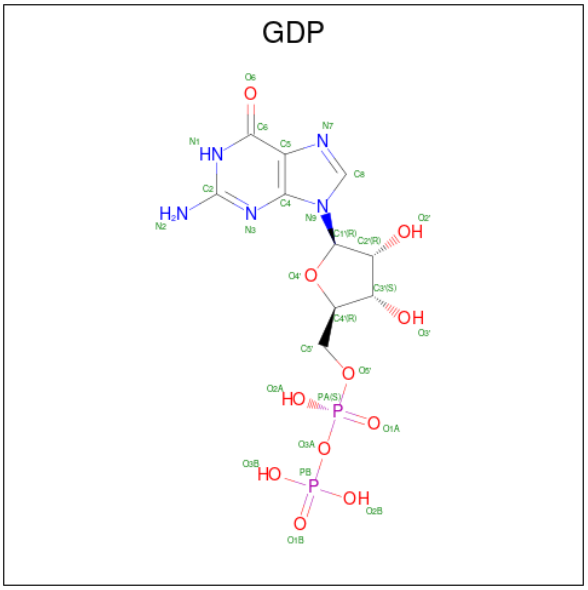
- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	b	47	364	227	64	67	6	0	0

- Molecule 36 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	9	1	28	10	5	11	2	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	9	1	1	1	0
37	A	1	1	1	0

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

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

- Molecule 39 is water.

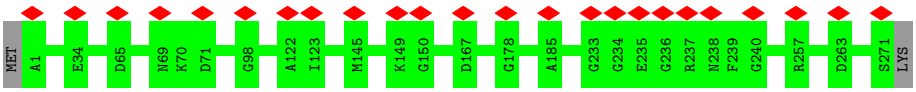
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	C	3	3	3	0
			Total	O	
39	D	1	1	1	0
			Total	O	
39	N	2	2	2	0
			Total	O	
39	S	1	1	1	0
			Total	O	
39	2	1	1	1	0
			Total	O	
39	B	1	1	1	0
			Total	O	
39	A	17	17	17	0
			Total	O	
39	F	1	1	1	0

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.

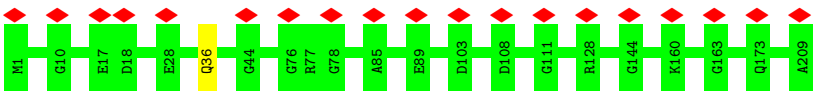
• Molecule 1: 50S ribosomal protein L2

Chain C: 9% 99%



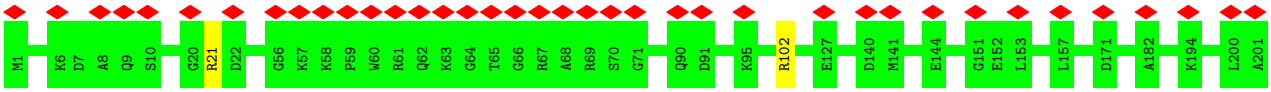
• Molecule 2: 50S ribosomal protein L3

Chain D: 9% 100%



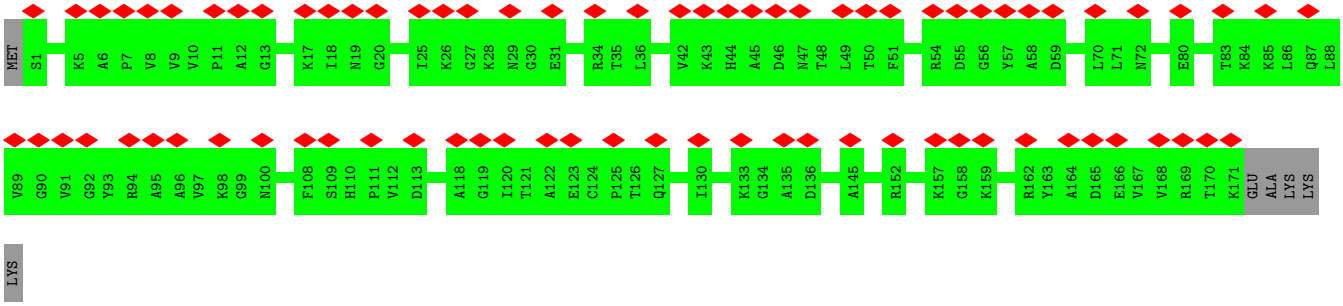
• Molecule 3: 50S ribosomal protein L4

Chain E: 19% 99%



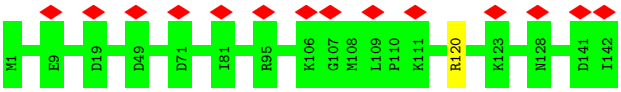
• Molecule 4: 50S ribosomal protein L6

Chain G: 44% 97%



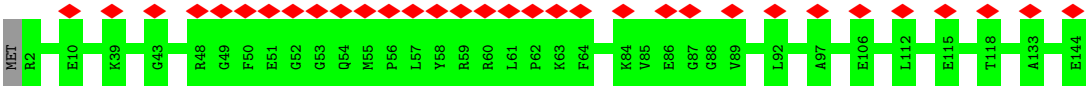
• Molecule 5: 50S ribosomal protein L13

Chain J: 10% 99%



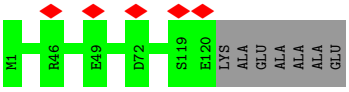
• Molecule 6: 50S ribosomal protein L15

Chain L: 22% 99%



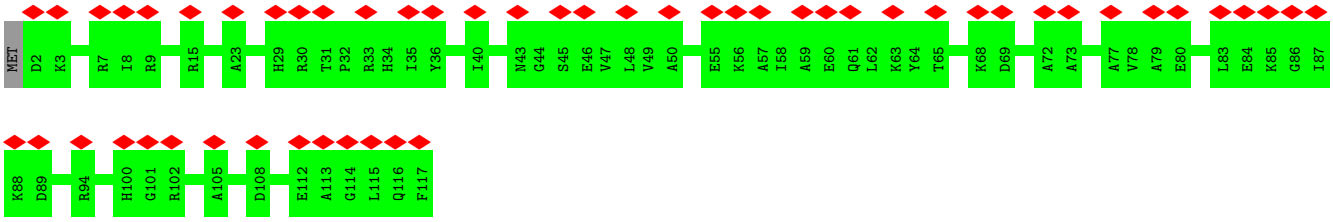
• Molecule 7: 50S ribosomal protein L17

Chain N: 94% 6%



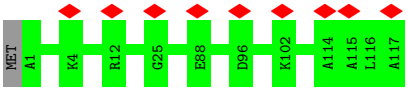
• Molecule 8: 50S ribosomal protein L18

Chain O: 45% 99%



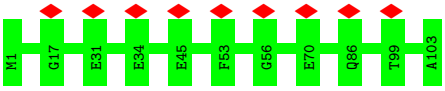
• Molecule 9: 50S ribosomal protein L20

Chain Q: 8% 99%



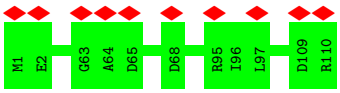
• Molecule 10: 50S ribosomal protein L21

Chain R: 9% 100%



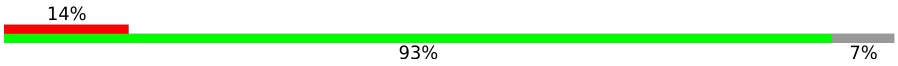
• Molecule 11: 50S ribosomal protein L22

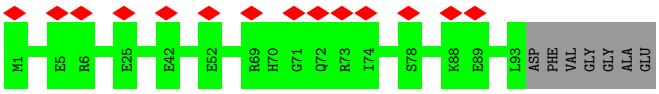
Chain S: 9% 100%



• Molecule 12: 50S ribosomal protein L23

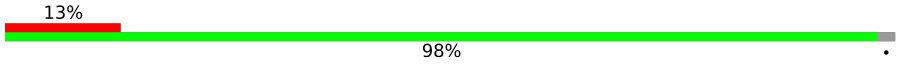
Chain T:

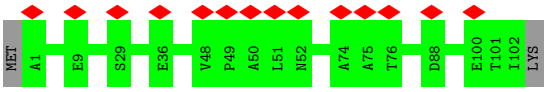




• Molecule 13: 50S ribosomal protein L24

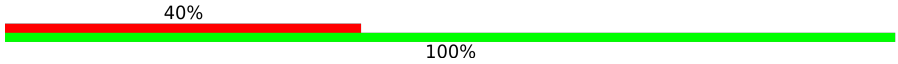
Chain U:

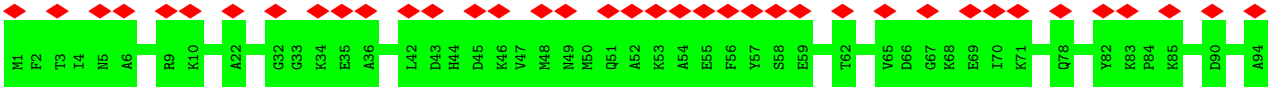




• Molecule 14: 50S ribosomal protein L25

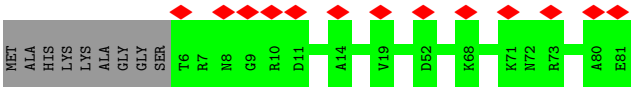
Chain V:





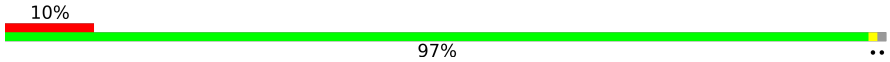
• Molecule 15: 50S ribosomal protein L27

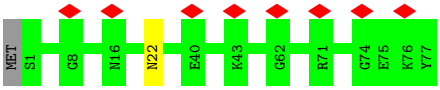
Chain W:



• Molecule 16: 50S ribosomal protein L28

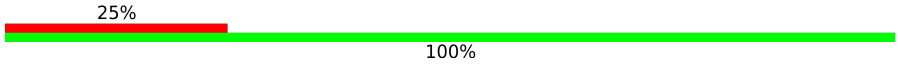
Chain X:

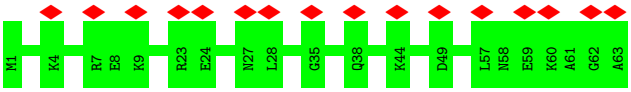




• Molecule 17: 50S ribosomal protein L29

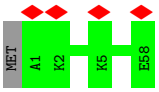
Chain Y:





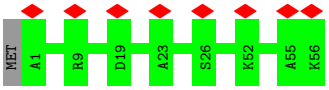
• Molecule 18: 50S ribosomal protein L30

Chain Z: 7% 98%



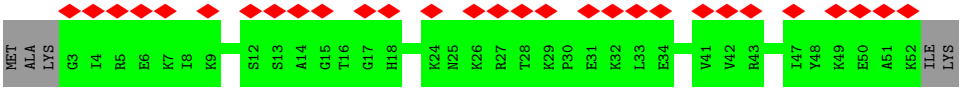
• Molecule 19: 50S ribosomal protein L32

Chain 0: 14% 98%



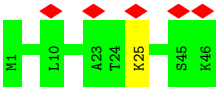
• Molecule 20: 50S ribosomal protein L33

Chain 1: 53% 91% 9%



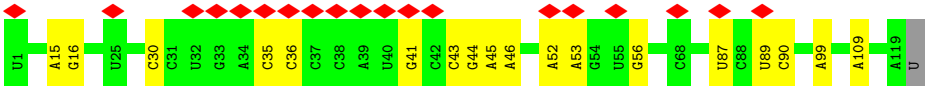
• Molecule 21: 50S ribosomal protein L34

Chain 2: 11% 98%



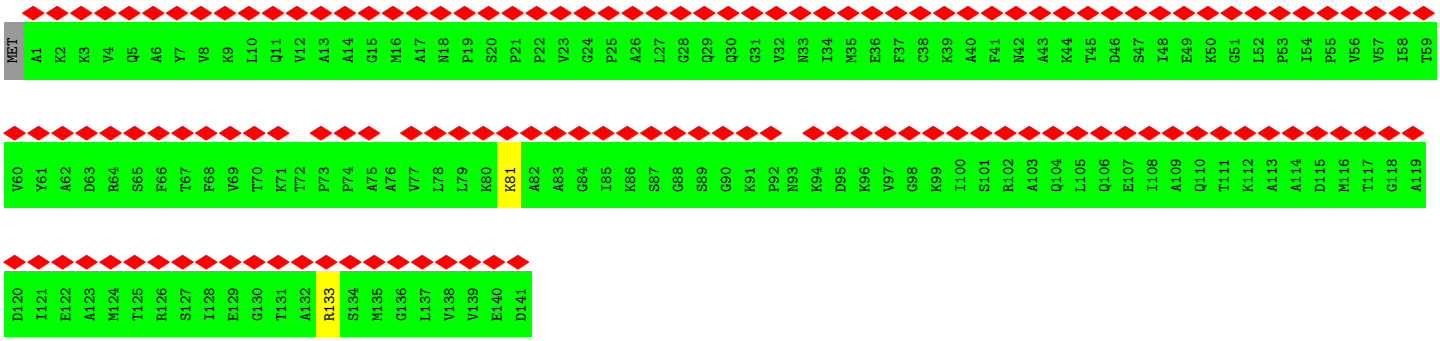
• Molecule 22: 5S ribosomal RNA

Chain B: 16% 84% 15%



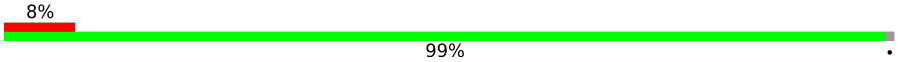
• Molecule 23: 50S ribosomal protein L11

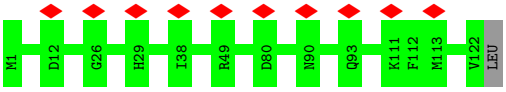
Chain I: 97% 98%



• Molecule 24: 50S ribosomal protein L14

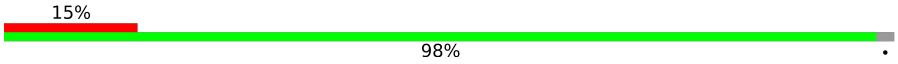
Chain K:

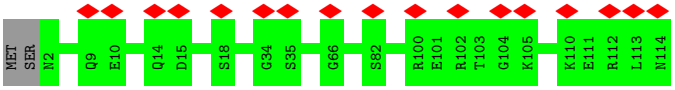




• Molecule 25: 50S ribosomal protein L19

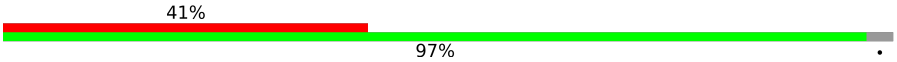
Chain P:

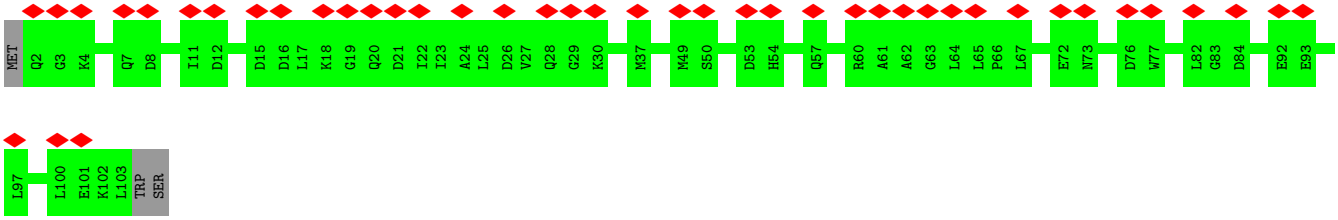




• Molecule 26: Ribosomal silencing factor RsfS

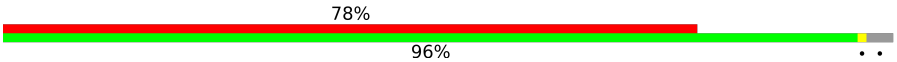
Chain 6:

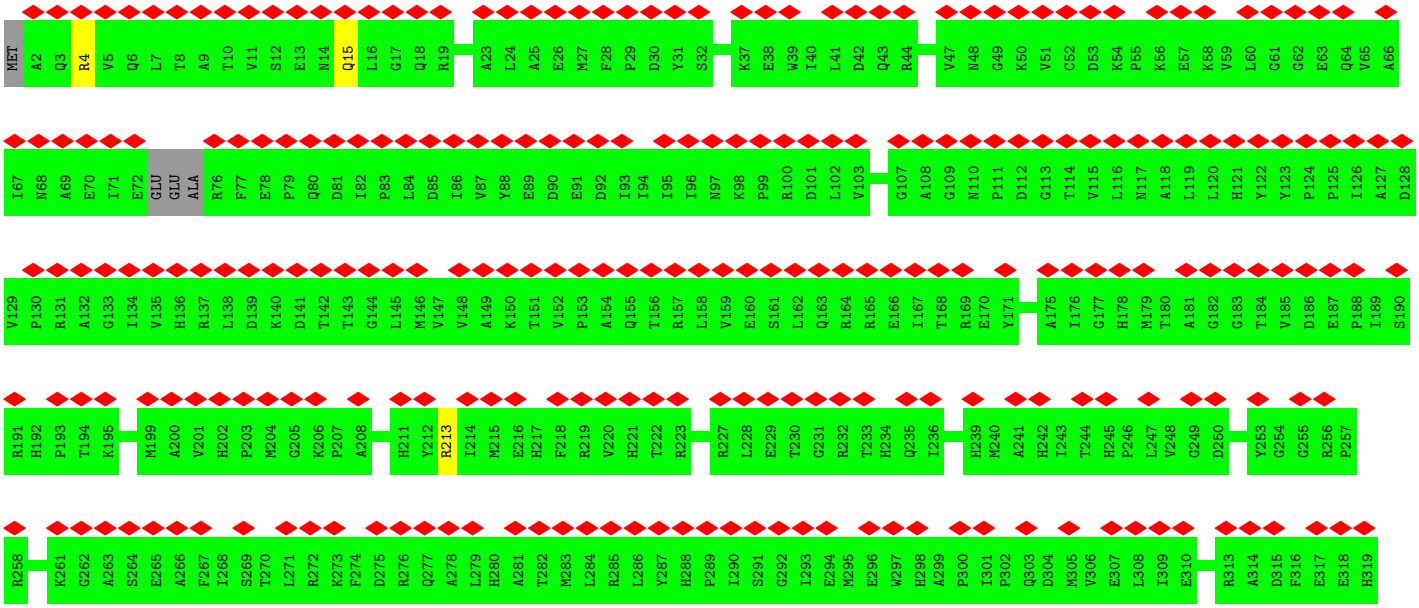


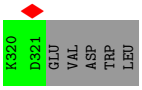


• Molecule 27: Ribosomal large subunit pseudouridine synthase D

Chain 7:

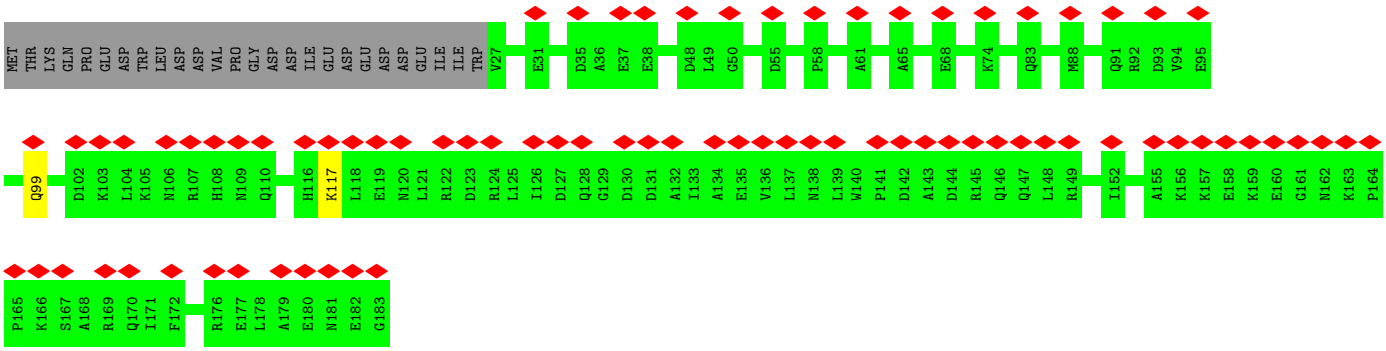






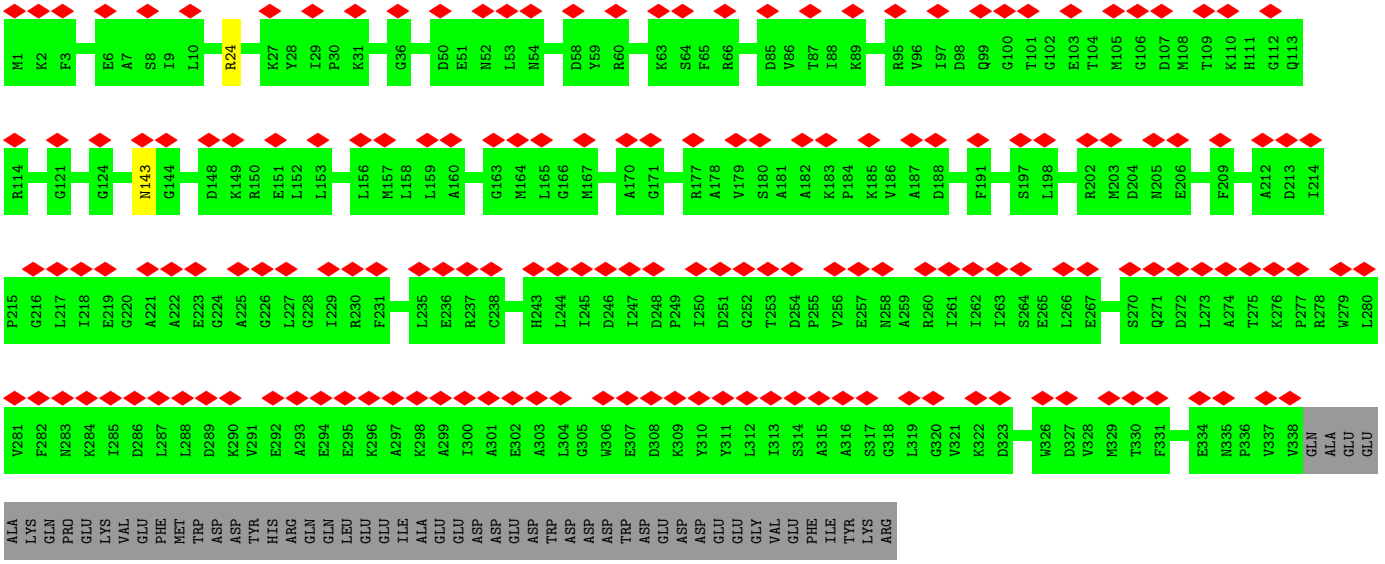
• Molecule 28: UPF0307 protein YjgA

Chain 8:



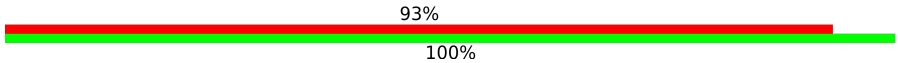
• Molecule 29: GTPase ObgE/CgtA

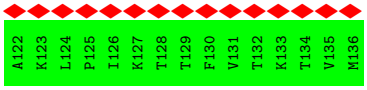
Chain 9:



• Molecule 30: 50S ribosomal protein L16

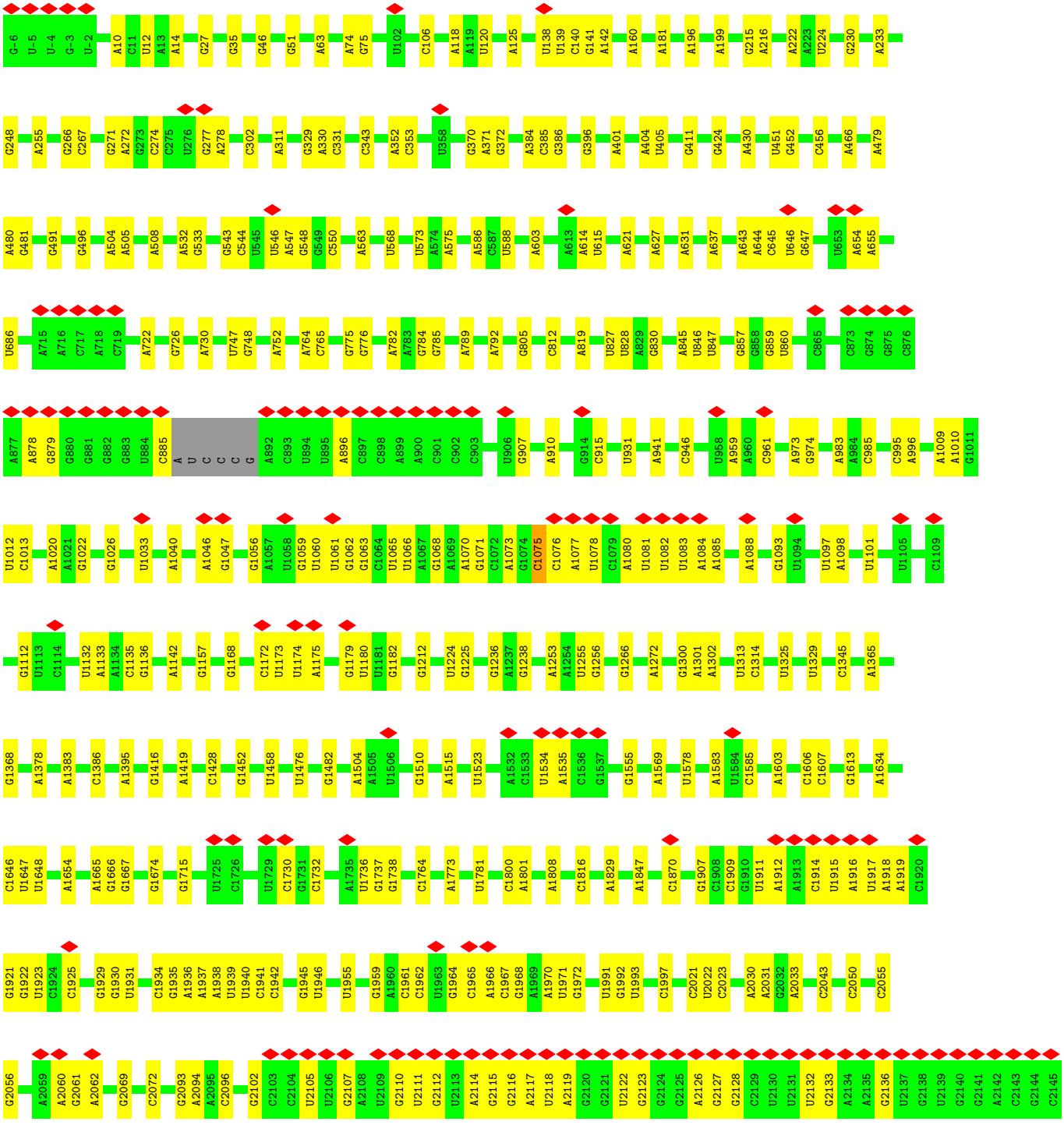
Chain M:





• Molecule 31: 23S ribosomal RNA

Chain A:



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 A2198 A2199 G2204 A2211 A2212 U2213 A2225 G2238 G2239 U2249 G2250 G2251

G2252 G2253 C2254 G2255 C2275 G2279 C2283 A2287 A2288 A2297 G2304 U2305 C2306 G2307 G2308 A2309 C2310 A2311 U2312 C2313 A2314 G2315 G2316 A2317 G2318 G2319 U2320 U2321 A2322 G2325 C2326 A2327 A2333 A2336 U2344 G2345 C2350 G2357 G2383 U2384 C2385 A2392 U2402 A2406

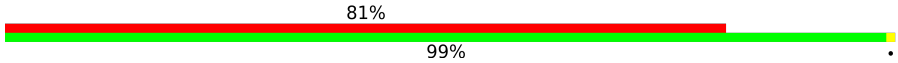
C2420 G2421 C2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 A2435 U2441 G2447 A2448 U2449 G2455 C2456 U2457 G2458 A2471 G2472 U2473 U2474 C2475 A2476 U2477 A2478 U2479 G2490 U2491 A2497 C2498 C2499 U2500 C2501 G2502 A2503 U2504 G2505 U2506 A2513 A2518 U2519 C2520 G2525 G2529

G2535 A2547 U2554 A2564 A2565 A2566 G2567 A2572 C2573 U2586 C2601 A2602 U2609 C2610 U2613 A2614 U2615 U2629 G2630 C2636 A2639 C2646 U2647 A2682 C2683 U2684 U2689 U2690 G2714 G2718 A2721 A2726 G2729 A2733 G2744 A2748 A2765

A2778 U2779 G2780 G2791 U2797 U2798 U2818 G2819 A2820 G2825 A2835 U2836 G2867 A2872 A2873 C2880 A2883 U2884 C2885 A2886 A2893 C2901 C2902 U2903 U2904 A2905 C2906 A2907 A2908 C2909 C2910 C2911 C2912

- Molecule 32: 50S ribosomal protein L9

Chain H:



M1 Q2 L5 L6 D7 A10 N11 S14 L15 G16 D17 Q18 V19 N20 G34 K35 A36 T40 K41 K42 N43 I44 E45 F46 F47 E48 A49 R50 R51 A52 E53 L54 E55 A56 K57 L58 A59 E60 V61 L62 A63 A64 A65 N66 A67 R68 A69 E70 K71 I72 N73 A74 L75 E76 T77

V78 T79 I80 A81 S82 K83 A84 G85 D86 E87 G88 K89 L90 F91 G92 S93 I94 G95 T96 R97 D98 I99 A100 D101 A102 V103 T104 A105 A106 G107 V108 R109 E110 V111 A112 K113 S114 E115 V116 R117 L118 P119 N120 G121 V122 L123 R124 T125 G126 E127 H128 E129 V130 S131 F132 Q133 V134 H135 S136 E137

V138 F139 A140 K141 V142 I143 V144 N145 V146 V147 A148 E149

- Molecule 33: 50S ribosomal protein L10

Chain e:

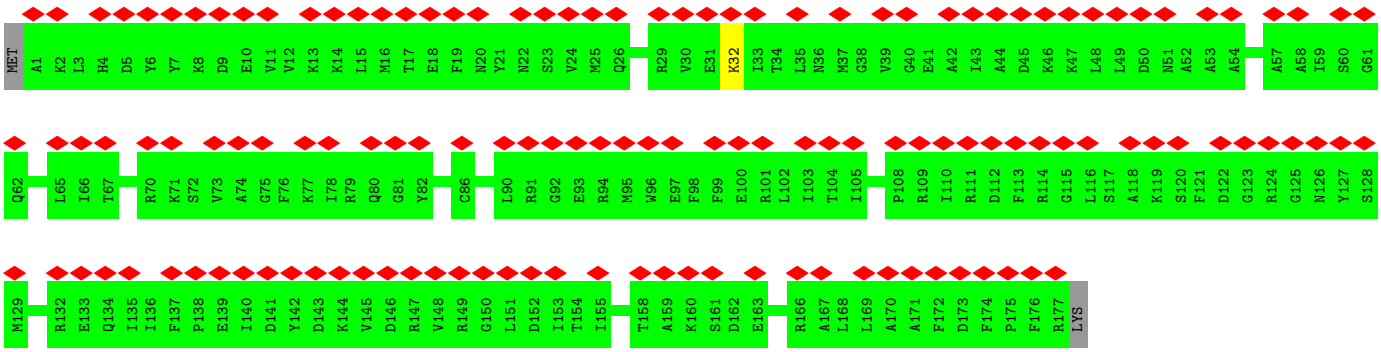
M1 A2 L3 N4 L5 Q6 D7 K8 Q9 A10 I11 V12 A13 E14 V15 S16 E17 V18 A19 K20 G21 A22 L23 S24 A25 V26 V27 A28 D29 S30 R31 G32 V33 T34 V35 D36 K37 M38 T39 E40 L41 R42 K43 A44 G45 R46 E47 A48 G49 V50 Y51 M52 R53 V54 V55 R56 N57 T58 L59 L60

R61 R62 A63 V64 E65 G66 T67 P68 F69 E70 C71 L72 K73 D74 A75 F76 V77 G78 P79 T80 M81 I82 A83 Y84 S85 M86 E87 H88 P89 G90 A91 A92 A93 R94 L95 F96 K97 E98 F99 A100 K101 A102 N103 A104 K105 F106 E107 V108 K109 A110 A111 A112 F113 E114 G115 E116 L117 I118 P119 A120

S121 Q122 I123 D124 R125 L126 A127 T128 L129 P130 T131 TYR GLU GLU ALA ILE ALA ARG LEU MET ALA THR MET LYS GLU ALA SER ALA GLY LYS LEU VAL ARG THR LEU ALA ALA VAL ARG ASP ALA LYS GLU ALA ALA

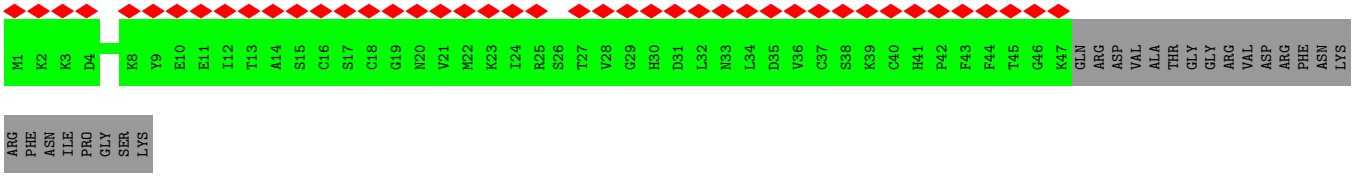
- Molecule 34: 50S ribosomal protein L5

Chain F: 75% 98%



- Molecule 35: 50S ribosomal protein L31

Chain b: 61% 67% 33%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	13.174	Depositor
Minimum map value	-5.976	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.789	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	334.8, 334.8, 334.8	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	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: ZN, GDP, 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	C	0.24	0/2121	0.44	0/2852
2	D	0.25	0/1586	0.48	0/2134
3	E	0.24	0/1571	0.42	0/2113
4	G	0.24	0/1301	0.45	0/1764
5	J	0.24	0/1152	0.42	0/1551
6	L	0.26	0/1054	0.55	0/1403
7	N	0.24	0/973	0.44	0/1301
8	O	0.25	0/902	0.42	0/1209
9	Q	0.24	0/960	0.36	0/1278
10	R	0.27	0/829	0.53	0/1107
11	S	0.23	0/864	0.44	0/1156
12	T	0.23	0/744	0.43	0/994
13	U	0.25	0/787	0.46	0/1051
14	V	0.24	0/766	0.48	0/1025
15	W	0.26	0/582	0.46	0/769
16	X	0.23	0/635	0.42	0/848
17	Y	0.24	0/510	0.50	0/677
18	Z	0.23	0/453	0.47	0/605
19	0	0.23	0/450	0.45	0/599
20	1	0.24	0/416	0.46	0/554
21	2	0.23	0/380	0.39	0/498
22	B	0.15	0/2847	0.71	0/4440
23	I	0.25	0/1046	0.47	0/1410
24	K	0.25	0/947	0.47	0/1268
25	P	0.25	0/923	0.45	0/1234
26	6	0.24	0/787	0.47	0/1062
27	7	0.23	0/2590	0.43	0/3513
28	8	0.23	0/1292	0.41	0/1727
29	9	0.25	0/2626	0.45	0/3542
30	M	0.24	0/1093	0.44	0/1460
31	A	0.17	0/70038	0.73	12/109262 (0.0%)
32	H	0.24	0/1121	0.45	0/1515

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.25	0/1001	0.47	0/1350
34	F	0.25	0/1434	0.44	0/1926
35	b	0.23	0/371	0.43	0/496
All	All	0.20	0/107152	0.66	12/159693 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	1313	U	C2-N1-C1'	7.05	126.17	117.70
31	A	106	C	N3-C2-O2	-6.91	117.07	121.90
31	A	1075	C	N3-C2-O2	-6.88	117.08	121.90
31	A	1075	C	N1-C2-O2	6.46	122.77	118.90
31	A	1939	U	C2-N1-C1'	6.37	125.34	117.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
2	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
3	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
4	G	169/177 (96%)	163 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
6	L	141/144 (98%)	119 (84%)	22 (16%)	0	100	100
7	N	118/127 (93%)	111 (94%)	7 (6%)	0	100	100
8	O	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
9	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
10	R	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
11	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
12	T	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
13	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
14	V	92/94 (98%)	92 (100%)	0	0	100	100
15	W	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
16	X	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
17	Y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
18	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
19	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
20	1	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
21	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
23	I	139/142 (98%)	116 (84%)	23 (16%)	0	100	100
24	K	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
25	P	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
26	6	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
27	7	313/326 (96%)	304 (97%)	9 (3%)	0	100	100
28	8	155/183 (85%)	152 (98%)	3 (2%)	0	100	100
29	9	336/390 (86%)	312 (93%)	24 (7%)	0	100	100
30	M	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
32	H	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
33	e	129/165 (78%)	113 (88%)	16 (12%)	0	100	100
34	F	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
35	b	45/70 (64%)	41 (91%)	4 (9%)	0	100	100
All	All	4280/4545 (94%)	4035 (94%)	245 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	C	216/218 (99%)	216 (100%)	0	100	100
2	D	164/164 (100%)	163 (99%)	1 (1%)	86	91
3	E	165/165 (100%)	163 (99%)	2 (1%)	71	83
4	G	133/138 (96%)	133 (100%)	0	100	100
5	J	116/116 (100%)	115 (99%)	1 (1%)	78	87
6	L	102/103 (99%)	102 (100%)	0	100	100
7	N	100/103 (97%)	100 (100%)	0	100	100
8	O	86/87 (99%)	86 (100%)	0	100	100
9	Q	89/90 (99%)	89 (100%)	0	100	100
10	R	84/84 (100%)	84 (100%)	0	100	100
11	S	93/93 (100%)	93 (100%)	0	100	100
12	T	80/84 (95%)	80 (100%)	0	100	100
13	U	83/85 (98%)	83 (100%)	0	100	100
14	V	78/78 (100%)	78 (100%)	0	100	100
15	W	56/63 (89%)	56 (100%)	0	100	100
16	X	67/68 (98%)	66 (98%)	1 (2%)	65	81
17	Y	55/55 (100%)	55 (100%)	0	100	100
18	Z	48/49 (98%)	48 (100%)	0	100	100
19	0	47/48 (98%)	47 (100%)	0	100	100
20	1	45/49 (92%)	45 (100%)	0	100	100
21	2	38/38 (100%)	37 (97%)	1 (3%)	46	71
23	I	109/110 (99%)	107 (98%)	2 (2%)	59	78
24	K	103/104 (99%)	103 (100%)	0	100	100
25	P	98/100 (98%)	98 (100%)	0	100	100
26	6	88/91 (97%)	88 (100%)	0	100	100
27	7	274/282 (97%)	271 (99%)	3 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	8	135/161 (84%)	133 (98%)	2 (2%)	65	81
29	9	273/321 (85%)	271 (99%)	2 (1%)	84	90
30	M	109/109 (100%)	109 (100%)	0	100	100
32	H	114/114 (100%)	113 (99%)	1 (1%)	78	87
33	e	100/123 (81%)	100 (100%)	0	100	100
34	F	148/150 (99%)	147 (99%)	1 (1%)	84	90
35	b	43/62 (69%)	43 (100%)	0	100	100
All	All	3539/3705 (96%)	3522 (100%)	17 (0%)	89	93

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	9	143	ASN
34	F	32	LYS
23	I	133	ARG
27	7	4	ARG
27	7	15	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
27	7	117	ASN
27	7	239	HIS
29	9	113	GLN
27	7	245	HIS
10	R	18	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	B	118/120 (98%)	18 (15%)	0
31	A	2911/2919 (99%)	474 (16%)	17 (0%)
All	All	3029/3039 (99%)	492 (16%)	17 (0%)

5 of 492 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	B	15	A
22	B	16	G
22	B	30	C
22	B	35	C
22	B	36	C

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	A	2249	U
31	A	2425	A
31	A	1224	U
31	A	1606	C
31	A	1666	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
36	GDP	9	1001	29,37	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)

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
36	GDP	9	1001	29,37	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	9	1001	GDP	C6-N1	-2.38	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	9	1001	GDP	PA-O3A-PB	-3.64	120.34	132.83
36	9	1001	GDP	C3'-C2'-C1'	2.92	105.37	100.98
36	9	1001	GDP	C8-N7-C5	2.36	107.50	102.99
36	9	1001	GDP	C5-C6-N1	2.26	117.95	113.95

There are no chirality outliers.

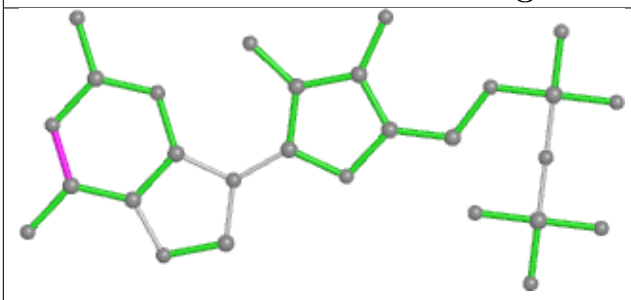
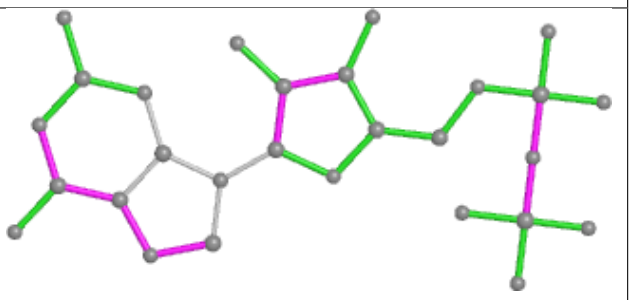
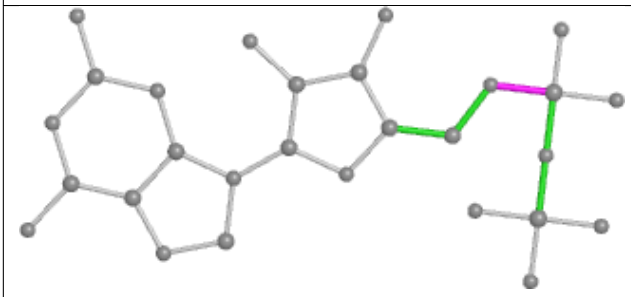
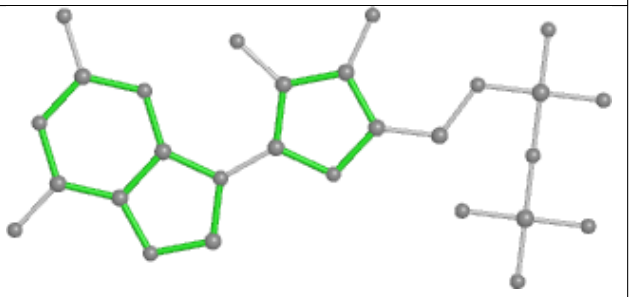
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	9	1001	GDP	C5'-O5'-PA-O1A
36	9	1001	GDP	C5'-O5'-PA-O2A
36	9	1001	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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 GDP 9 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

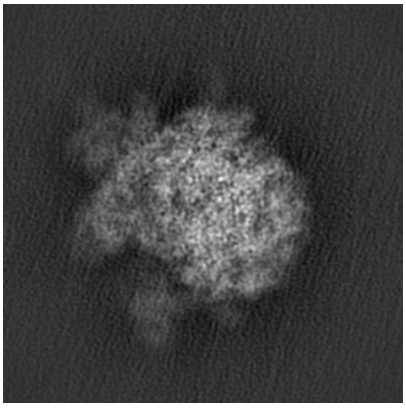
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12218. These allow visual inspection of the internal detail of the map and identification of artifacts.

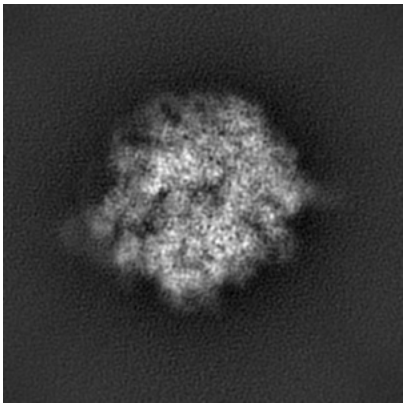
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

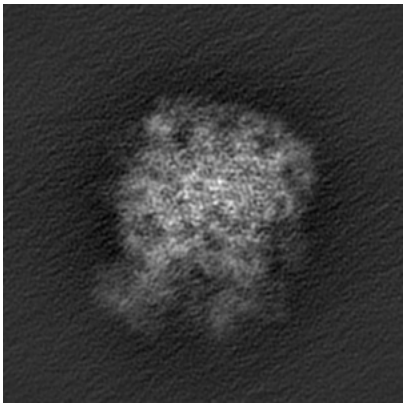
6.1.1 Primary map



X



Y

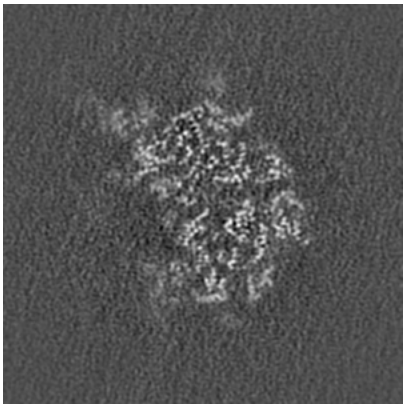


Z

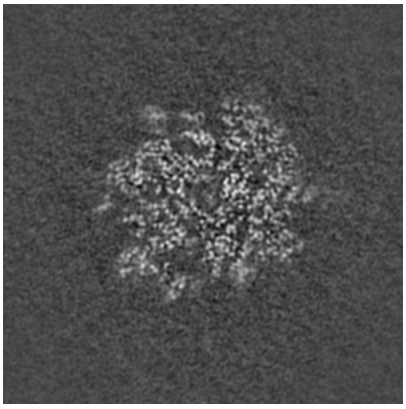
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

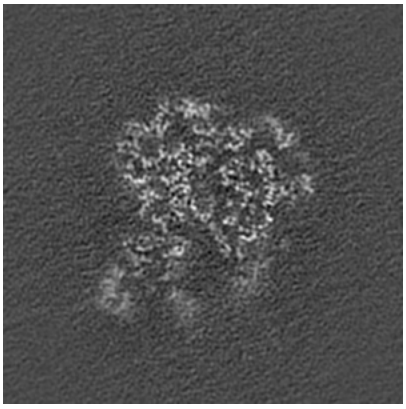
6.2.1 Primary map



X Index: 135



Y Index: 135

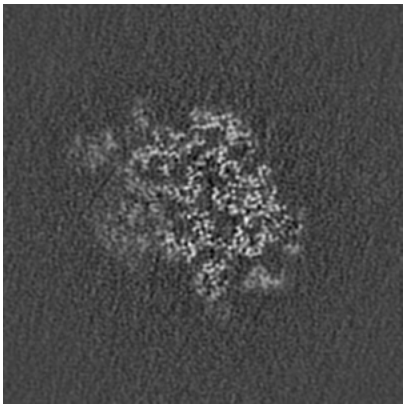


Z Index: 135

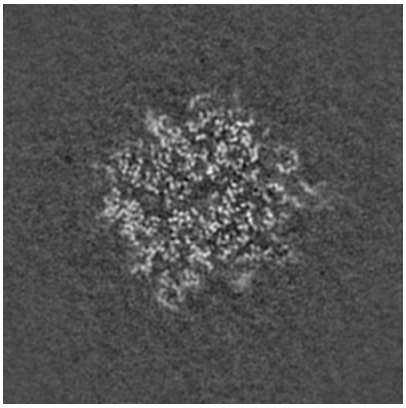
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

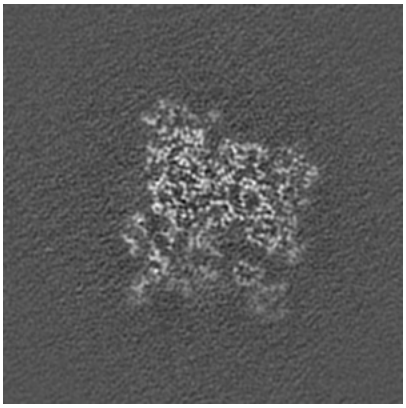
6.3.1 Primary map



X Index: 157



Y Index: 142



Z Index: 151

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

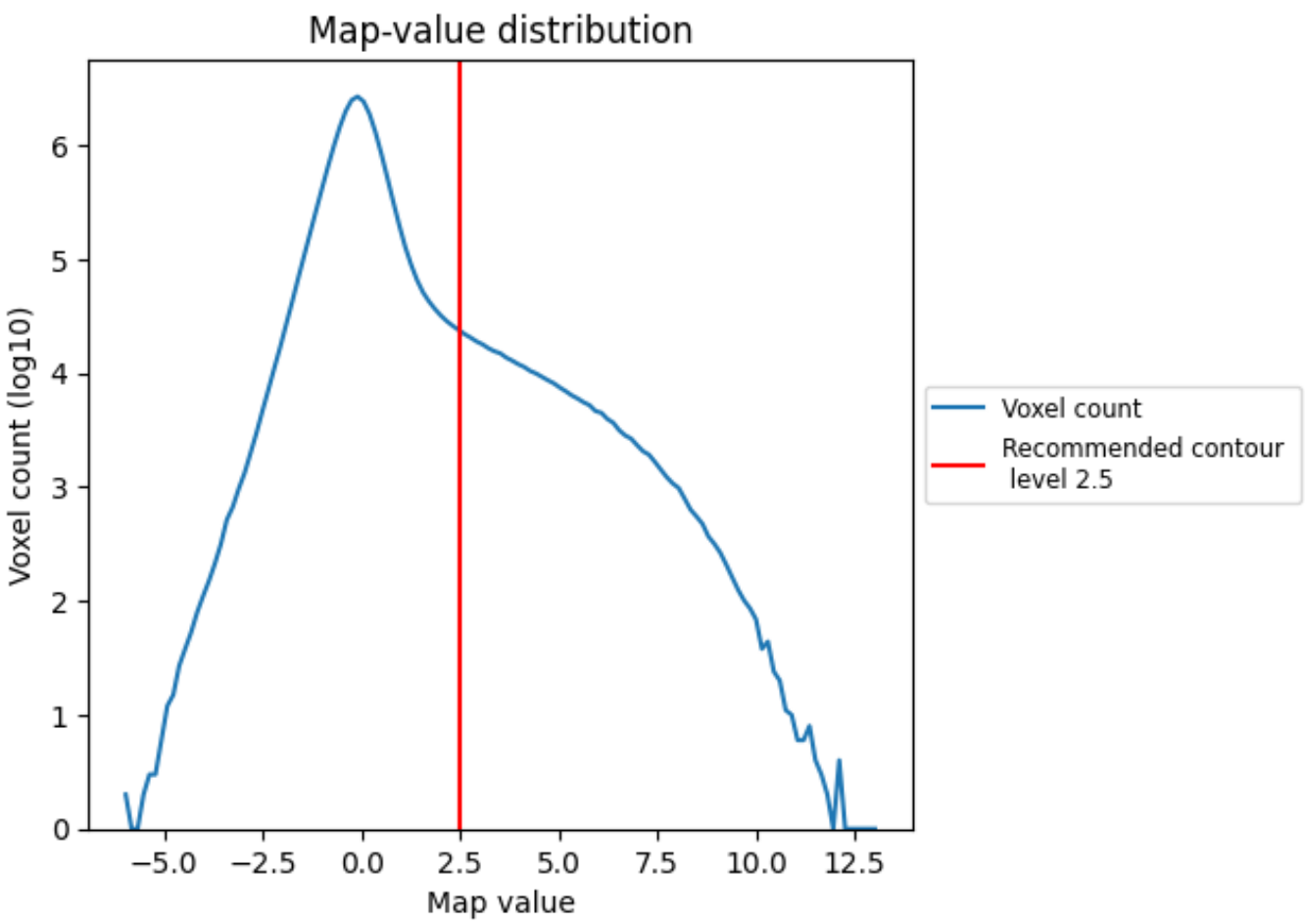
6.5 Mask visualisation (i)

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

7 Map analysis (i)

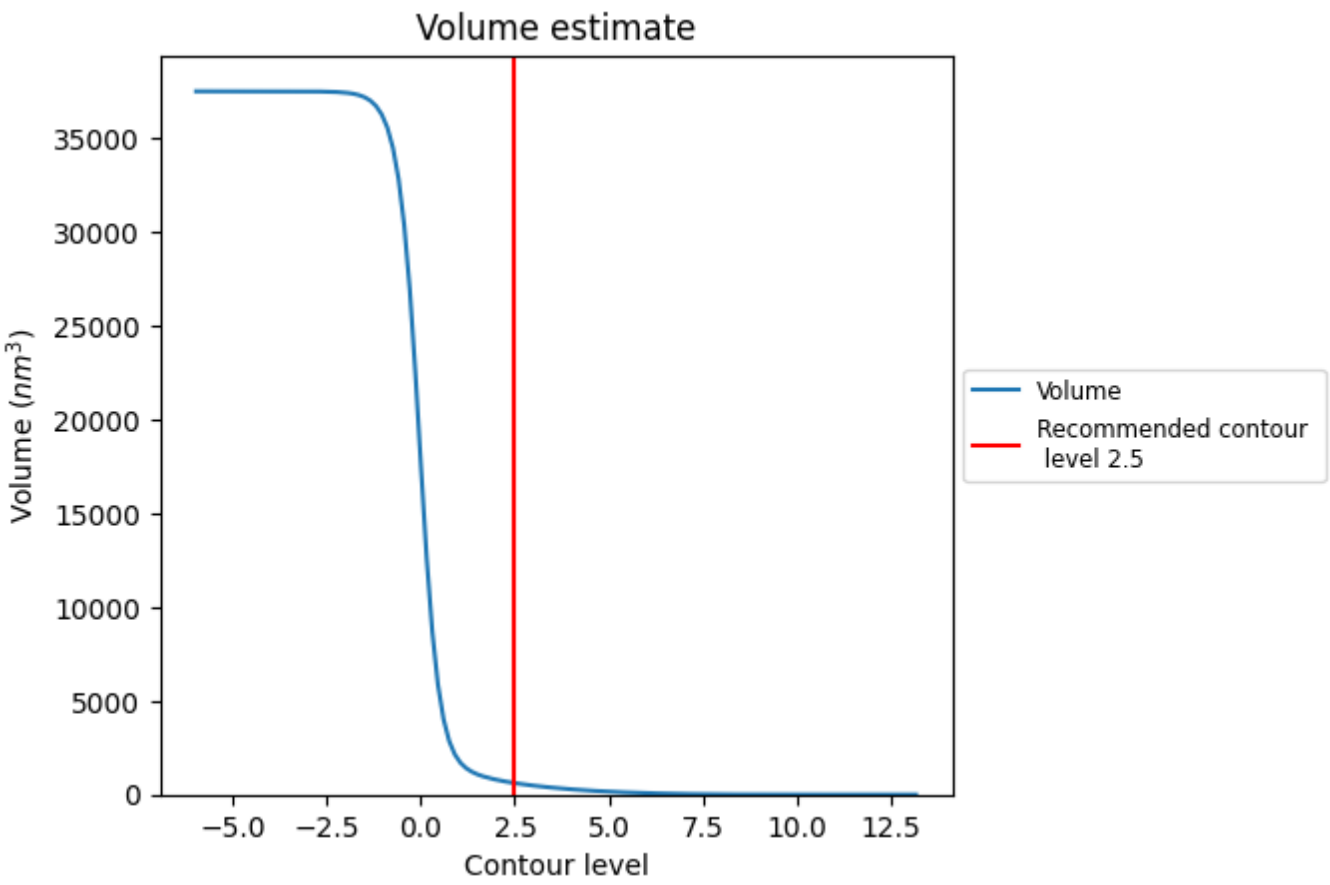
This section contains the results of statistical analysis of the map.

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.

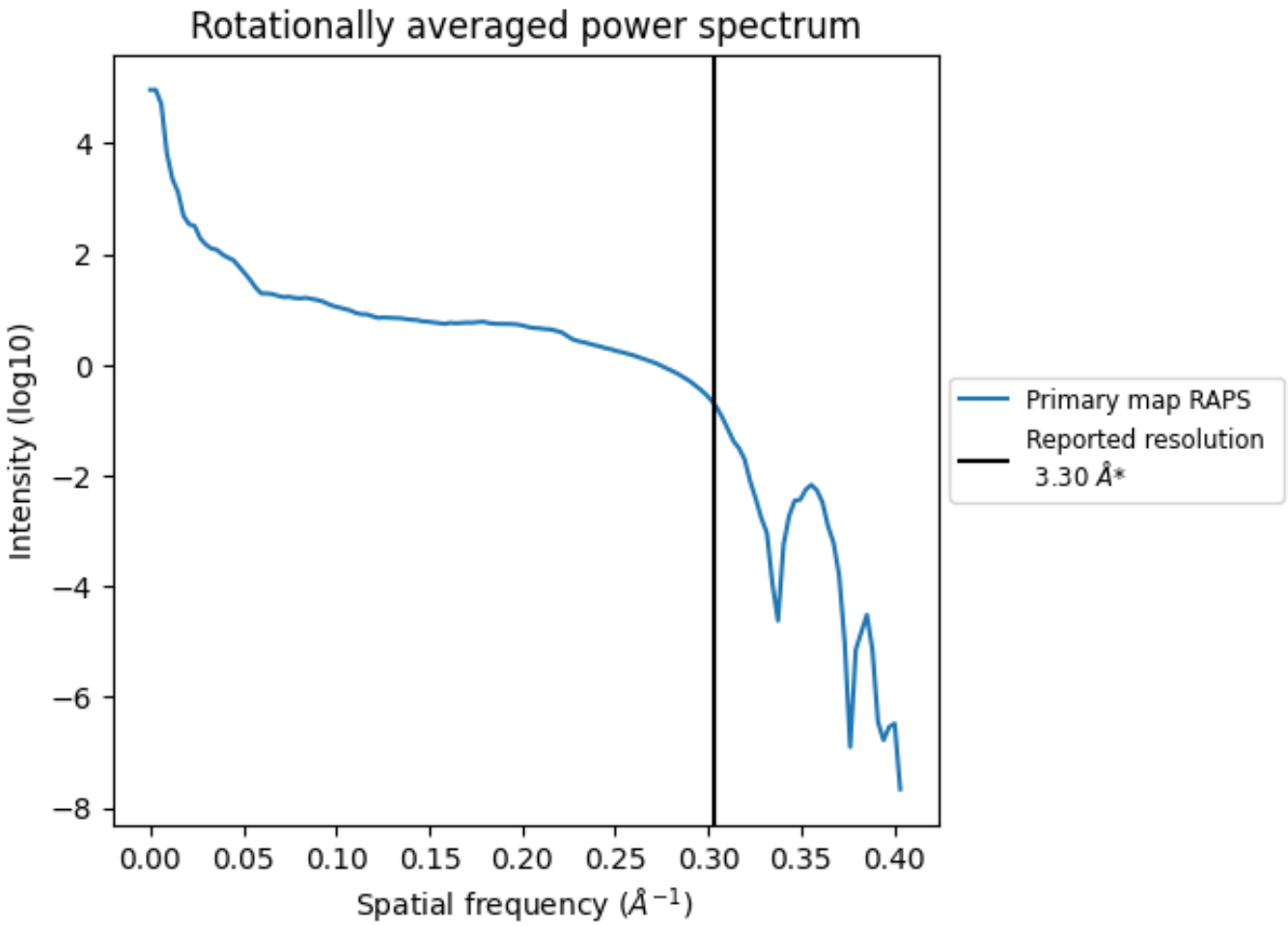
7.2 Volume estimate (i)



The volume at the recommended contour level is 613 nm^3; this corresponds to an approximate mass of 554 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)

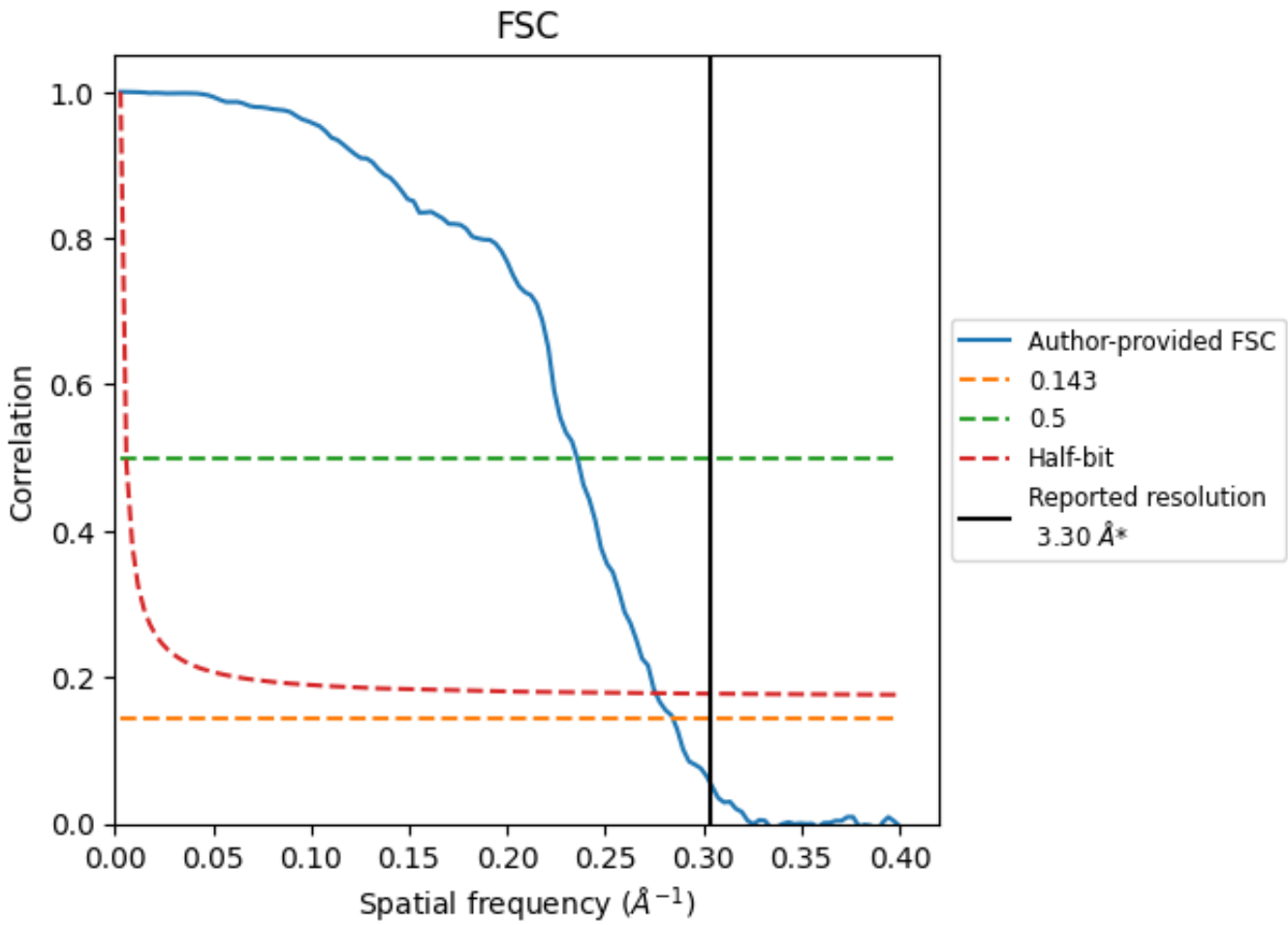


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

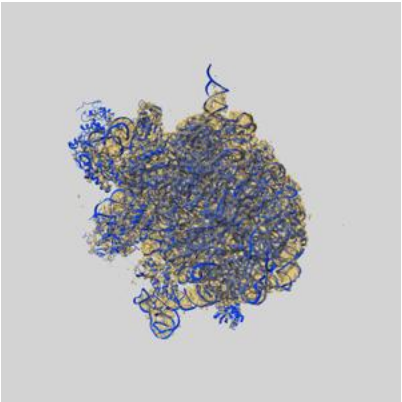
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.51	4.24	3.63
Unmasked-calculated*	-	-	-

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

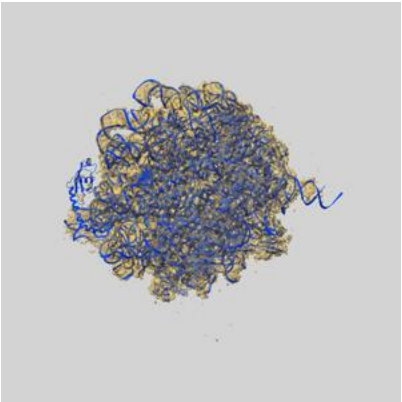
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12218 and PDB model 7BL5. Per-residue inclusion information can be found in section 3 on page 12.

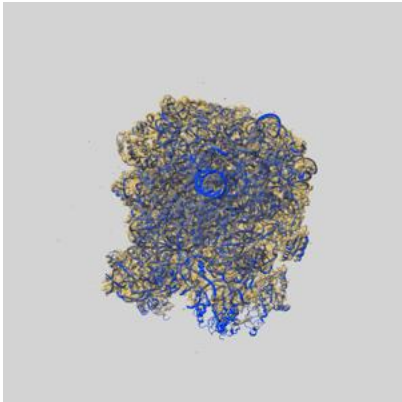
9.1 Map-model overlay (i)



X



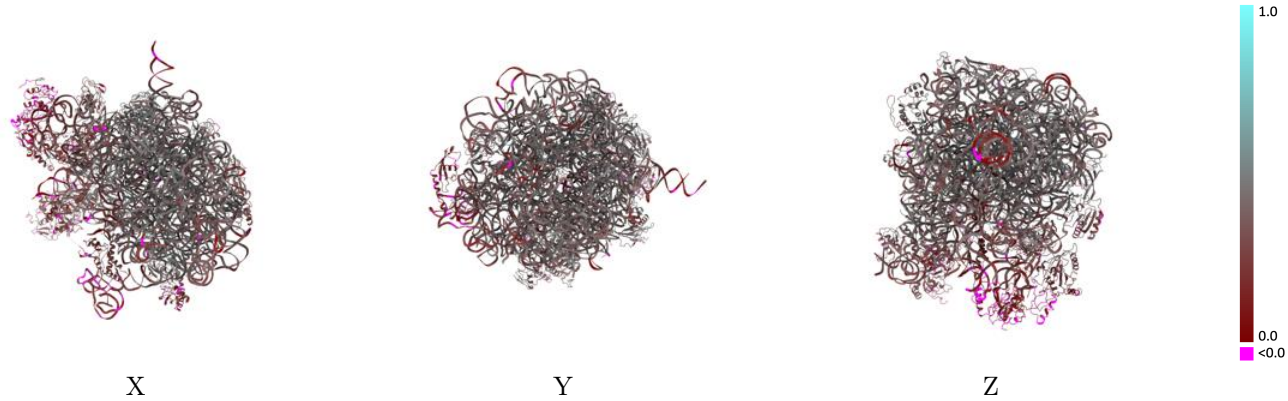
Y



Z

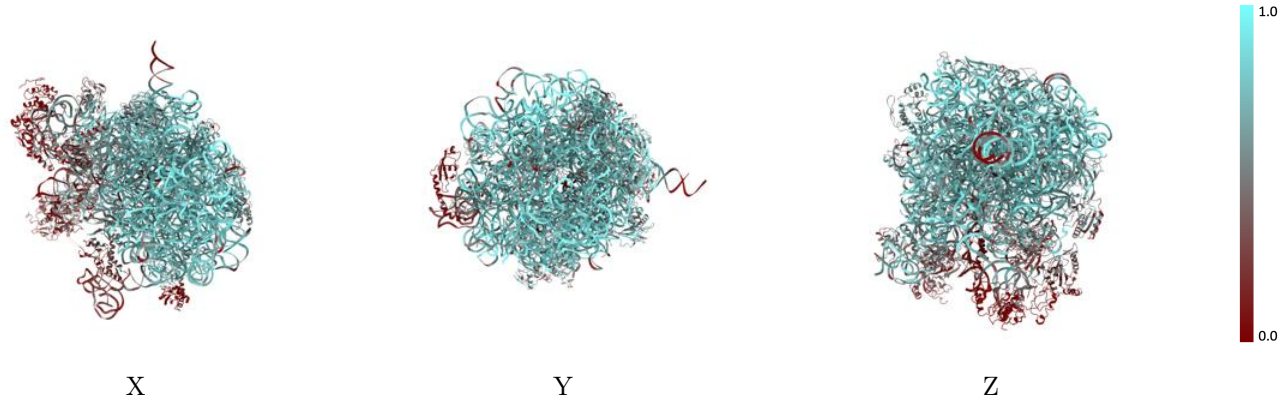
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



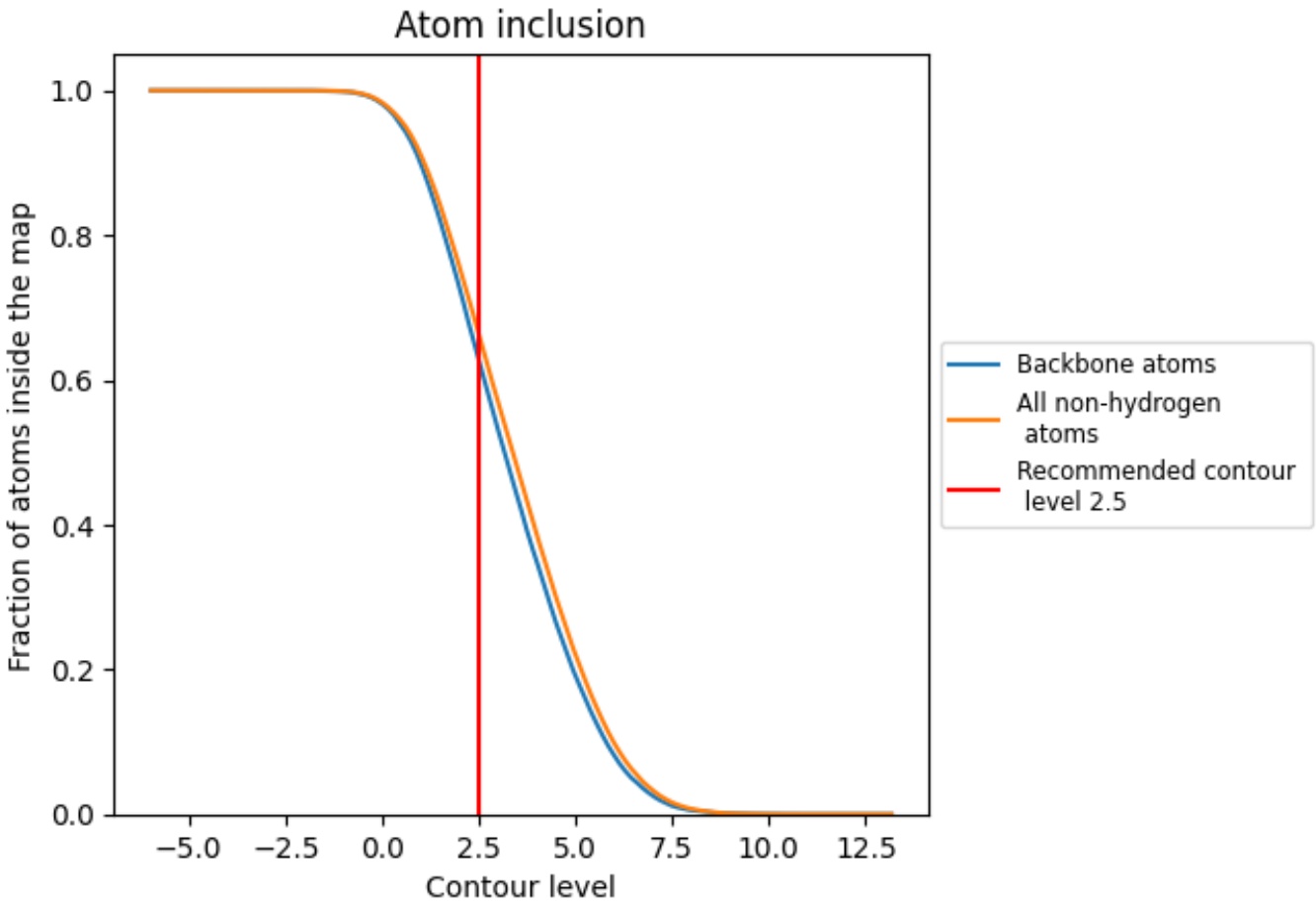
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 66% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6643	0.3630
0	0.6472	0.4120
1	0.3541	0.3060
2	0.6648	0.4390
6	0.4117	0.3080
7	0.2521	0.2880
8	0.3918	0.3140
9	0.3891	0.3330
A	0.7731	0.3750
B	0.6601	0.3140
C	0.6766	0.4390
D	0.6658	0.4400
E	0.5829	0.3860
F	0.2418	0.2380
G	0.4303	0.3270
H	0.1589	0.1980
I	0.0440	0.0980
J	0.6636	0.4410
K	0.6473	0.4360
L	0.5571	0.3700
M	0.1363	0.2670
N	0.6974	0.4440
O	0.4368	0.3040
P	0.6474	0.4240
Q	0.6718	0.4340
R	0.6612	0.4270
S	0.6722	0.4340
T	0.6150	0.4050
U	0.6154	0.4020
V	0.4485	0.3160
W	0.6082	0.4200
X	0.6639	0.4450
Y	0.5734	0.3310
Z	0.6636	0.4210
b	0.0912	0.1770
e	0.0238	0.0660