wwPDB EM Validation Summary Report (i)

Mar 20, 2023 – 07:27 PM EDT

PDB ID	:	8FIZ
EMDB ID	:	EMD-29214
Title	:	Cryo-EM structure of E. coli 70S Ribosome containing mRNA and tRNA (in the transcription-translation complex)
Authors	:	Florez Ariza, A.; Wee, L.; Tong, A.; Canari, C.; Grob, P.; Nogales, E.; Bustamante, C.
Deposited on	:	2022-12-18
Resolution	:	3.80 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 (i)) were used in the production of this report:

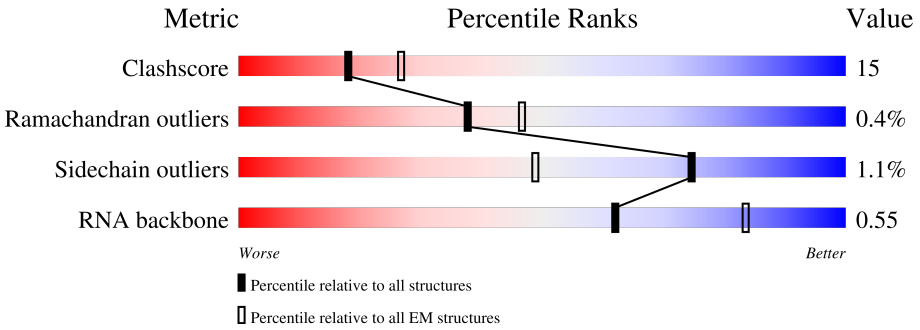
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	AA	1534	37% 47% 16%
2	AB	87	75% 24%
3	AC	124	62% 31% 5%
4	AD	92	55% 29% 14%
5	AE	118	65% 31%
6	AF	101	56% 43%
7	AG	233	63% 25% 12%

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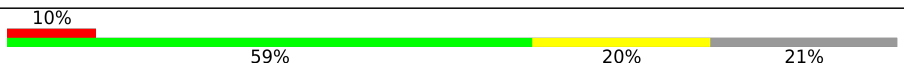
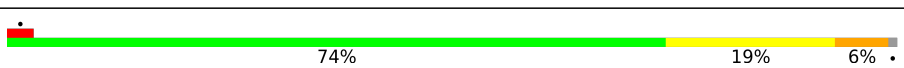
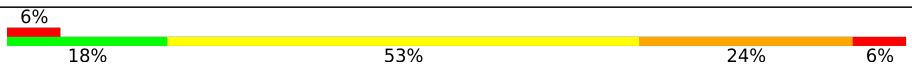
Mol	Chain	Length	Quality of chain
8	AH	103	
9	AI	206	
10	AJ	241	
11	AK	130	
12	AL	179	
13	AM	129	
14	AN	135	
15	AO	82	
16	AP	167	
17	AQ	130	
18	AR	89	
19	AS	84	
20	AT	75	
21	AU	71	
22	AV	70	
23	AW	17	
24	BA	2904	
25	BB	77	
26	BC	120	
27	BD	273	
28	BE	209	
29	BF	201	
30	BG	179	
31	BH	117	
32	BI	55	

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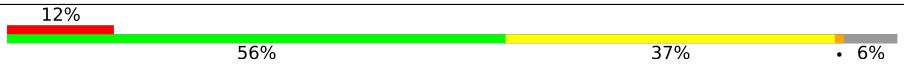
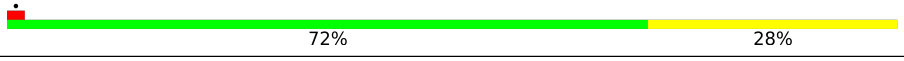
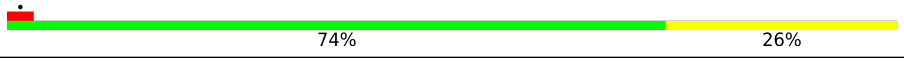
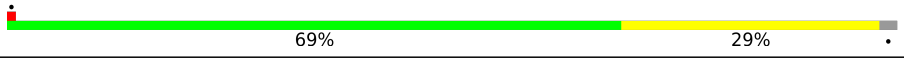
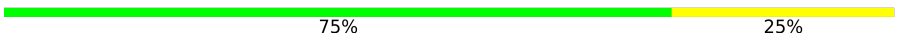
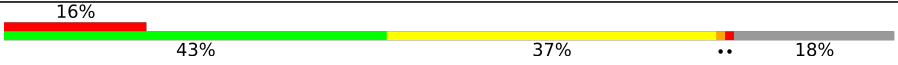
Mol	Chain	Length	Quality of chain
33	BJ	177	
34	BK	149	
35	BL	142	
36	BM	57	
37	BN	46	
38	BO	65	
39	BP	38	
40	BQ	59	
41	BR	142	
42	BS	123	
43	BT	144	
44	BU	136	
45	BV	127	
46	BW	115	
47	BX	118	
48	BY	103	
49	BZ	110	
50	DA	100	
51	DB	104	
52	DC	94	
53	DD	85	
54	DE	78	
55	DF	63	
56	DG	165	

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 146125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1534	Total 32917	C 14681	N 6041	O 10661	P 1534	0	0

- Molecule 2 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	86	Total 670	C 414	N 138	O 115	S 3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	122	Total 947	C 586	N 195	O 162	S 4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S19.

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

- Molecule 5 is a protein called 30S ribosomal protein S13.

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

- Molecule 6 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total 805	C 499	N 164	O 139	S 3	0	0

- Molecule 7 is a protein called 30S ribosomal protein S3.

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

- Molecule 8 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S7.

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

- Molecule 13 is a protein called 30S ribosomal protein S11.

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

- Molecule 14 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 17 is a protein called 30S ribosomal protein S8.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 19 is a protein called 30S ribosomal protein S17.

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

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	69	Total	C	N	O	S	0	0
			539	333	102	98	6		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	17	Total	C	N	O	P	0	0
			365	162	65	121	17		

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BA	2897	Total	C	N	O	P	2	0
			62218	27755	11451	20114	2898		

- Molecule 25 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BB	75	Total	C	N	O	P	0	0
			1598	713	290	521	74		

- Molecule 26 is a RNA chain called 5s rRNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BE	208	Total	C	N	O	S	0	0
			1556	974	286	292	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L18.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L11.

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

- Molecule 36 is a protein called 50S ribosomal protein L32.

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

- Molecule 37 is a protein called 50S ribosomal protein L34.

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

- Molecule 38 is a protein called 50S ribosomal protein L35.

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

- Molecule 39 is a protein called 50S ribosomal protein L36.

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

- Molecule 40 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BQ	58	Total	C	N	O	S	2	0
			463	290	90	81	2		

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L14.

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

- Molecule 43 is a protein called 50S ribosomal protein L15.

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

- Molecule 44 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BU	136	Total	C	N	O	S	1	0
			1082	691	208	177	6		

- Molecule 45 is a protein called 50S ribosomal protein L17.

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

- Molecule 46 is a protein called 50S ribosomal protein L19.

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

- Molecule 47 is a protein called 50S ribosomal protein L20.

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

- Molecule 48 is a protein called Ribosomal protein L21.

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

- Molecule 49 is a protein called 50S ribosomal protein L22.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L24.

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

- Molecule 52 is a protein called 50S ribosomal protein L25.

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

- Molecule 53 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	DD	76	Total	C	N	O	S	1	0
			591	365	121	104	1		

- Molecule 54 is a protein called 50S ribosomal protein L28.

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

- Molecule 55 is a protein called 50S ribosomal protein L29.

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

- Molecule 56 is a protein called 50S ribosomal protein L10.

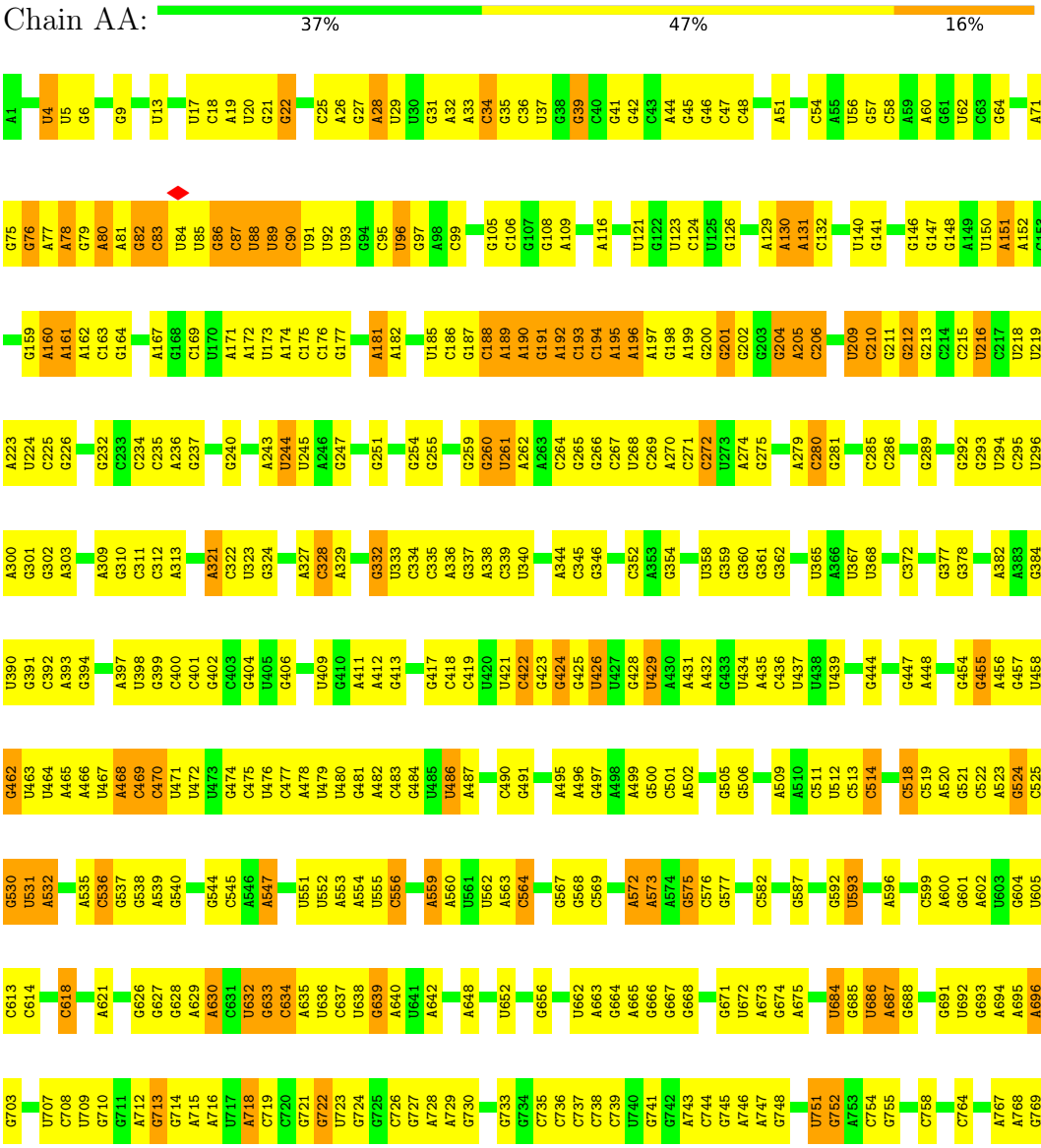
Mol	Chain	Residues	Atoms					AltConf	Trace
56	DG	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

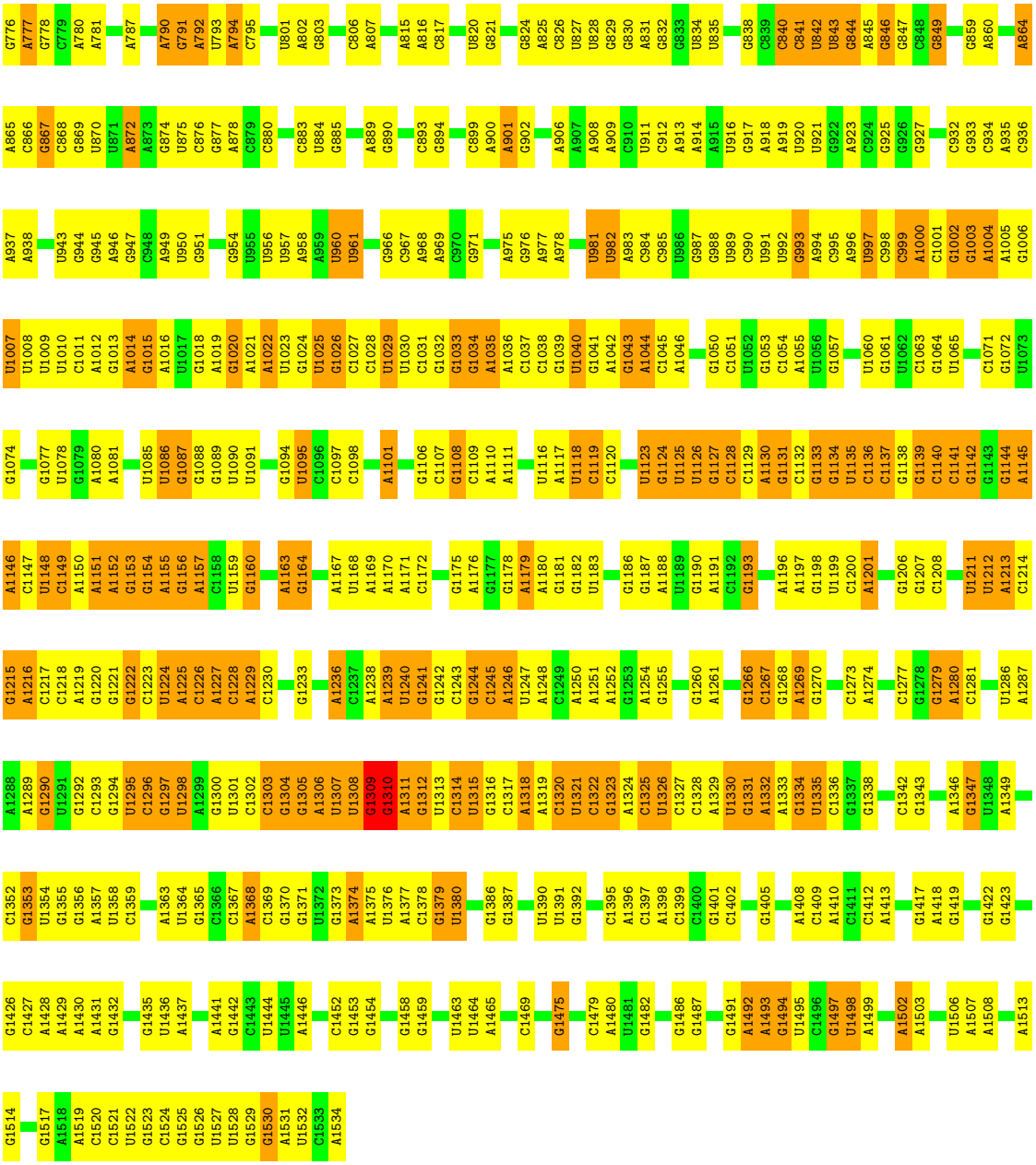
3 Residue-property plots (i)

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: 16S rRNA

Chain AA:



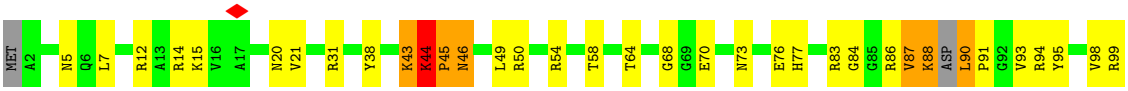


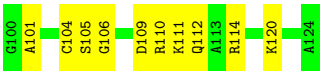
• Molecule 2: 30S ribosomal protein S20

Chain AB:

• Molecule 3: 30S ribosomal protein S12

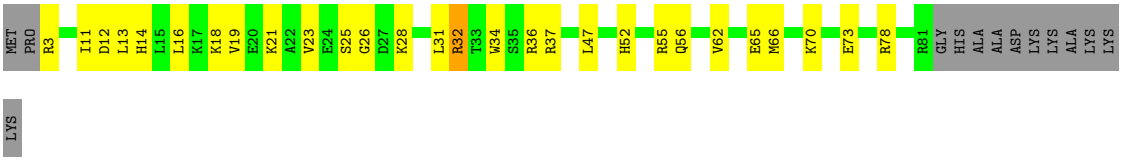
Chain AC:





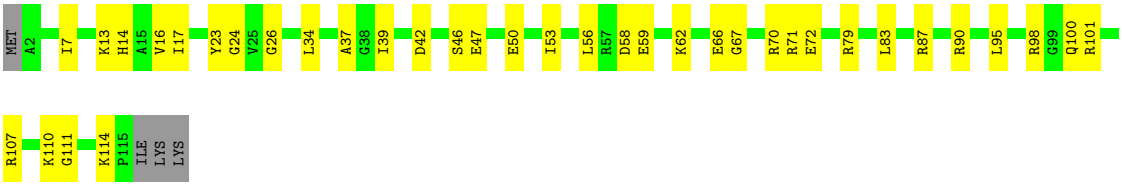
• Molecule 4: 30S ribosomal protein S19

Chain AD:



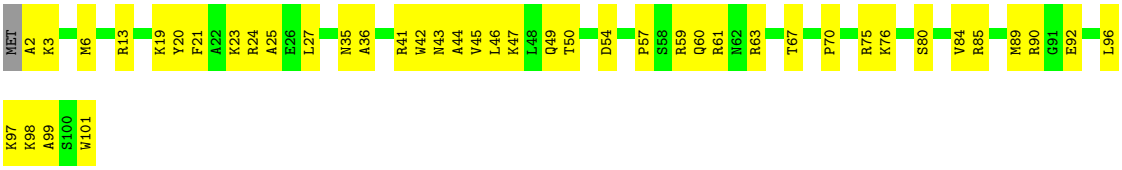
• Molecule 5: 30S ribosomal protein S13

Chain AE:



• Molecule 6: 30S ribosomal protein S14

Chain AF:

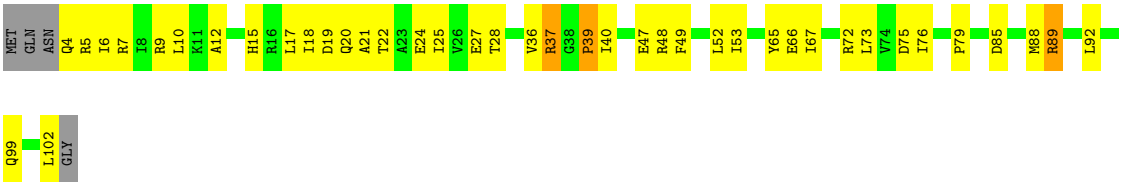


• Molecule 7: 30S ribosomal protein S3

Chain AG:

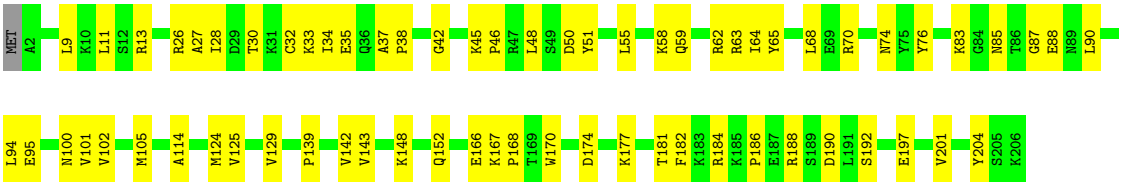
• Molecule 8: 30S ribosomal protein S10

Chain AH:



• Molecule 9: 30S ribosomal protein S4

Chain AI:

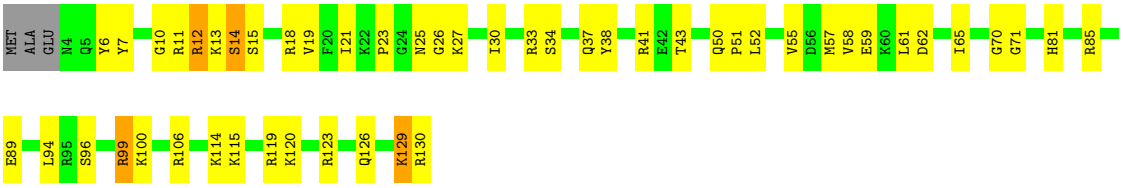


• Molecule 10: 30S ribosomal protein S2

Chain AJ:

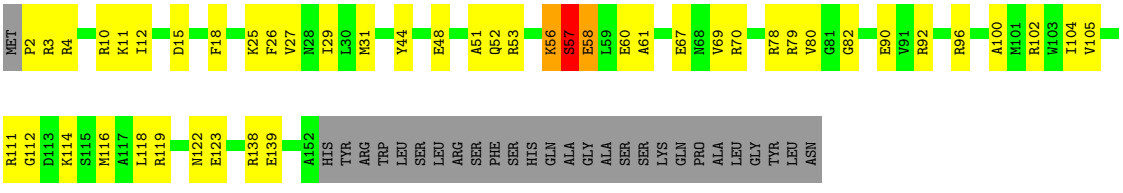
• Molecule 11: 30S ribosomal protein S9

Chain AK:



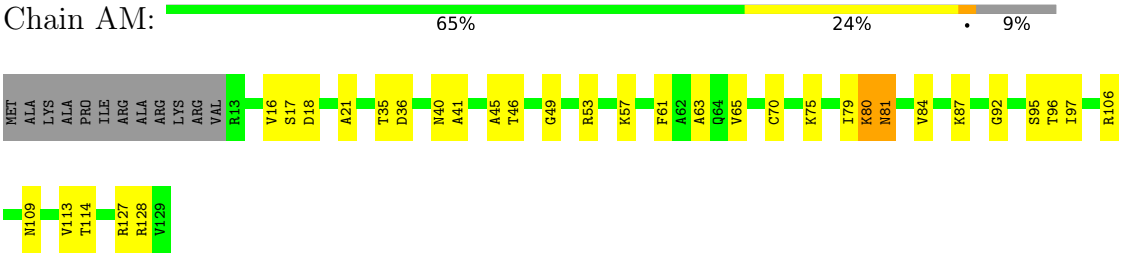
• Molecule 12: 30S ribosomal protein S7

Chain AL:



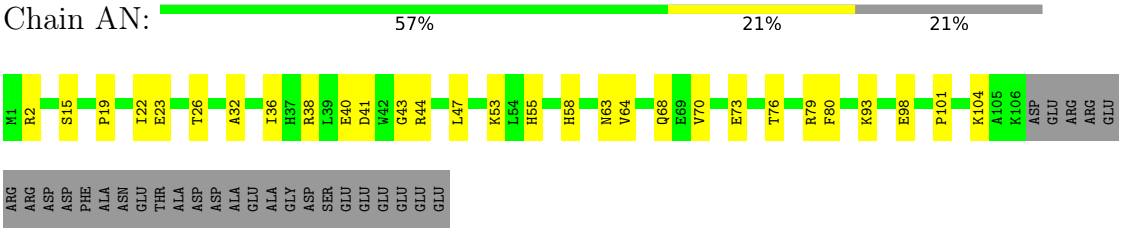
• Molecule 13: 30S ribosomal protein S11

Chain AM:



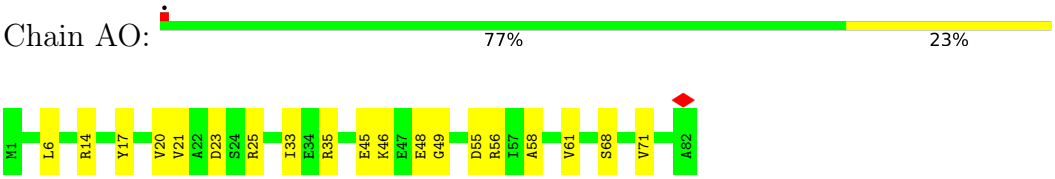
• Molecule 14: 30S ribosomal protein S6

Chain AN:



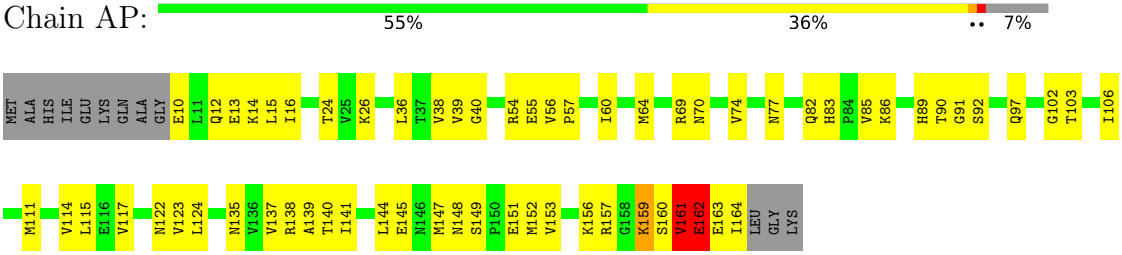
• Molecule 15: 30S ribosomal protein S16

Chain AO:



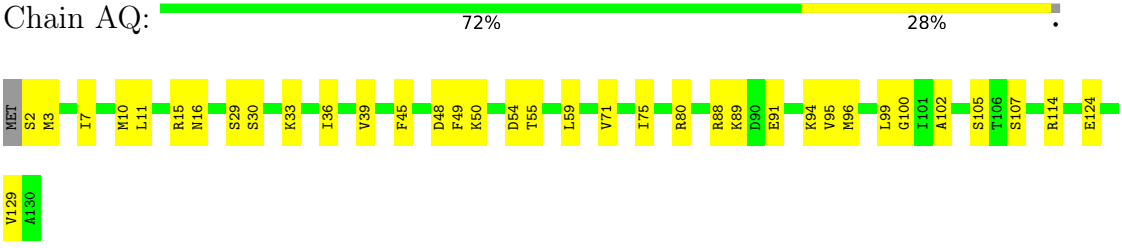
• Molecule 16: 30S ribosomal protein S5

Chain AP:



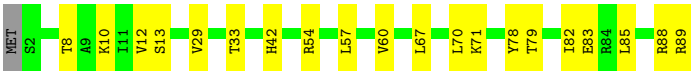
• Molecule 17: 30S ribosomal protein S8

Chain AQ:

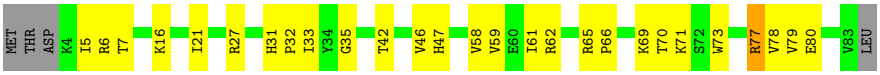


• Molecule 18: 30S ribosomal protein S15

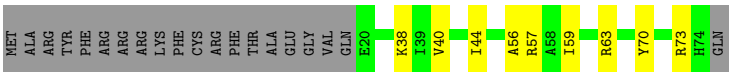
Chain AR:



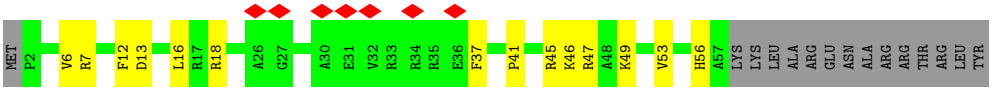
• Molecule 19: 30S ribosomal protein S17



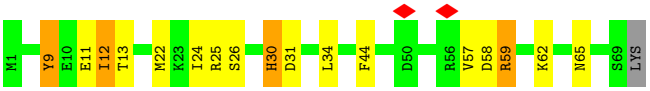
• Molecule 20: 30S ribosomal protein S18



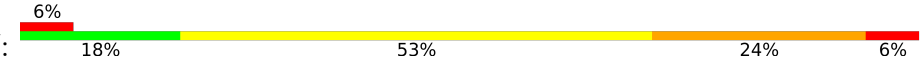
• Molecule 21: 30S ribosomal protein S21

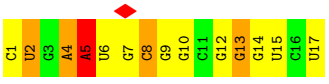


• Molecule 22: 50S ribosomal protein L31

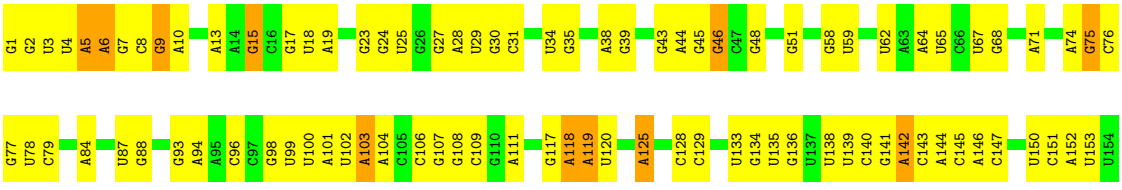


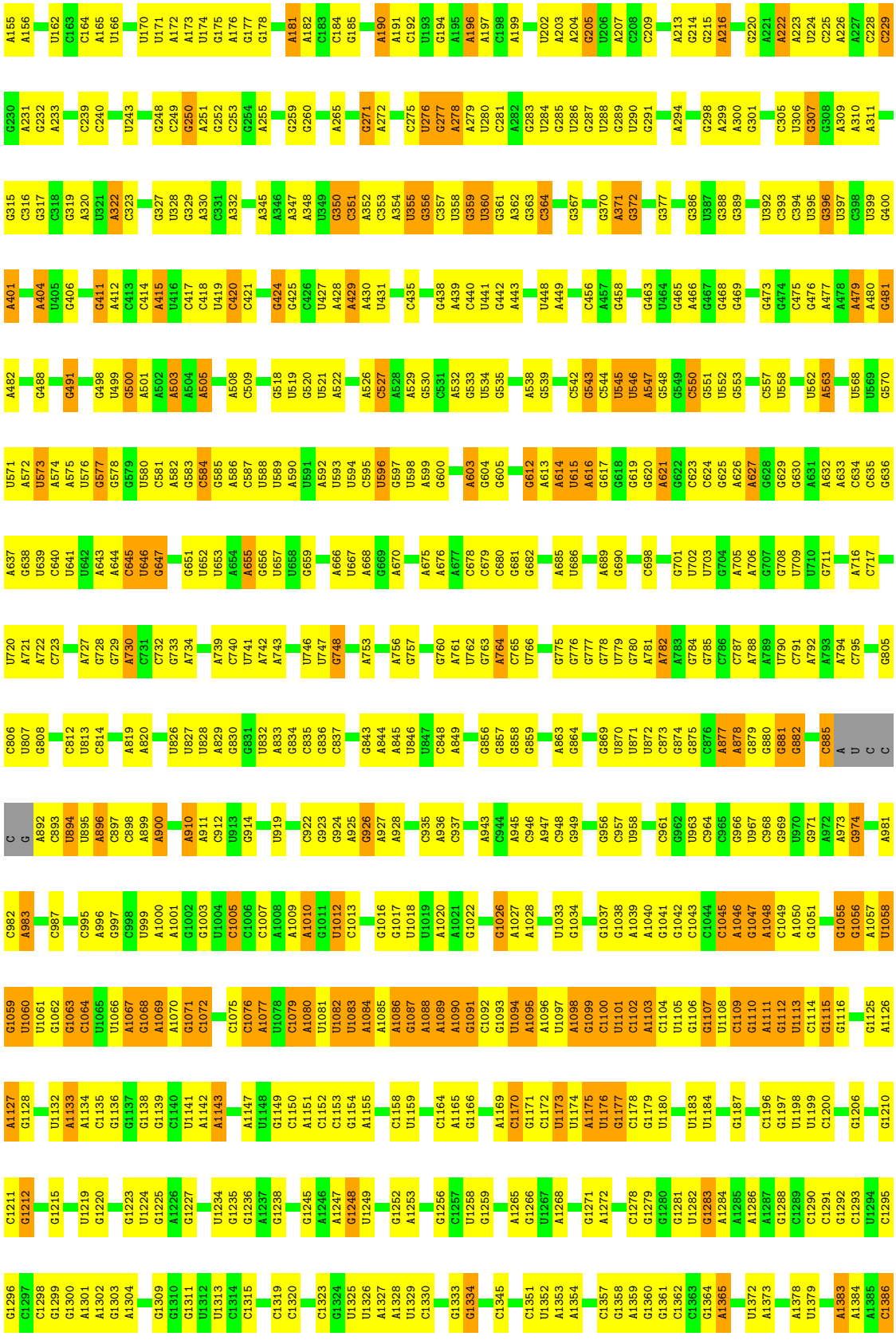
• Molecule 23: mRNA

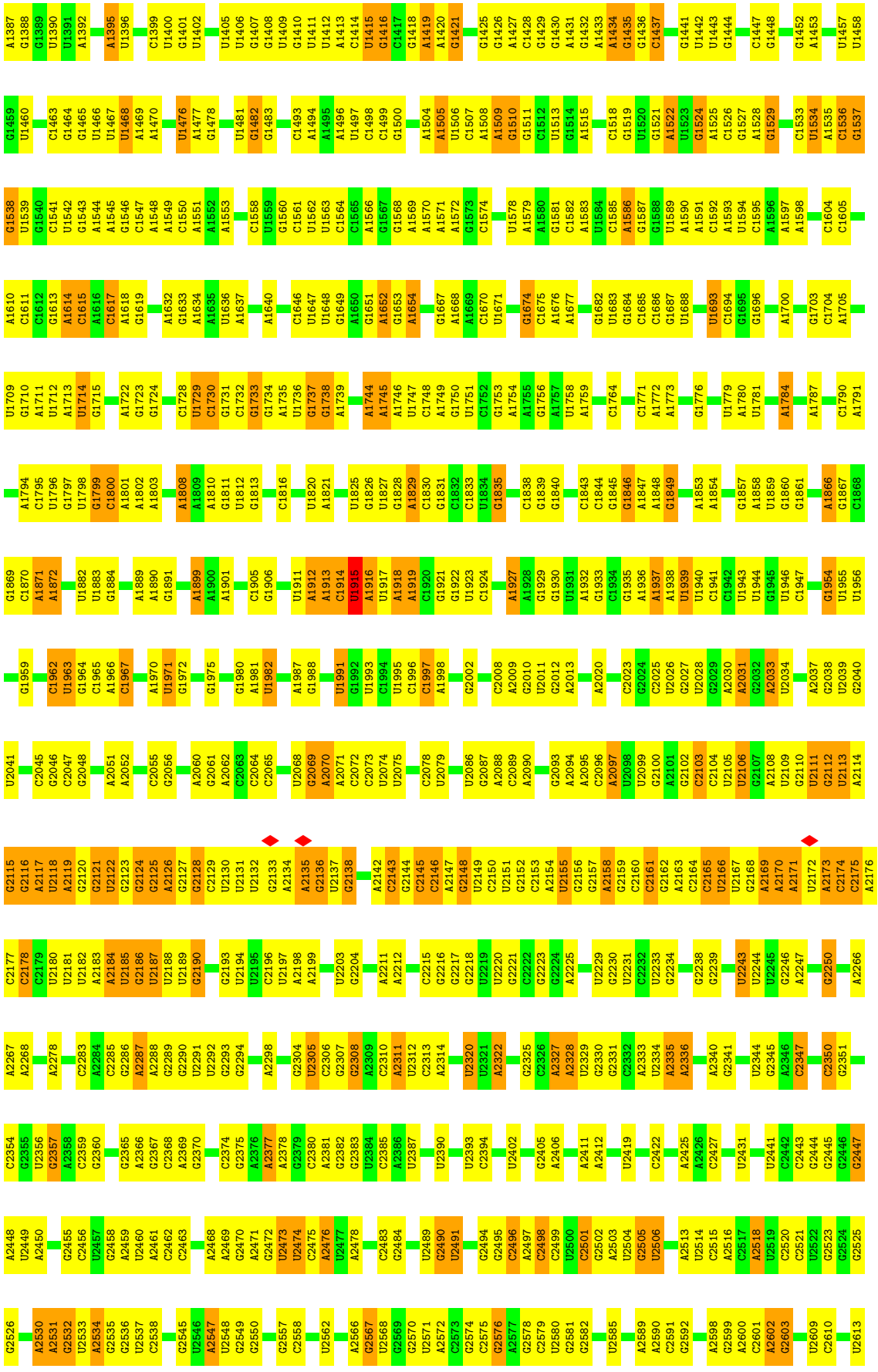


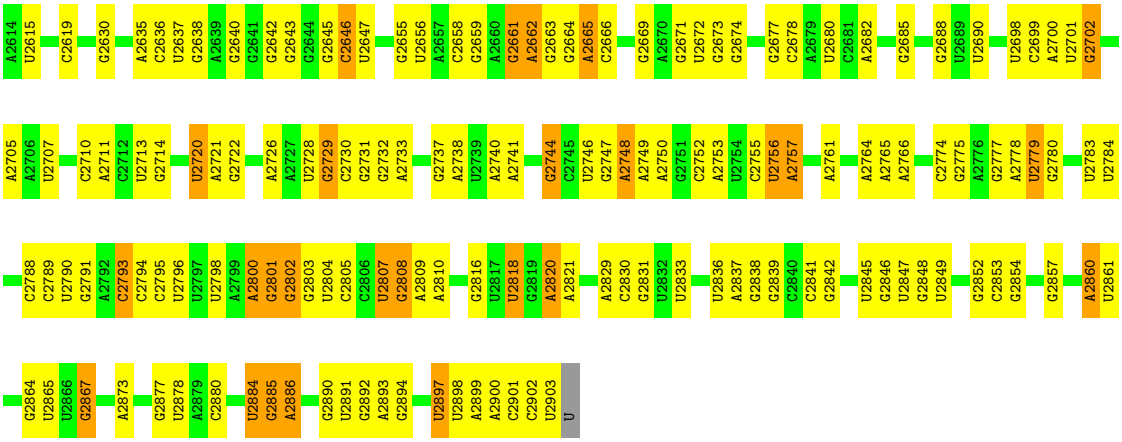


• Molecule 24: 23S rRNA









• Molecule 25: P-site tRNA

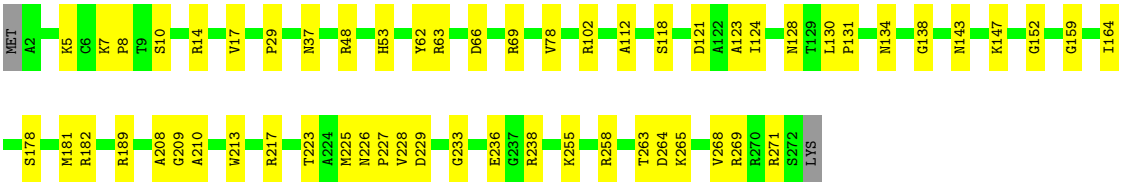
Chain BB:

• Molecule 26: 5s rRNA

Chain BC:

• Molecule 27: 50S ribosomal protein L2

Chain BD:

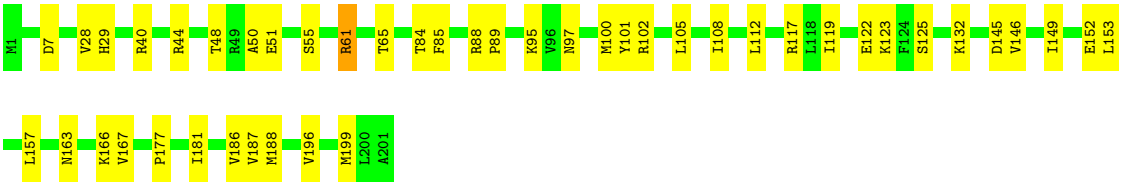


• Molecule 28: 50S ribosomal protein L3

Chain BE:

• Molecule 29: 50S ribosomal protein L4

Chain BF:

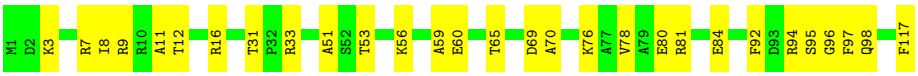


• Molecule 30: 50S ribosomal protein L5

Chain BG:

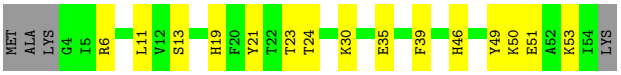
• Molecule 31: 50S ribosomal protein L18

Chain BH:



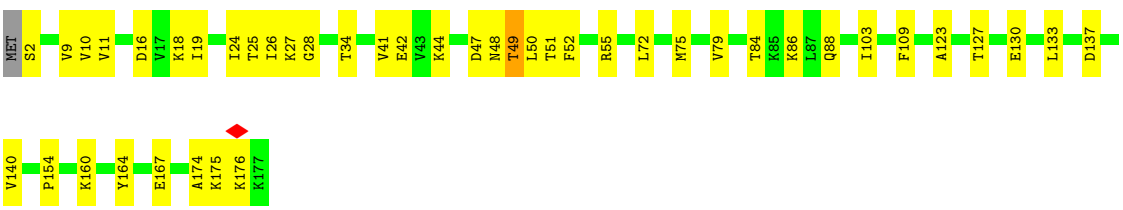
• Molecule 32: 50S ribosomal protein L33

Chain BI:



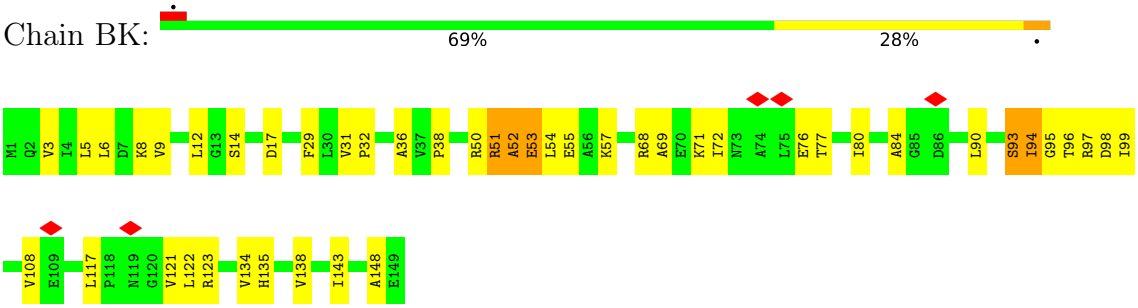
• Molecule 33: 50S ribosomal protein L6

Chain BJ:



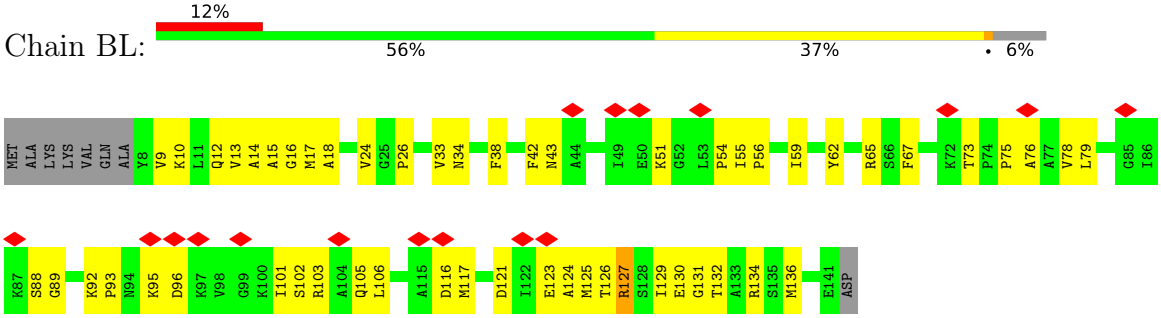
• Molecule 34: 50S ribosomal protein L9

Chain BK:



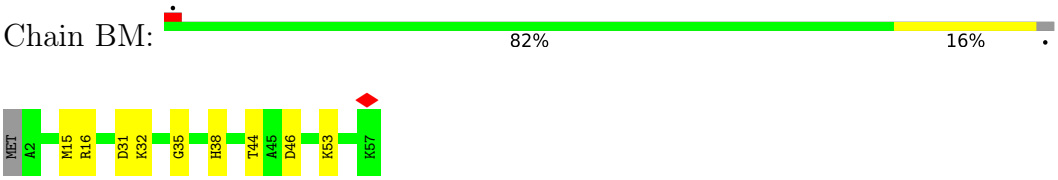
• Molecule 35: 50S ribosomal protein L11

Chain BL:



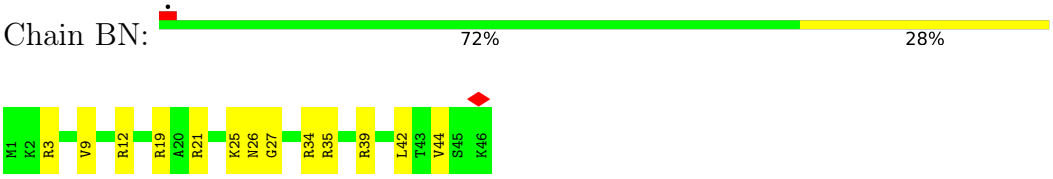
• Molecule 36: 50S ribosomal protein L32

Chain BM:



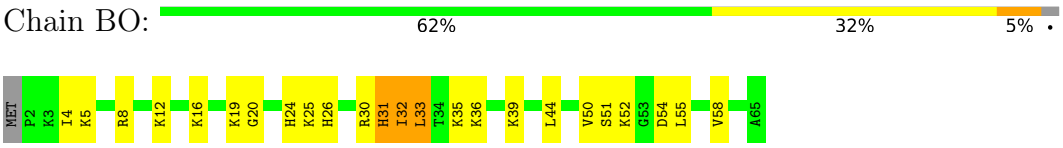
• Molecule 37: 50S ribosomal protein L34

Chain BN:



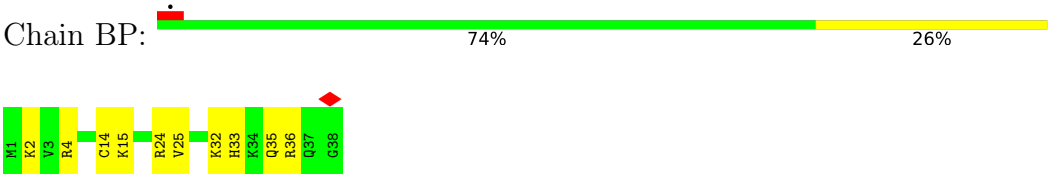
• Molecule 38: 50S ribosomal protein L35

Chain BO:



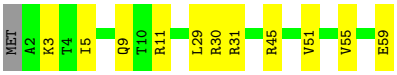
• Molecule 39: 50S ribosomal protein L36

Chain BP:



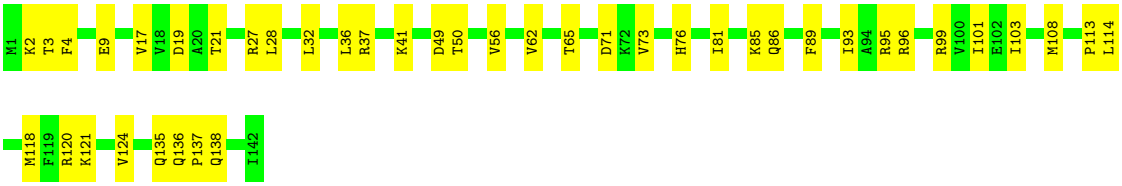
• Molecule 40: 50S ribosomal protein L30

Chain BQ:



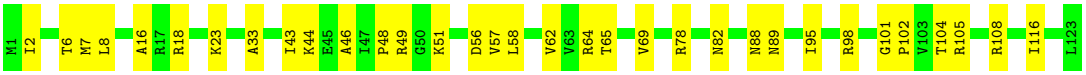
• Molecule 41: 50S ribosomal protein L13

Chain BR:



• Molecule 42: 50S ribosomal protein L14

Chain BS:

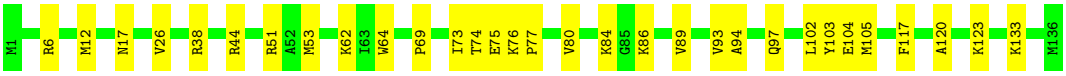


• Molecule 43: 50S ribosomal protein L15

Chain BT:

• Molecule 44: 50S ribosomal protein L16

Chain BU:

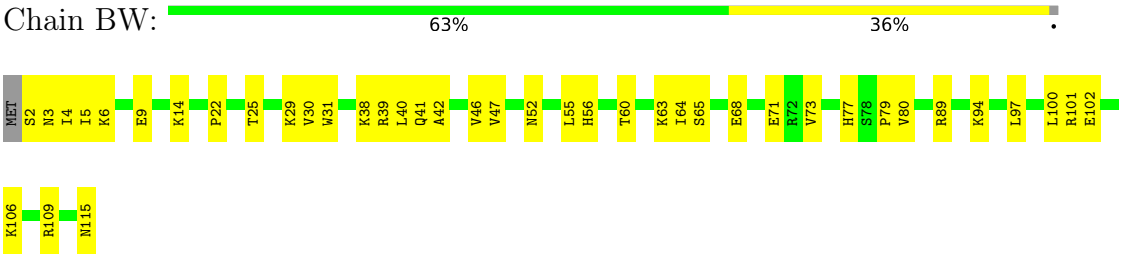


• Molecule 45: 50S ribosomal protein L17

Chain BV:

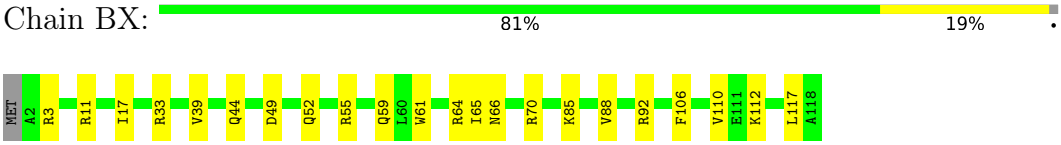
• Molecule 46: 50S ribosomal protein L19

Chain BW:



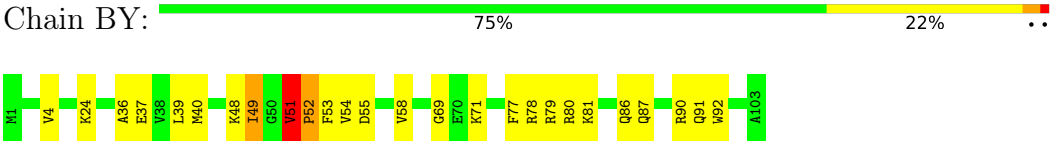
• Molecule 47: 50S ribosomal protein L20

Chain BX:



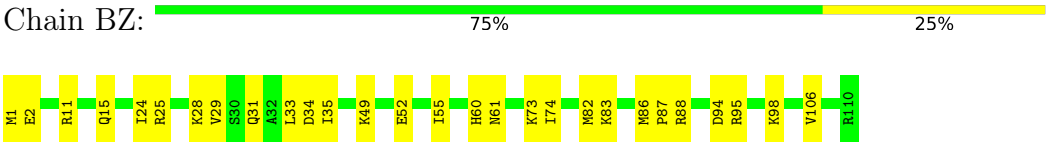
• Molecule 48: Ribosomal protein L21

Chain BY:



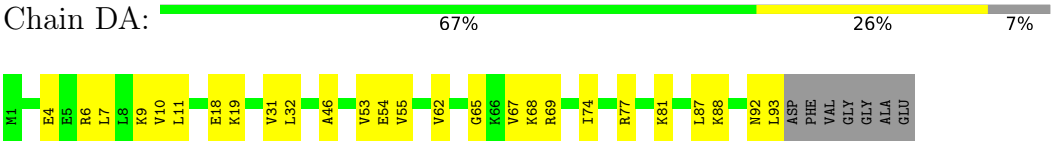
• Molecule 49: 50S ribosomal protein L22

Chain BZ:



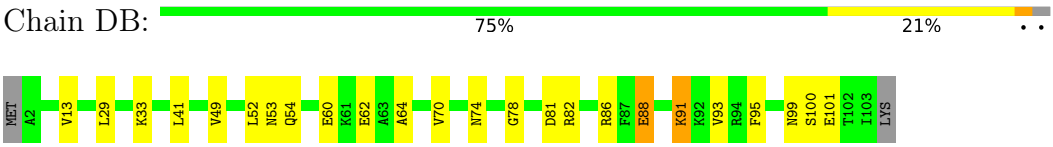
• Molecule 50: 50S ribosomal protein L23

Chain DA:



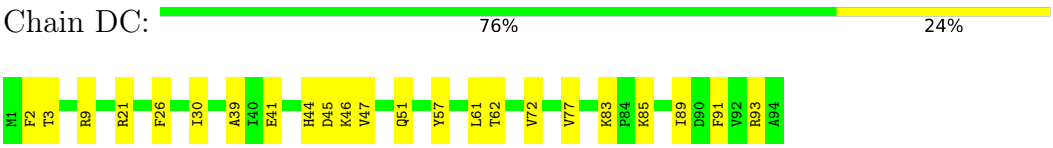
• Molecule 51: 50S ribosomal protein L24

Chain DB:



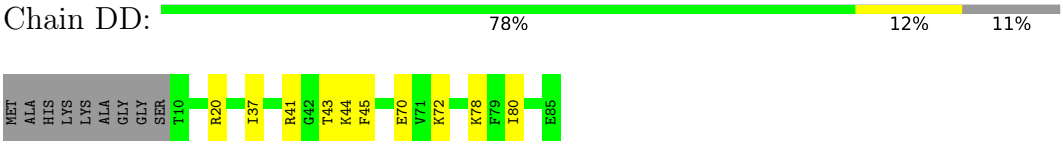
• Molecule 52: 50S ribosomal protein L25

Chain DC:



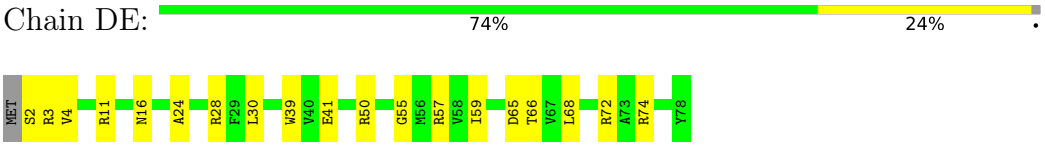
• Molecule 53: 50S ribosomal protein L27

Chain DD:



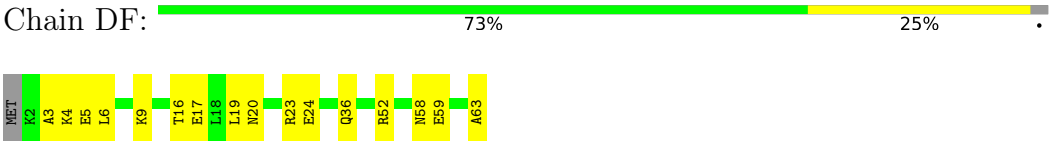
• Molecule 54: 50S ribosomal protein L28

Chain DE:



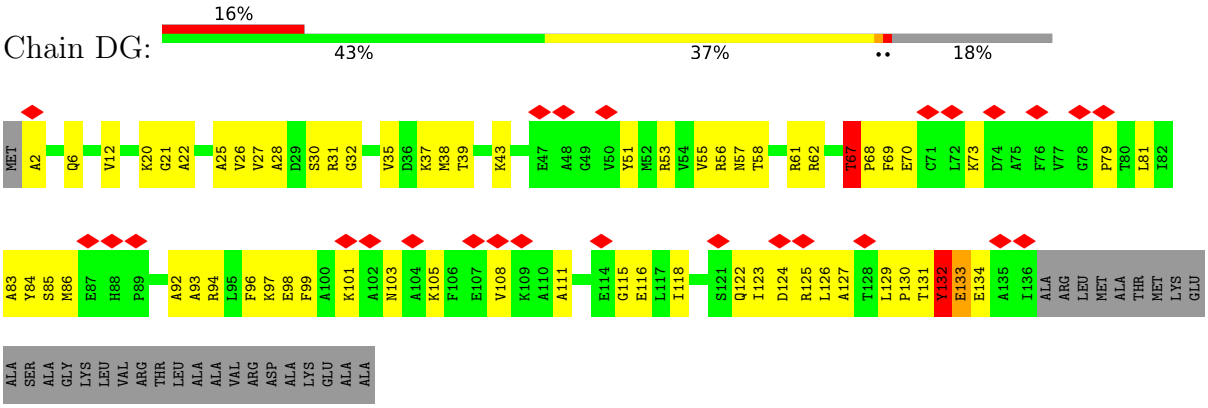
• Molecule 55: 50S ribosomal protein L29

Chain DF:



• Molecule 56: 50S ribosomal protein L10

Chain DG:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18629	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.405	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	601.952, 601.952, 601.952	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.447, 1.447, 1.447	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.30	0/36859	0.81	4/57501 (0.0%)
2	AB	0.26	0/676	0.50	0/895
3	AC	0.30	0/960	0.65	0/1286
4	AD	0.26	0/652	0.55	0/877
5	AE	0.25	0/892	0.59	0/1193
6	AF	0.25	0/817	0.60	0/1088
7	AG	0.27	0/1651	0.56	0/2225
8	AH	0.39	0/805	0.72	1/1089 (0.1%)
9	AI	0.26	0/1665	0.53	0/2227
10	AJ	0.25	0/1784	0.53	0/2403
11	AK	0.36	1/1034 (0.1%)	0.63	0/1375
12	AL	0.28	0/1195	0.55	0/1602
13	AM	0.27	0/893	0.56	0/1205
14	AN	0.27	0/881	0.55	0/1189
15	AO	0.26	0/659	0.58	0/884
16	AP	0.30	0/1157	0.60	0/1557
17	AQ	0.27	0/989	0.56	0/1326
18	AR	0.27	0/722	0.60	0/964
19	AS	0.28	0/657	0.62	0/881
20	AT	0.26	0/462	0.58	0/621
21	AU	0.26	0/472	0.58	0/627
22	AV	0.72	0/549	1.14	1/734 (0.1%)
23	AW	0.60	1/407 (0.2%)	0.98	1/633 (0.2%)
24	BA	0.30	1/69710 (0.0%)	0.79	0/108752
25	BB	0.40	0/1784	0.90	0/2778
26	BC	0.27	0/2872	0.77	0/4478
27	BD	0.27	0/2121	0.57	0/2852
28	BE	0.29	0/1576	0.55	0/2119
29	BF	0.26	0/1571	0.51	0/2113
30	BG	0.32	0/1434	0.56	0/1926
31	BH	0.26	0/910	0.59	0/1219
32	BI	0.25	0/421	0.53	0/561
33	BJ	0.28	0/1343	0.53	0/1816
34	BK	0.29	0/1121	0.56	0/1515

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	BL	0.26	0/993	0.55	0/1341
36	BM	0.25	0/450	0.56	0/599
37	BN	0.25	0/380	0.65	0/498
38	BO	0.29	0/513	0.54	0/676
39	BP	0.26	0/303	0.55	0/397
40	BQ	0.25	0/467	0.55	0/623
41	BR	0.27	0/1152	0.55	0/1551
42	BS	0.27	0/955	0.59	0/1279
43	BT	0.27	0/1062	0.59	0/1413
44	BU	0.29	0/1104	0.60	0/1474
45	BV	0.27	0/1006	0.58	0/1345
46	BW	0.27	0/929	0.56	0/1242
47	BX	0.27	0/960	0.53	0/1278
48	BY	0.34	0/829	0.58	0/1107
49	BZ	0.25	0/864	0.55	0/1156
50	DA	0.26	0/744	0.58	0/994
51	DB	0.29	0/787	0.53	0/1051
52	DC	0.27	0/766	0.55	0/1025
53	DD	0.26	0/598	0.55	0/790
54	DE	0.26	0/635	0.59	0/848
55	DF	0.27	0/502	0.60	0/667
56	DG	0.29	0/1037	0.56	0/1400
All	All	0.30	3/158737 (0.0%)	0.74	7/237265 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AK	129	LYS	C-N	7.15	1.50	1.34
24	BA	1915	U	C1'-N1	7.07	1.59	1.48
23	AW	2	U	C1'-N1	5.88	1.57	1.48

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1310	G	O3'-P-O5'	-15.99	73.61	104.00
8	AH	39	PRO	CA-N-CD	-8.58	99.49	111.50
1	AA	1310	G	OP2-P-O3'	7.77	122.29	105.20
1	AA	1310	G	C3'-C2'-C1'	-7.29	95.67	101.50
23	AW	5	A	C3'-C2'-C1'	-6.70	96.14	101.50

There are no chirality outliers.

There are no planarity outliers.

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	AA	32917	0	16563	855	0
2	AB	670	0	719	14	0
3	AC	947	0	1011	71	0
4	AD	637	0	665	23	0
5	AE	883	0	941	34	0
6	AF	805	0	844	32	0
7	AG	1624	0	1696	40	0
8	AH	795	0	836	46	0
9	AI	1643	0	1707	52	0
10	AJ	1753	0	1780	48	0
11	AK	1022	0	1070	50	0
12	AL	1181	0	1238	38	0
13	AM	877	0	887	25	0
14	AN	862	0	864	25	0
15	AO	649	0	666	12	0
16	AP	1144	0	1185	57	0
17	AQ	979	0	1031	34	0
18	AR	714	0	734	14	0
19	AS	648	0	691	24	0
20	AT	455	0	478	11	0
21	AU	465	0	491	9	0
22	AV	539	0	539	31	0
23	AW	365	0	184	22	0
24	BA	62218	0	31285	1365	0
25	BB	1598	0	817	97	0
26	BC	2569	0	1301	30	0
27	BD	2082	0	2154	42	0
28	BE	1556	0	1607	63	0
29	BF	1552	0	1619	38	0
30	BG	1410	0	1444	69	0
31	BH	900	0	935	22	0
32	BI	414	0	442	12	0
33	BJ	1323	0	1371	35	0
34	BK	1110	0	1148	57	0
35	BL	979	0	1028	44	0
36	BM	444	0	458	9	0
37	BN	377	0	418	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BO	504	0	572	25	0
39	BP	302	0	343	7	0
40	BQ	463	0	504	8	0
41	BR	1129	0	1162	34	0
42	BS	946	0	1023	25	0
43	BT	1053	0	1129	28	0
44	BU	1082	0	1170	24	0
45	BV	993	0	1034	30	0
46	BW	917	0	962	29	0
47	BX	947	0	1019	22	0
48	BY	816	0	839	44	0
49	BZ	857	0	922	21	0
50	DA	738	0	807	21	0
51	DB	779	0	831	29	0
52	DC	753	0	780	14	0
53	DD	591	0	606	10	0
54	DE	625	0	652	18	0
55	DF	501	0	531	17	0
56	DG	1023	0	1050	90	0
All	All	146125	0	98783	3535	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 15.

The worst 5 of 3535 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:AA:523:A:C2	3:AC:88:LYS:CB	1.94	1.48
24:BA:222:A:H62	24:BA:232:G:N2	1.14	1.46
3:AC:44:LYS:CG	3:AC:45:PRO:HD2	1.44	1.45
24:BA:222:A:N6	24:BA:232:G:H21	1.15	1.45
1:AA:1347:G:N7	11:AK:13:LYS:HE2	1.14	1.43

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
2	AB	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
3	AC	118/124 (95%)	110 (93%)	6 (5%)	2 (2%)	9 43
4	AD	77/92 (84%)	73 (95%)	4 (5%)	0	100 100
5	AE	112/118 (95%)	104 (93%)	8 (7%)	0	100 100
6	AF	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
7	AG	204/233 (88%)	198 (97%)	6 (3%)	0	100 100
8	AH	97/103 (94%)	89 (92%)	8 (8%)	0	100 100
9	AI	203/206 (98%)	201 (99%)	2 (1%)	0	100 100
10	AJ	222/241 (92%)	208 (94%)	14 (6%)	0	100 100
11	AK	125/130 (96%)	116 (93%)	9 (7%)	0	100 100
12	AL	149/179 (83%)	142 (95%)	6 (4%)	1 (1%)	22 60
13	AM	115/129 (89%)	110 (96%)	5 (4%)	0	100 100
14	AN	104/135 (77%)	103 (99%)	1 (1%)	0	100 100
15	AO	80/82 (98%)	73 (91%)	7 (9%)	0	100 100
16	AP	153/167 (92%)	143 (94%)	6 (4%)	4 (3%)	5 36
17	AQ	127/130 (98%)	123 (97%)	4 (3%)	0	100 100
18	AR	86/89 (97%)	86 (100%)	0	0	100 100
19	AS	78/84 (93%)	75 (96%)	3 (4%)	0	100 100
20	AT	53/75 (71%)	53 (100%)	0	0	100 100
21	AU	54/71 (76%)	53 (98%)	1 (2%)	0	100 100
22	AV	67/70 (96%)	53 (79%)	11 (16%)	3 (4%)	2 25
27	BD	269/273 (98%)	260 (97%)	9 (3%)	0	100 100
28	BE	204/209 (98%)	197 (97%)	6 (3%)	1 (0%)	29 66
29	BF	199/201 (99%)	194 (98%)	5 (2%)	0	100 100
30	BG	175/179 (98%)	159 (91%)	15 (9%)	1 (1%)	25 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
32	BI	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
33	BJ	174/177 (98%)	166 (95%)	6 (3%)	2 (1%)	14	51
34	BK	147/149 (99%)	133 (90%)	11 (8%)	3 (2%)	7	41
35	BL	132/142 (93%)	123 (93%)	9 (7%)	0	100	100
36	BM	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
37	BN	44/46 (96%)	44 (100%)	0	0	100	100
38	BO	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	9	44
39	BP	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
40	BQ	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
41	BR	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
42	BS	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
43	BT	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
44	BU	135/136 (99%)	130 (96%)	5 (4%)	0	100	100
45	BV	123/127 (97%)	112 (91%)	11 (9%)	0	100	100
46	BW	112/115 (97%)	112 (100%)	0	0	100	100
47	BX	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
48	BY	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	7	41
49	BZ	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
50	DA	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
51	DB	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
52	DC	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
53	DD	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
54	DE	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
55	DF	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
56	DG	133/165 (81%)	114 (86%)	15 (11%)	4 (3%)	4	33
All	All	5846/6220 (94%)	5567 (95%)	255 (4%)	24 (0%)	38	70

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	44	LYS
16	AP	160	SER

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Mol	Chain	Res	Type
22	AV	31	ASP
22	AV	62	LYS
22	AV	65	ASN

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	
2	AB	65/66 (98%)	65 (100%)	0	100	100
3	AC	102/104 (98%)	96 (94%)	6 (6%)	19	51
4	AD	70/79 (89%)	69 (99%)	1 (1%)	67	81
5	AE	92/96 (96%)	92 (100%)	0	100	100
6	AF	83/84 (99%)	81 (98%)	2 (2%)	49	71
7	AG	170/190 (90%)	169 (99%)	1 (1%)	86	92
8	AH	87/90 (97%)	85 (98%)	2 (2%)	50	72
9	AI	172/173 (99%)	172 (100%)	0	100	100
10	AJ	186/199 (94%)	186 (100%)	0	100	100
11	AK	105/107 (98%)	102 (97%)	3 (3%)	42	67
12	AL	124/147 (84%)	121 (98%)	3 (2%)	49	71
13	AM	90/99 (91%)	86 (96%)	4 (4%)	28	57
14	AN	92/116 (79%)	92 (100%)	0	100	100
15	AO	65/65 (100%)	65 (100%)	0	100	100
16	AP	118/126 (94%)	115 (98%)	3 (2%)	47	70
17	AQ	104/105 (99%)	104 (100%)	0	100	100
18	AR	76/77 (99%)	76 (100%)	0	100	100
19	AS	74/78 (95%)	72 (97%)	2 (3%)	44	69
20	AT	48/65 (74%)	48 (100%)	0	100	100
21	AU	48/61 (79%)	48 (100%)	0	100	100
22	AV	61/62 (98%)	57 (93%)	4 (7%)	16	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BD	216/218 (99%)	216 (100%)	0	100	100
28	BE	163/164 (99%)	163 (100%)	0	100	100
29	BF	165/165 (100%)	164 (99%)	1 (1%)	86	92
30	BG	148/150 (99%)	145 (98%)	3 (2%)	55	75
31	BH	87/87 (100%)	87 (100%)	0	100	100
32	BI	45/49 (92%)	44 (98%)	1 (2%)	52	72
33	BJ	137/138 (99%)	137 (100%)	0	100	100
34	BK	114/114 (100%)	111 (97%)	3 (3%)	46	69
35	BL	104/110 (94%)	103 (99%)	1 (1%)	76	86
36	BM	47/48 (98%)	47 (100%)	0	100	100
37	BN	38/38 (100%)	37 (97%)	1 (3%)	46	69
38	BO	51/52 (98%)	49 (96%)	2 (4%)	32	60
39	BP	34/34 (100%)	34 (100%)	0	100	100
40	BQ	49/49 (100%)	49 (100%)	0	100	100
41	BR	116/116 (100%)	116 (100%)	0	100	100
42	BS	104/104 (100%)	104 (100%)	0	100	100
43	BT	103/103 (100%)	103 (100%)	0	100	100
44	BU	110/109 (101%)	110 (100%)	0	100	100
45	BV	102/103 (99%)	102 (100%)	0	100	100
46	BW	99/100 (99%)	99 (100%)	0	100	100
47	BX	89/90 (99%)	89 (100%)	0	100	100
48	BY	84/84 (100%)	80 (95%)	4 (5%)	25	56
49	BZ	93/93 (100%)	93 (100%)	0	100	100
50	DA	80/84 (95%)	80 (100%)	0	100	100
51	DB	83/85 (98%)	81 (98%)	2 (2%)	49	71
52	DC	78/78 (100%)	77 (99%)	1 (1%)	69	82
53	DD	58/63 (92%)	58 (100%)	0	100	100
54	DE	67/68 (98%)	67 (100%)	0	100	100
55	DF	54/55 (98%)	53 (98%)	1 (2%)	57	76
56	DG	103/123 (84%)	100 (97%)	3 (3%)	42	67
All	All	4853/5063 (96%)	4799 (99%)	54 (1%)	74	85

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	AV	12	ILE
32	BI	53	LYS
52	DC	21	ARG
22	AV	30	HIS
30	BG	146	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
27	BD	53	HIS
27	BD	153	GLN
47	BX	59	GLN
35	BL	105	GLN
44	BU	13	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	420 (27%)	36 (2%)
23	AW	16/17 (94%)	5 (31%)	0
24	BA	2893/2904 (99%)	637 (22%)	35 (1%)
25	BB	74/77 (96%)	28 (37%)	1 (1%)
26	BC	119/120 (99%)	14 (11%)	0
All	All	4635/4652 (99%)	1104 (23%)	72 (1%)

5 of 1104 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	13	U

5 of 72 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2145	C
25	BB	1	C

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Mol	Chain	Res	Type
24	BA	2184	A
24	BA	2504	U
1	AA	1225	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

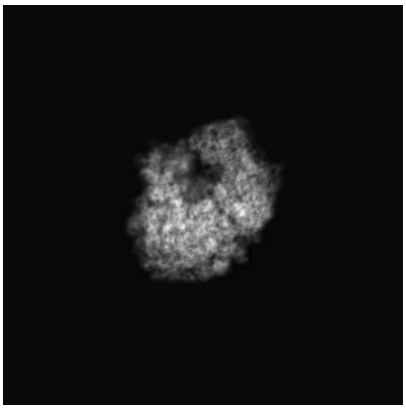
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29214. These allow visual inspection of the internal detail of the map and identification of artifacts.

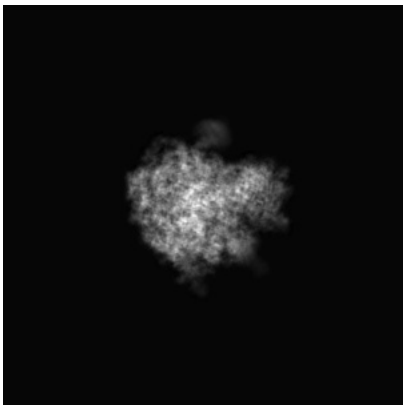
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

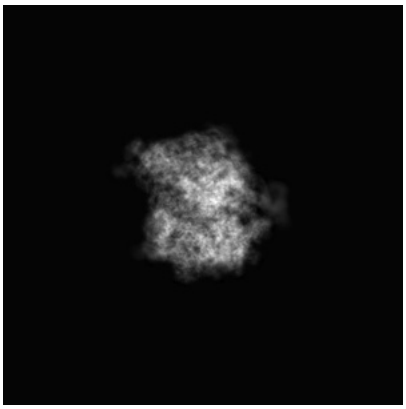
6.1.1 Primary map



X

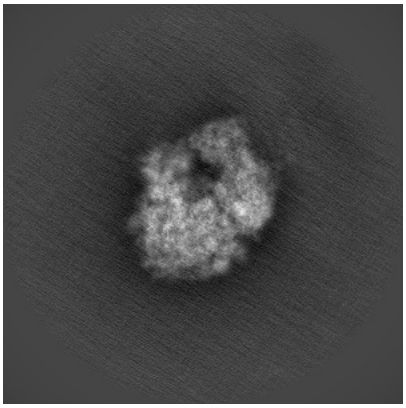


Y

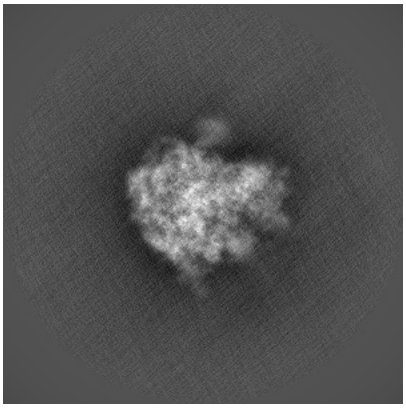


Z

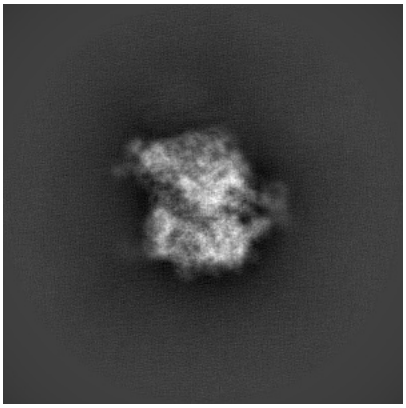
6.1.2 Raw map



X



Y

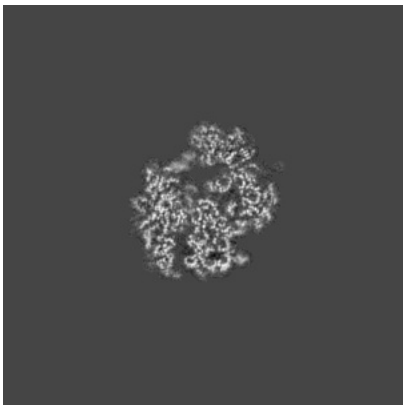


Z

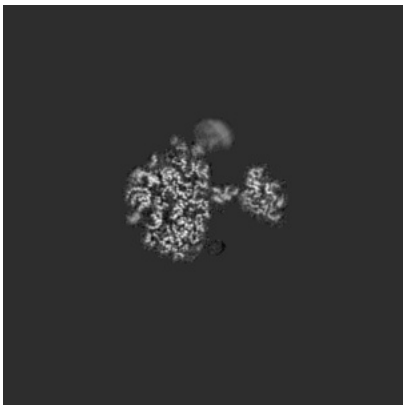
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



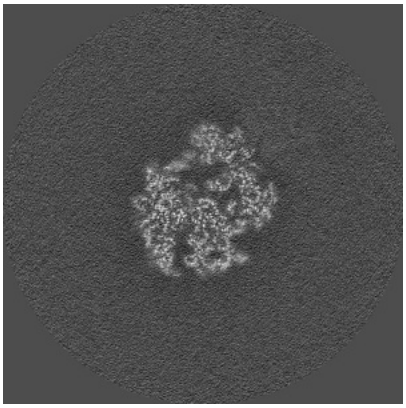
X Index: 208



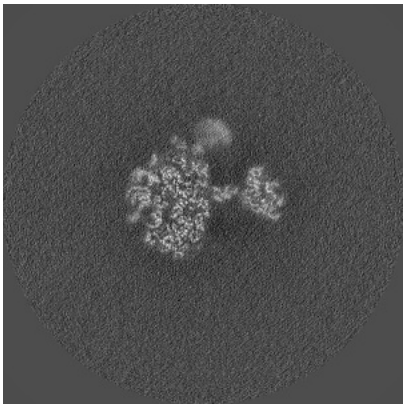
Y Index: 208

Z Index: 208

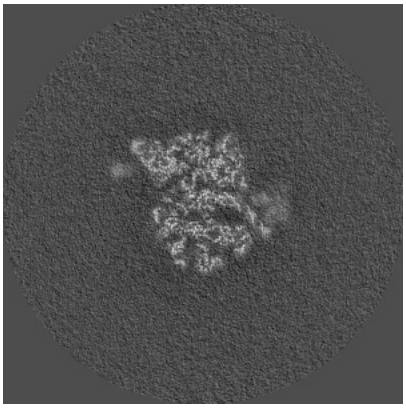
6.2.2 Raw map



X Index: 208



Y Index: 208

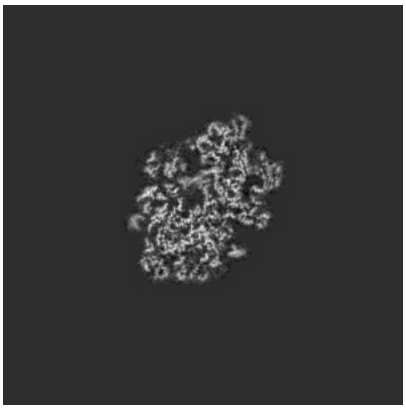


Z Index: 208

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

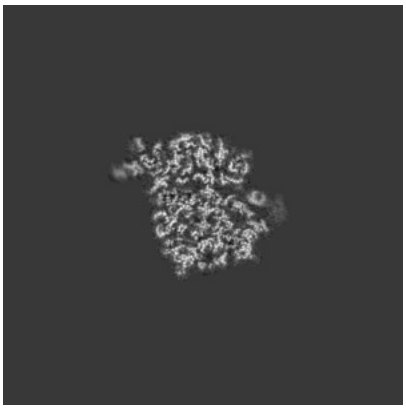
6.3 Largest variance slices (i)

6.3.1 Primary map



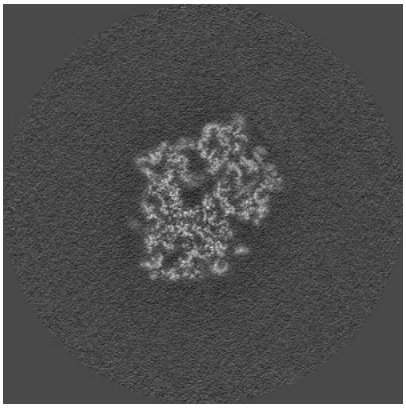
X Index: 221

Y Index: 231

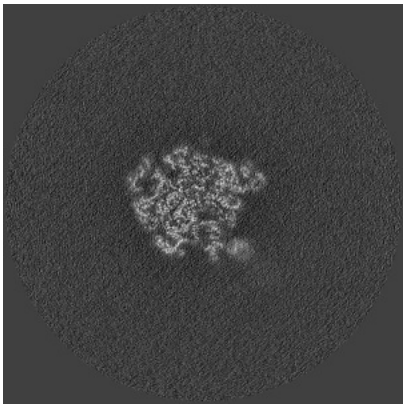


Z Index: 202

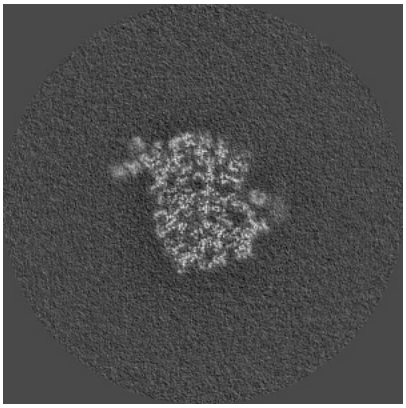
6.3.2 Raw map



X Index: 227



Y Index: 171

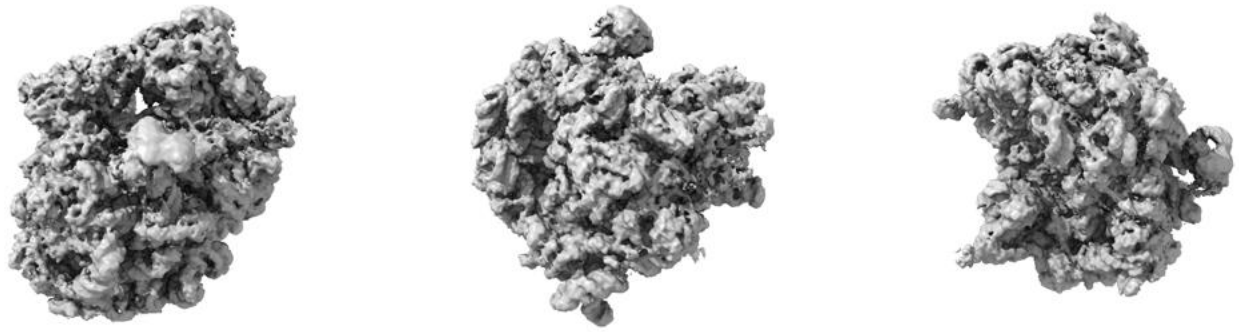


Z Index: 203

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

6.4 Orthogonal surface views (i)

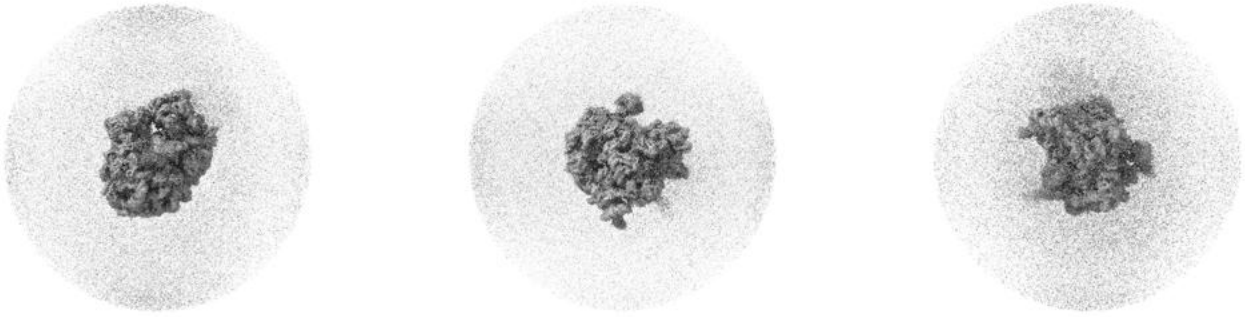
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

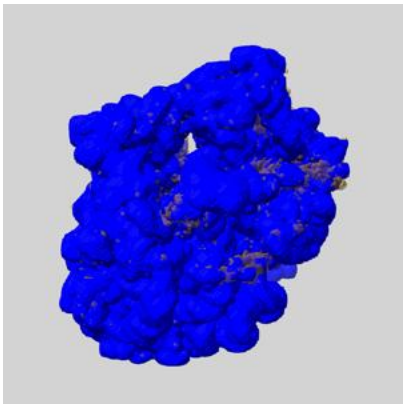
6.5 Mask visualisation

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

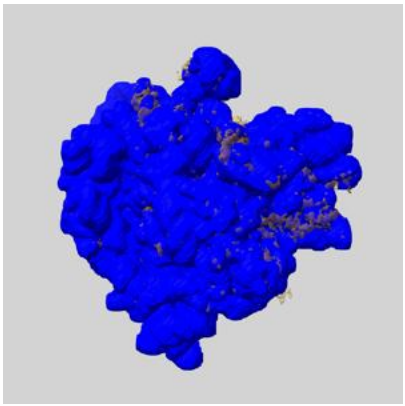
A mask typically either:

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

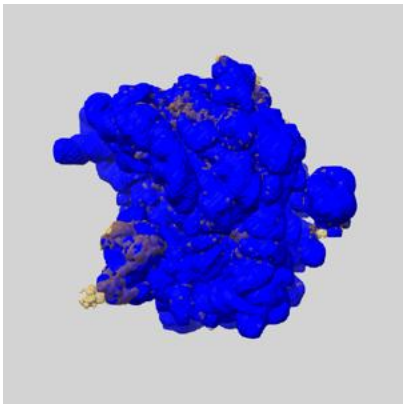
6.5.1 emd_29214_msk_1.map



X



Y

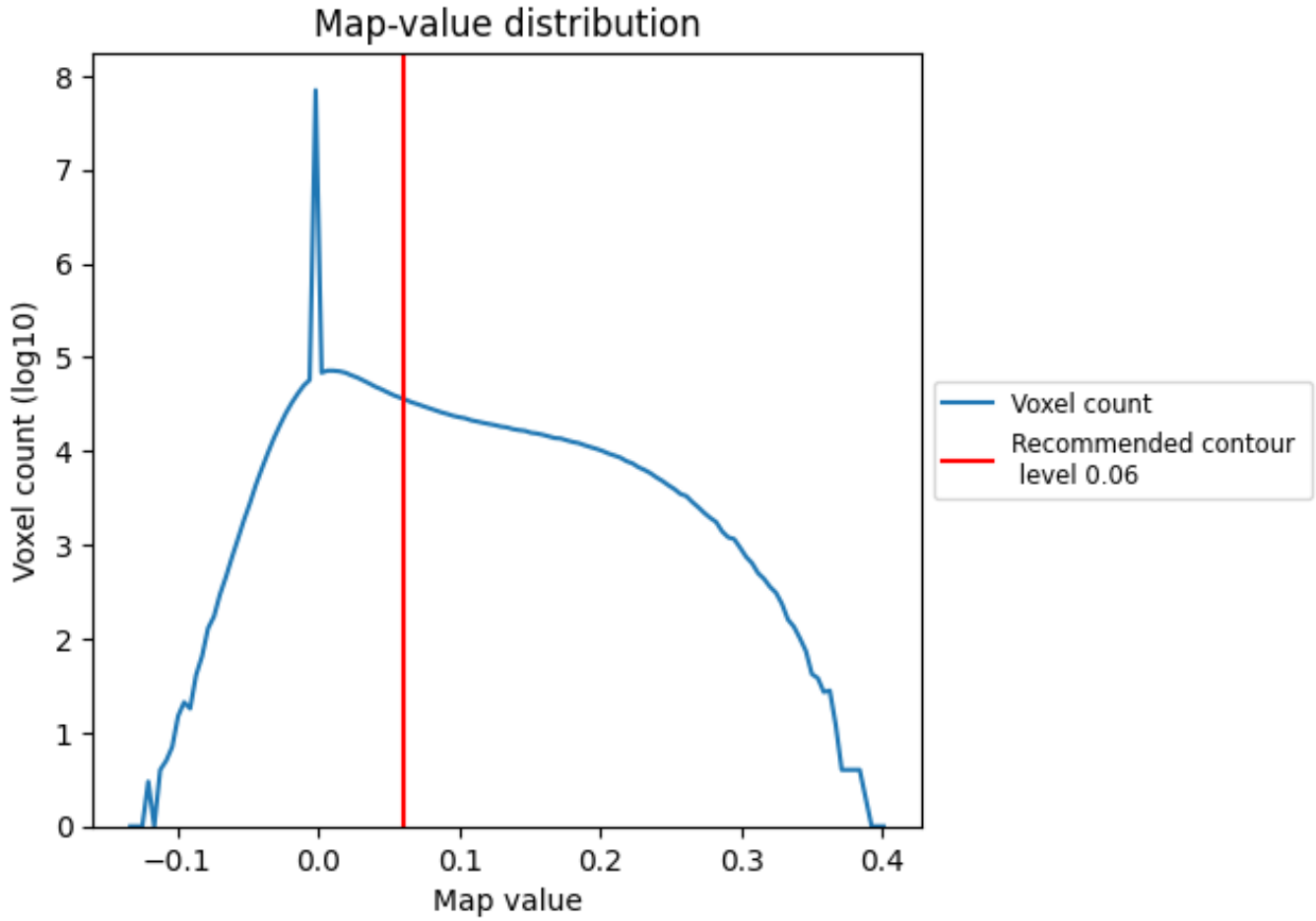


Z

7 Map analysis

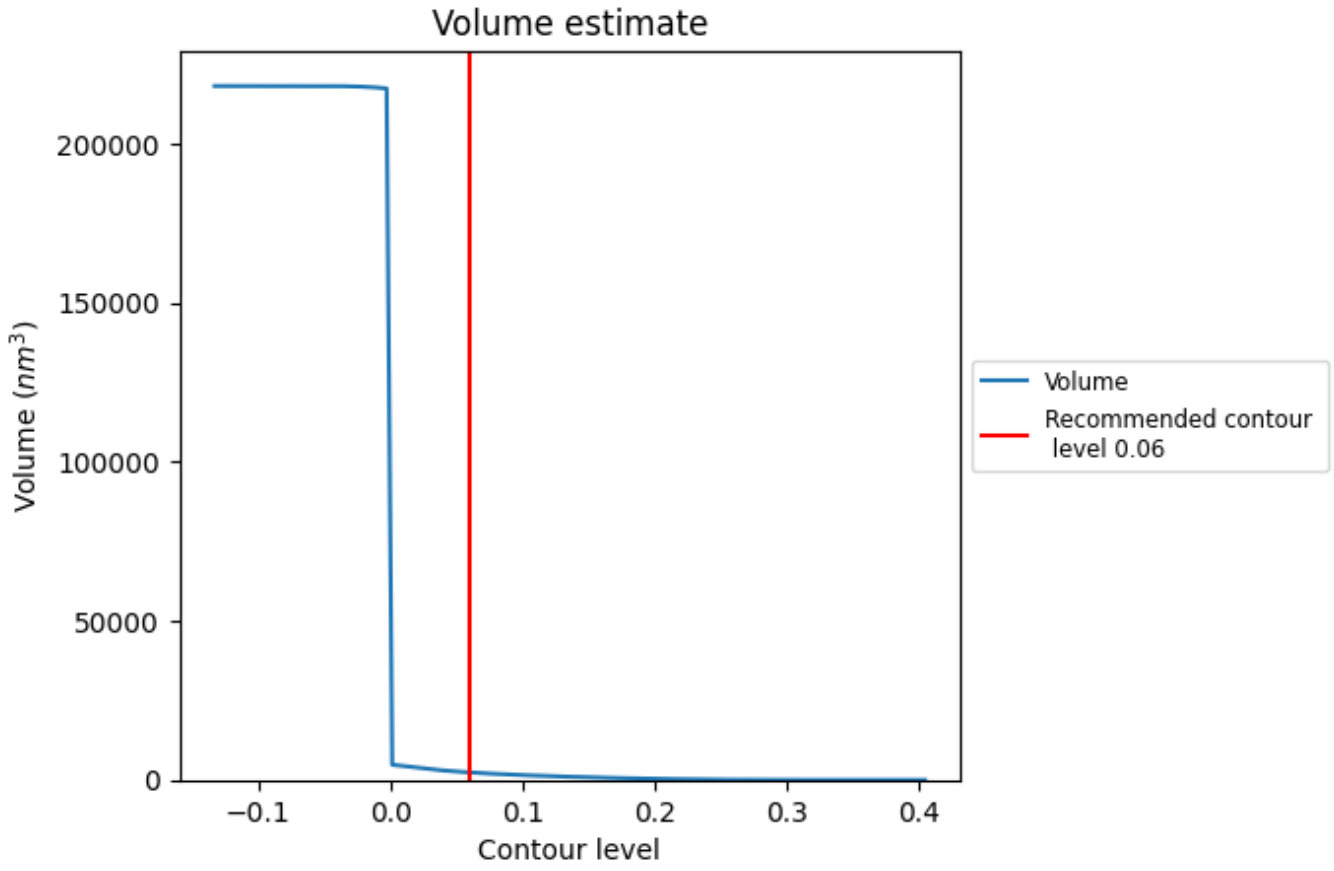
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

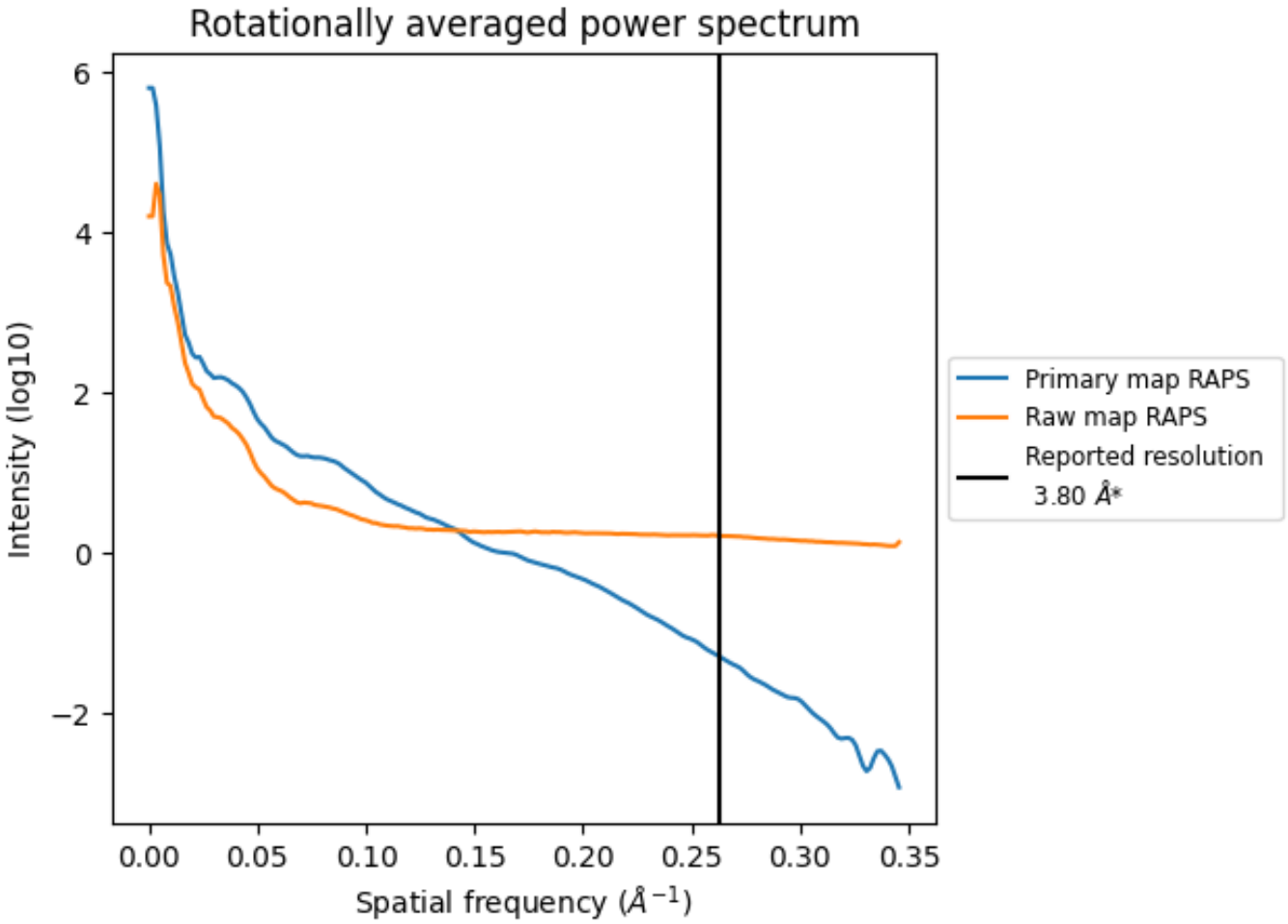
7.2 Volume estimate (i)



The volume at the recommended contour level is 2370 nm^3; this corresponds to an approximate mass of 2141 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)

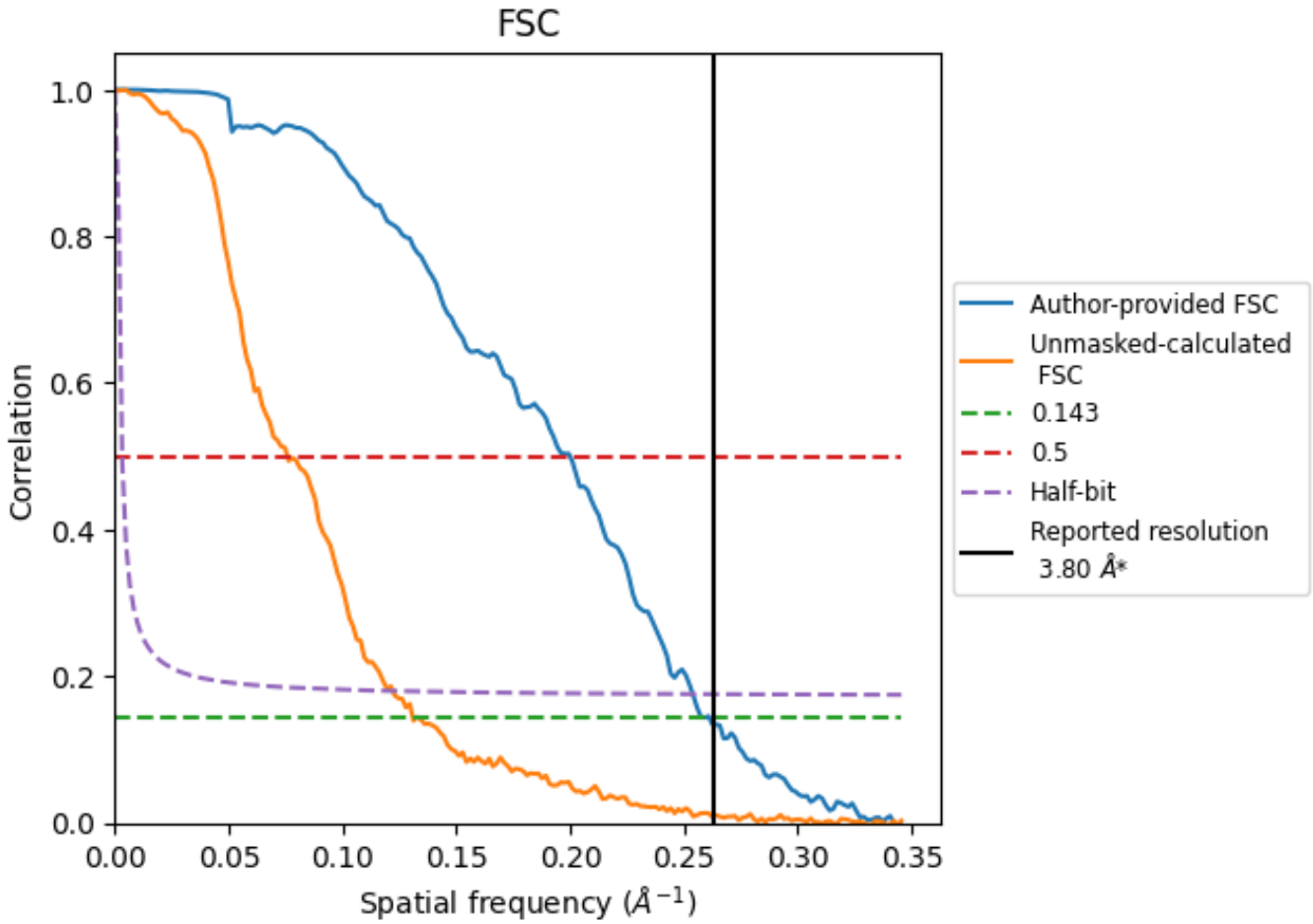


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

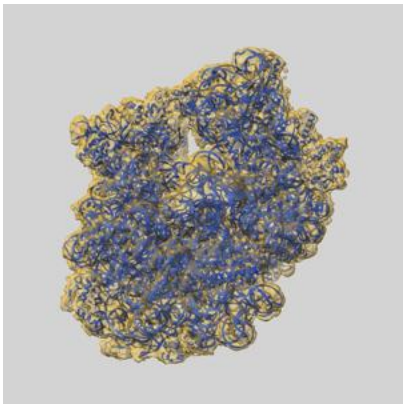
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	5.00	3.94
Unmasked-calculated*	7.63	13.19	8.19

*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 7.63 differs from the reported value 3.8 by more than 10 %

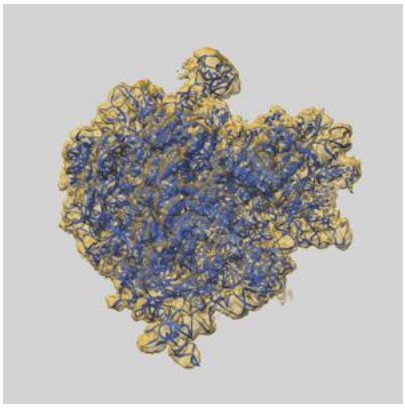
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29214 and PDB model 8FIZ. Per-residue inclusion information can be found in section 3 on page 14.

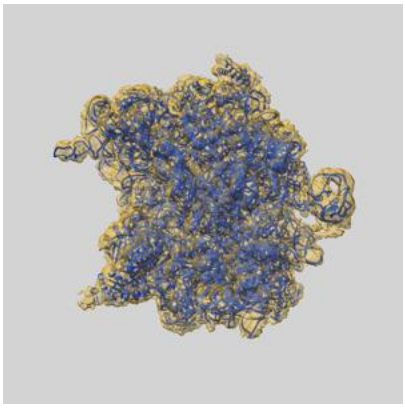
9.1 Map-model overlay



X



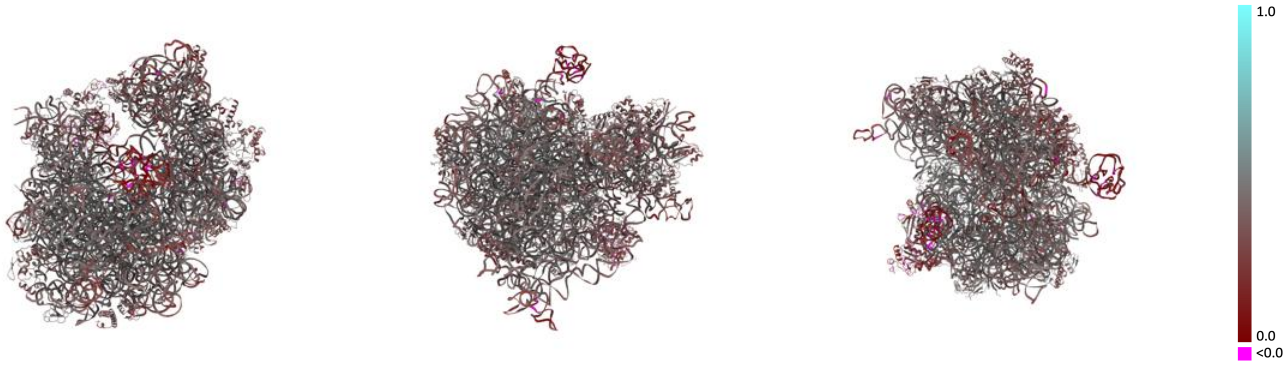
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

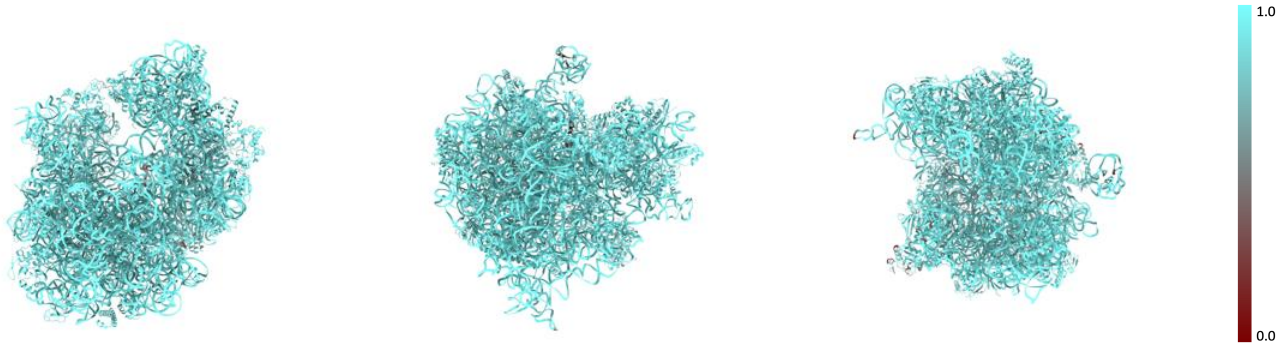
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

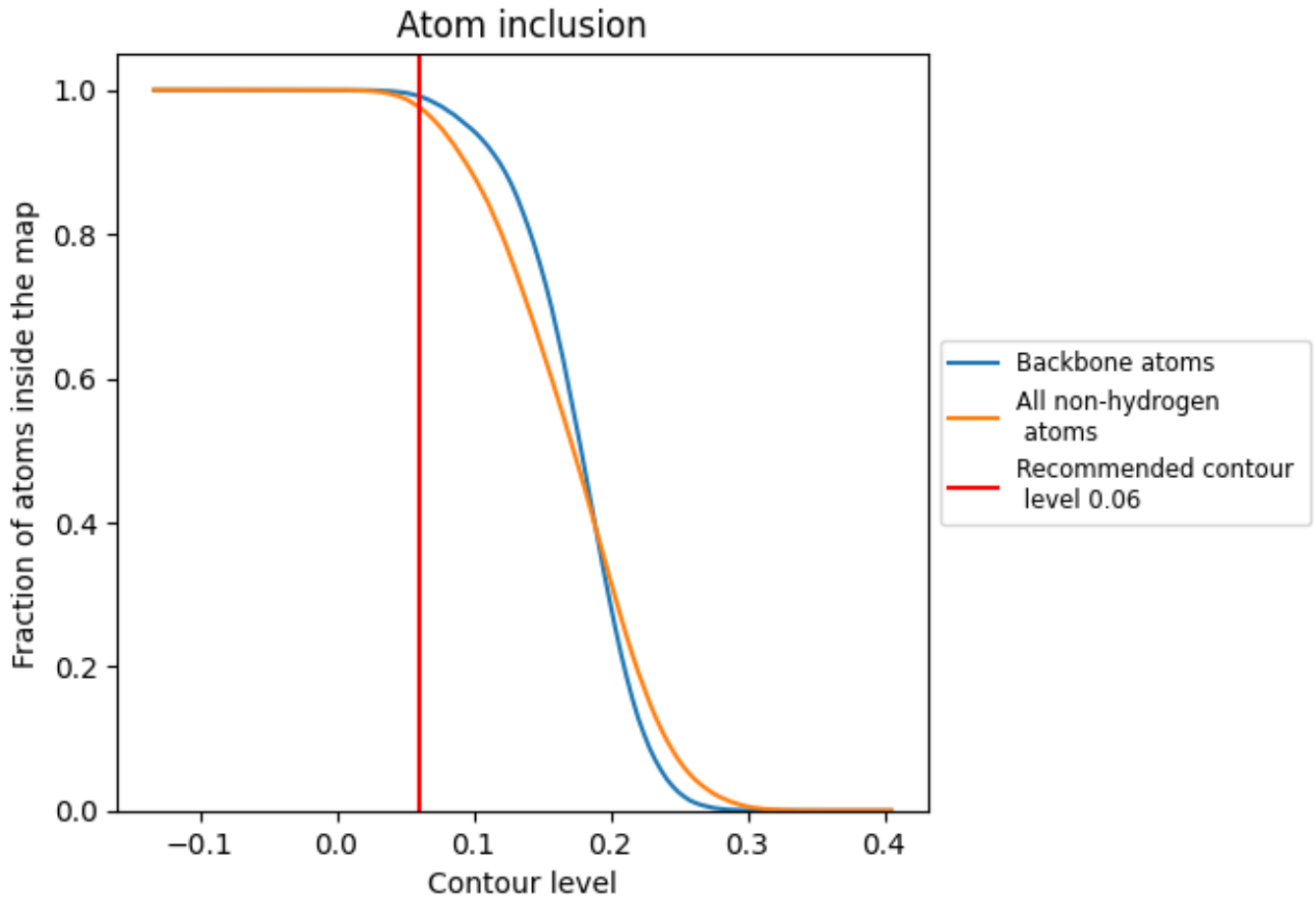
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9767	0.3940
AA	0.9930	0.3980
AB	0.9282	0.3370
AC	0.9562	0.4160
AD	0.9533	0.3690
AE	0.9800	0.3710
AF	0.9574	0.3720
AG	0.9354	0.3930
AH	0.9545	0.3630
AI	0.9415	0.3770
AJ	0.9309	0.3390
AK	0.9602	0.3680
AL	0.9327	0.3320
AM	0.9730	0.3840
AN	0.9774	0.3740
AO	0.9410	0.4140
AP	0.9724	0.4120
AQ	0.9615	0.4070
AR	0.9725	0.3750
AS	0.9494	0.3750
AT	0.9633	0.3780
AU	0.7320	0.3420
AV	0.8750	0.2720
AW	0.8740	0.2470
BA	0.9946	0.4060
BB	0.9731	0.3040
BC	0.9996	0.4080
BD	0.9707	0.4410
BE	0.9614	0.4240
BF	0.9599	0.4020
BG	0.9534	0.3730
BH	0.9690	0.3930
BI	0.9409	0.4180
BJ	0.9383	0.3760
BK	0.8183	0.3130

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Chain	Atom inclusion	Q-score
BL	0.8091	0.1180
BM	0.9626	0.4190
BN	0.9437	0.4260
BO	0.9511	0.4420
BP	0.9452	0.4480
BQ	0.9428	0.4190
BR	0.9655	0.4210
BS	0.9392	0.4250
BT	0.9561	0.4250
BU	0.9549	0.4250
BV	0.9529	0.4020
BW	0.9595	0.4180
BX	0.9802	0.4030
BY	0.9849	0.4140
BZ	0.9390	0.4170
DA	0.9404	0.3820
DB	0.9465	0.3880
DC	0.9702	0.4010
DD	0.9645	0.4420
DE	0.9567	0.4190
DF	0.9325	0.3100
DG	0.7116	0.1490