wwPDB EM Validation Summary Report (i)

Nov 2, 2024 – 03:46 PM EDT

PDB ID	:	6BU8
EMDB ID	:	EMD-7289
Title	:	70S ribosome with S1 domains 1 and 2 (Class 1)
Authors	:	Loveland, A.B.; Korostelev, A.A.
Deposited on	:	2017-12-08
Resolution	:	3.50 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:

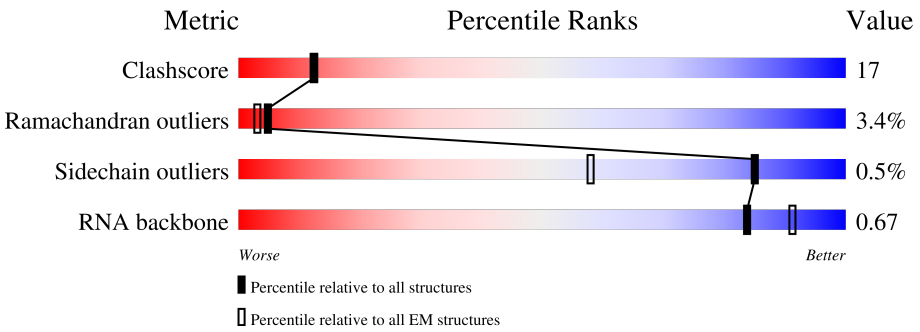
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	04	271	50% 48% •
2	05	209	58% 42%
3	06	201	51% 48% •
4	07	177	42% 57% • •
5	08	176	• 61% 38% •
6	09	149	13% 50% 46% •
7	10	131	26% 38% 58% •

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Mol	Chain	Length	Quality of chain
8	11	141	26% 44% 55%
9	12	142	49% 49%
10	13	122	58% 41%
11	14	143	57% 42%
12	15	136	57% 40%
13	16	120	48% 50%
14	17	116	52% 45%
15	18	114	48% 48%
16	19	117	52% 45%
17	20	103	53% 45%
18	21	110	43% 55%
19	22	93	55% 45%
20	23	102	59% 40%
21	24	94	61% 37%
22	25	75	67% 33%
23	26	77	60% 39%
24	27	63	5% 52% 43% 5%
25	28	58	52% 48%
26	29	66	8% 59% 41%
27	30	56	39% 59%
28	31	50	60% 40%
29	32	46	50% 46%
30	33	64	55% 44%
31	34	38	47% 53%
32	B	225	64% 35%

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Mol	Chain	Length	Quality of chain
33	C	206	52% 45% •
34	D	205	43% 51% 6%
35	E	157	40% 57% •
36	F	126	18% 55% 43% •
37	G	151	50% 48% •
38	H	129	• 52% 47% •
39	I	127	• 44% 52% •
40	J	98	• 39% 57% •
41	K	116	42% 55% •
42	L	123	• 45% 52% •
43	M	114	• 48% 48% •
44	N	100	46% 51% •
45	O	88	• 58% 41% •
46	P	82	• 37% 61% •
47	Q	80	48% 51% •
48	R	65	42% 52% 6%
49	S	79	• 52% 47% •
50	T	85	49% 49% •
51	U	65	5% 29% 66% 5%
52	03	223	• 26% 34% 40%
53	A	1539	57% 38% •
54	01	2903	54% 41% 5%
55	02	120	55% 37% 8%
56	W	77	• 69% 27% •
56	X	77	• 60% 34% 6%

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Mol	Chain	Length	Quality of chain
57	V	27	48% 19% 33%
58	Y	76	63% 29% 8%
59	Z	554	19% 19% 9% 72%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 152151 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	04	271	2083	1288	423	365	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	05	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	06	201	1552	974	283	290	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	07	177	1411	899	249	257	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	08	176	1323	832	243	246	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	09	149	1111	699	197	214	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	10	131	989	625	175	184	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	11	141	1032	651	179	196	6	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	12	142	1129	714	212	199	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	13	122	939	587	180	166	6	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	14	143	1045	649	206	189	1	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	15	136	1074	686	205	177	6	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	16	120	961	593	196	167	5	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	17	116	892	552	178	162	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	18	114	917	574	179	163	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	19	117	947	604	192	151	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	20	103	816	516	153	145	2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	21	110	857	532	166	156	3	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	22	93	739	466	139	132	2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	23	102	780	492	146	142	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	24	94	753	479	137	134	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	25	75	575	356	116	102	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	26	77	625	388	129	106	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	27	63	509	313	99	95	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	28	58	449	281	87	79	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	29	66	523	323	99	95	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	30	56	444	269	94	80	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	31	50	410	263	75	72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	32	46	377	228	90	57	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	33	64	504	323	105	74	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	34	38	302	185	65	48	4	0	0

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	B	225	1757	1111	315	323	8	0	0

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	C	206	1625	1028	305	289	3	0	0

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	E	157	1157	719	218	214	6	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	F	126	1028	638	189	194	7	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	G	151	1182	735	227	216	4	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	J	98	787	493	150	143	1	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	K	116	870	535	173	159	3	0	0

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	M	114	884	546	178	157	3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Q	80	649	411	121	114	3	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	R	65	536	339	100	96	1	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	S	79	638	408	120	108	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	U	65	545	335	117	92	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	03	134	1027	645	186	194	2	0	0

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	A	1539	33012	14725	6052	10697	1538	0	0

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	01	2903	62317	27801	11468	20146	2902	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
01	747	C	U	SEE REMARK 999	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	02	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
02	120	A	-	SEE REMARK 999	GB 1266961702

- Molecule 56 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	X	77	1640	732	297	535	76	0	0
56	W	77	1640	732	297	535	76	0	0

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	V	18	388	175	76	120	17	0	0

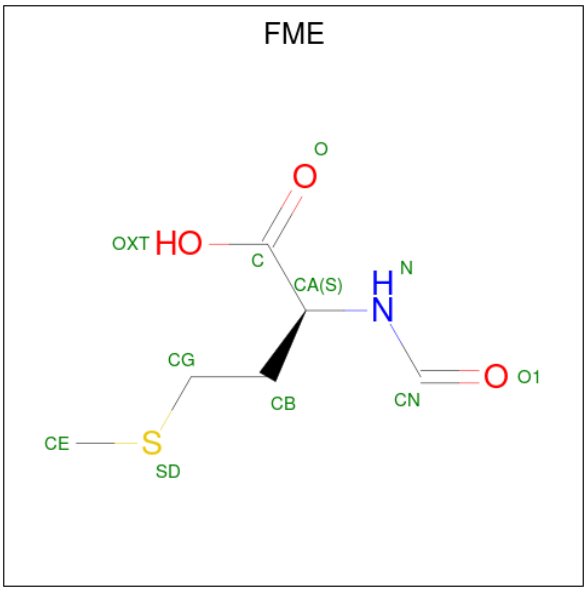
- Molecule 58 is a RNA chain called tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	Y	76	1622	723	290	533	76	0	0

- Molecule 59 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
59	Z	156	1204	760	209	235	0	0

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



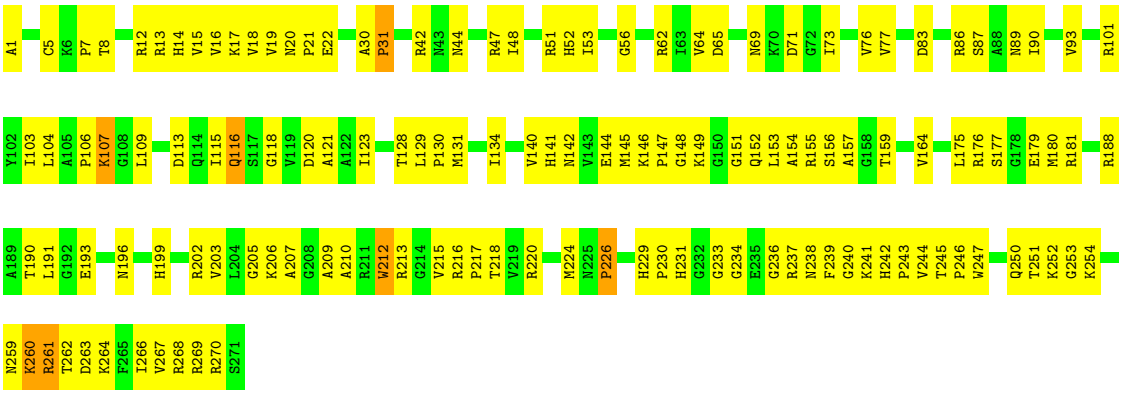
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	W	1	10	6	1	2	1	0

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.

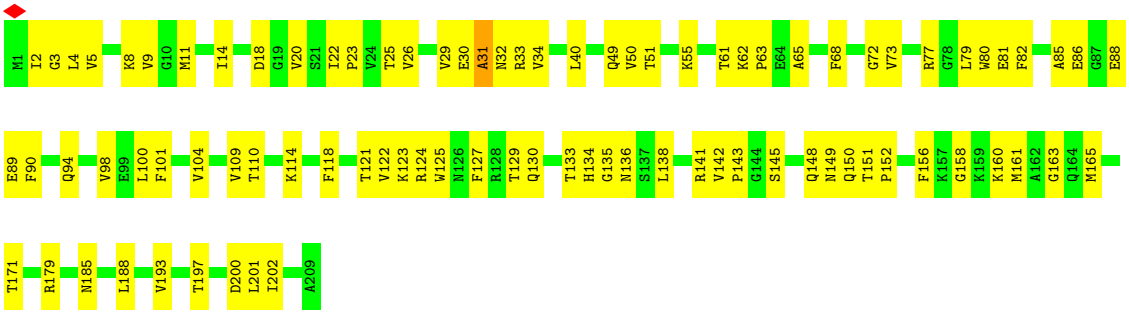
- Molecule 1: 50S ribosomal protein L2

Chain 04:



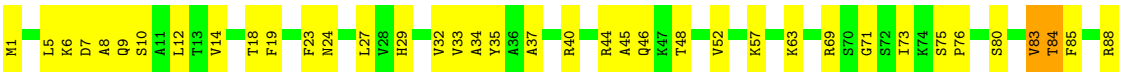
- Molecule 2: 50S ribosomal protein L3

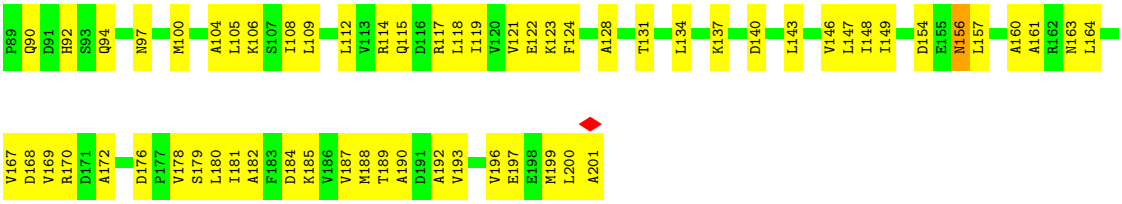
Chain 05:



- Molecule 3: 50S ribosomal protein L4

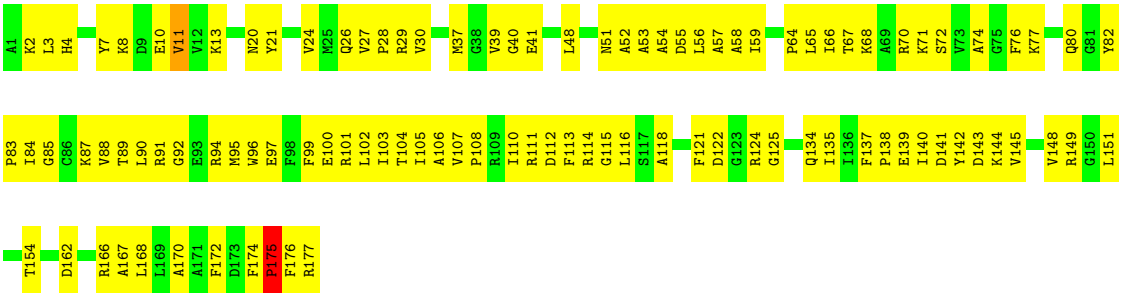
Chain 06:





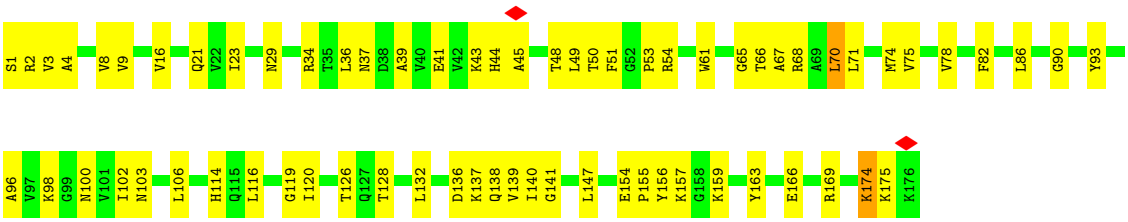
- Molecule 4: 50S ribosomal protein L5

Chain 07:



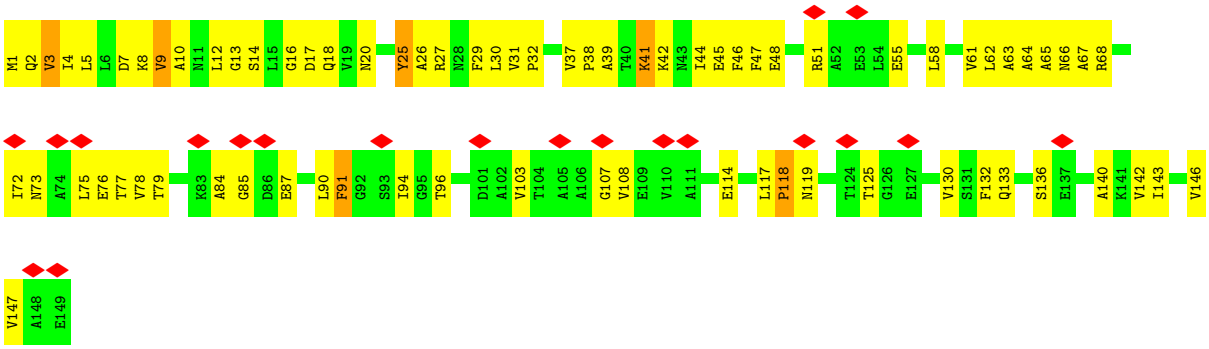
- Molecule 5: 50S ribosomal protein L6

Chain 08:



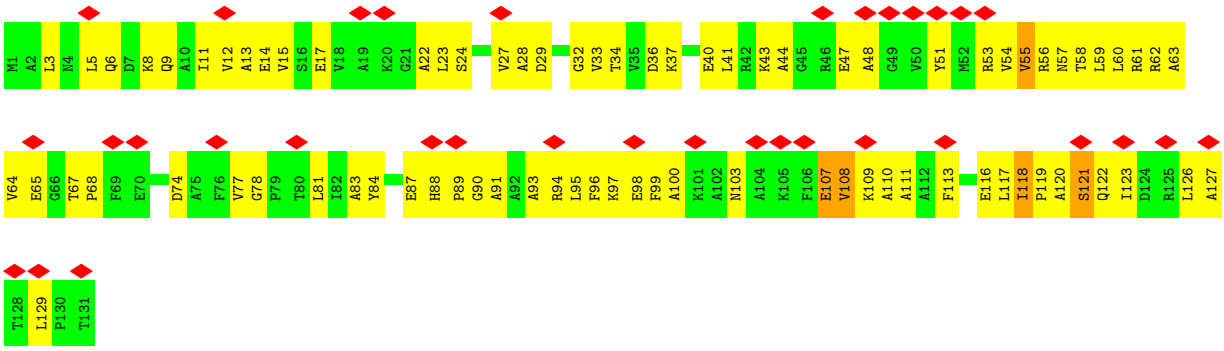
- Molecule 6: 50S ribosomal protein L9

Chain 09:



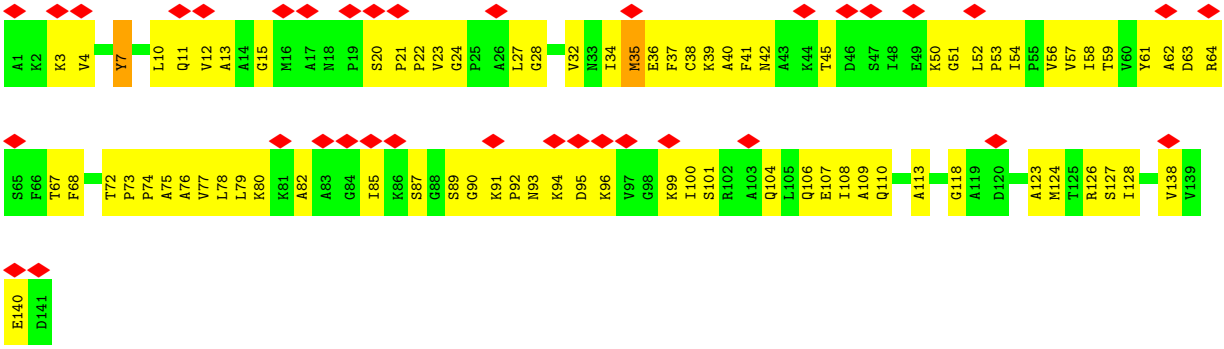
- Molecule 7: 50S ribosomal protein L10

Chain 10:



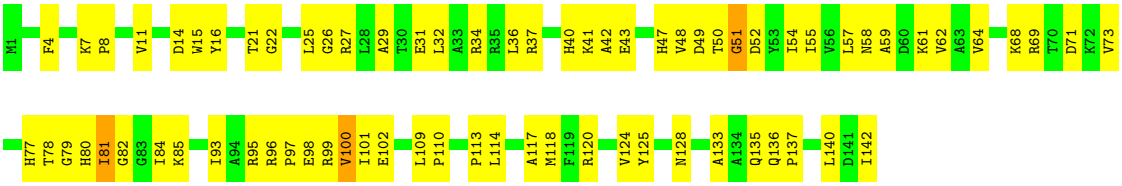
• Molecule 8: 50S ribosomal protein L11

Chain 11:



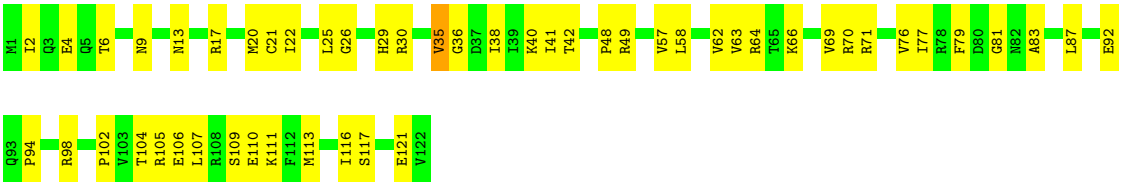
• Molecule 9: 50S ribosomal protein L13

Chain 12:



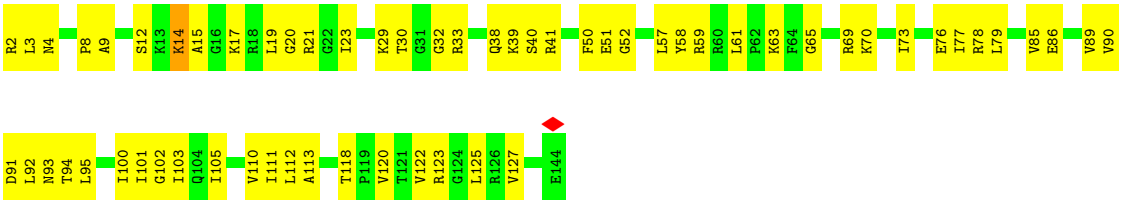
• Molecule 10: 50S ribosomal protein L14

Chain 13:



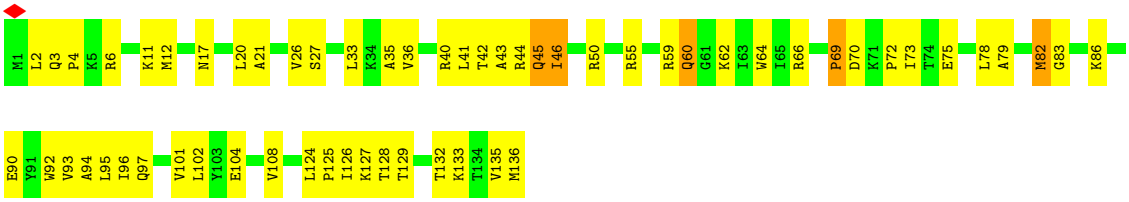
• Molecule 11: 50S ribosomal protein L15

Chain 14:



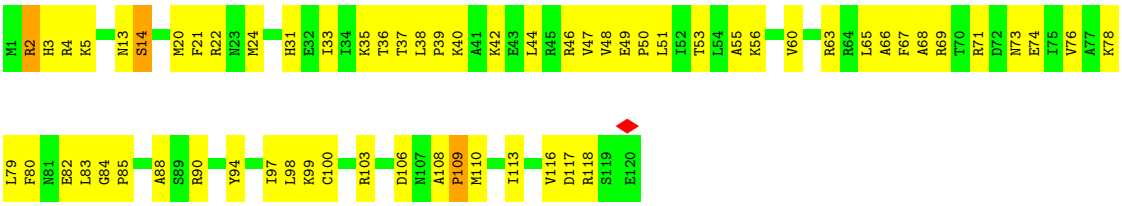
• Molecule 12: 50S ribosomal protein L16

Chain 15:



• Molecule 13: 50S ribosomal protein L17

Chain 16:

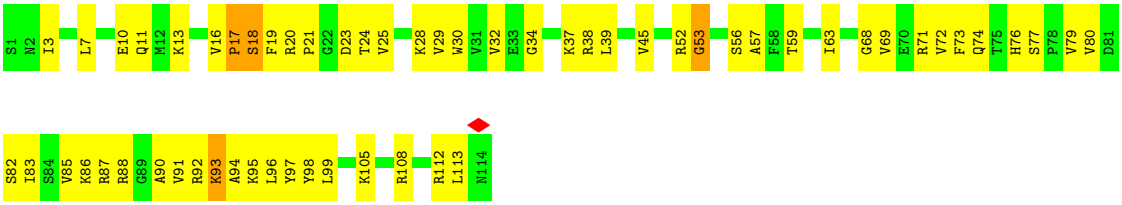


• Molecule 14: 50S ribosomal protein L18

Chain 17:

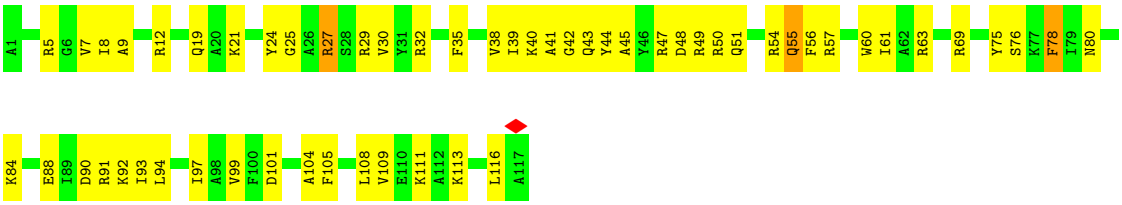
• Molecule 15: 50S ribosomal protein L19

Chain 18:



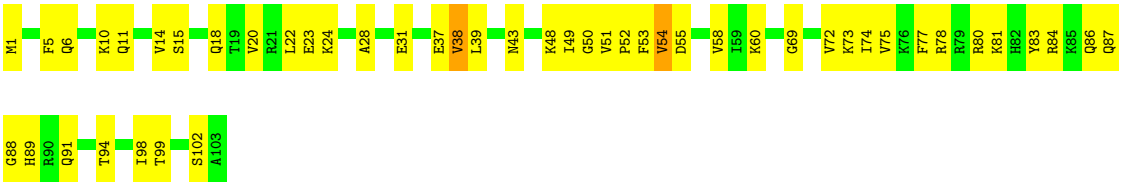
• Molecule 16: 50S ribosomal protein L20

Chain 19:



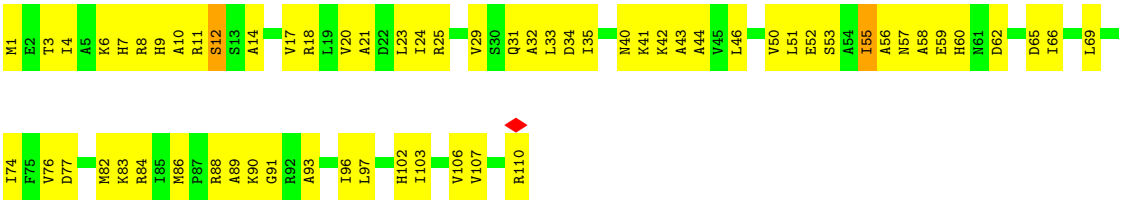
- Molecule 17: 50S ribosomal protein L21

Chain 20:



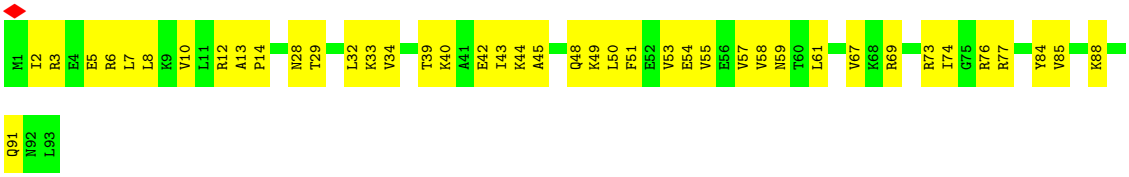
- Molecule 18: 50S ribosomal protein L22

Chain 21:



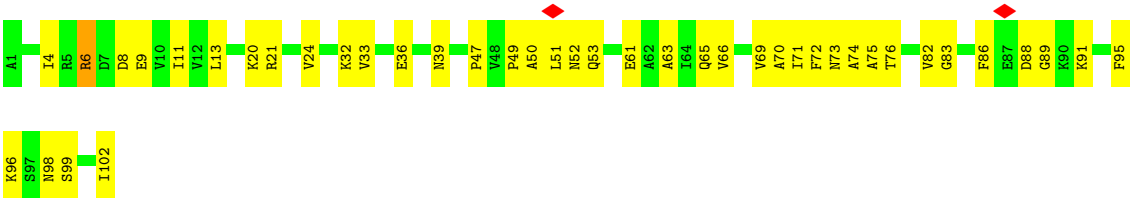
- Molecule 19: 50S ribosomal protein L23

Chain 22:



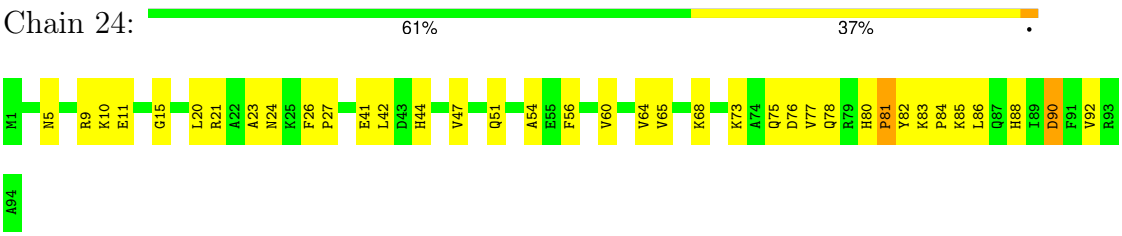
- Molecule 20: 50S ribosomal protein L24

Chain 23:



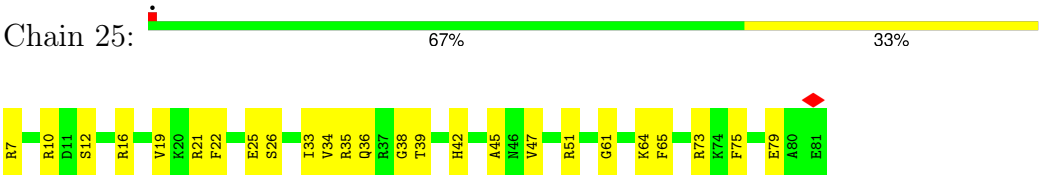
- Molecule 21: 50S ribosomal protein L25

Chain 24:



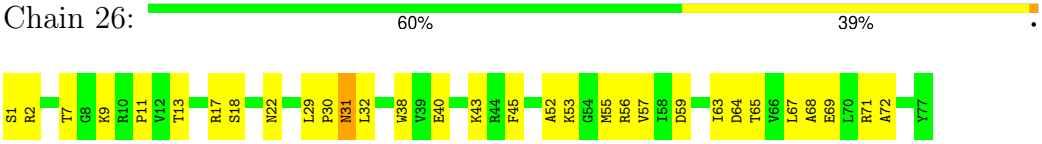
- Molecule 22: 50S ribosomal protein L27

Chain 25:



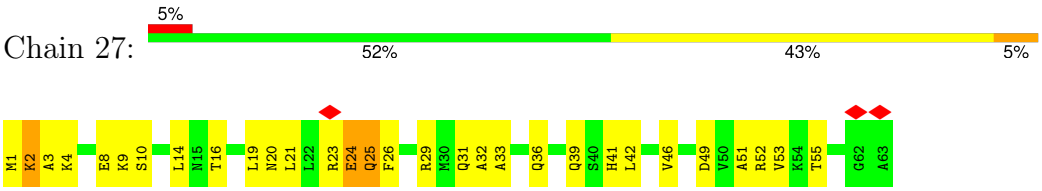
- Molecule 23: 50S ribosomal protein L28

Chain 26:



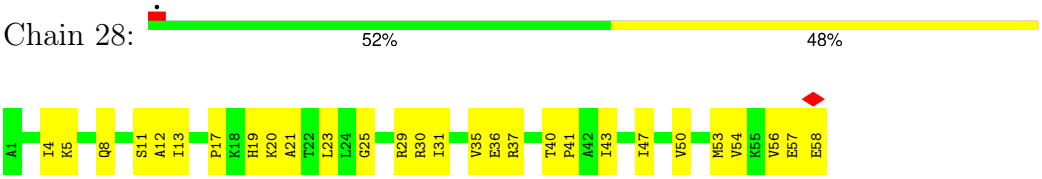
- Molecule 24: 50S ribosomal protein L29

Chain 27:



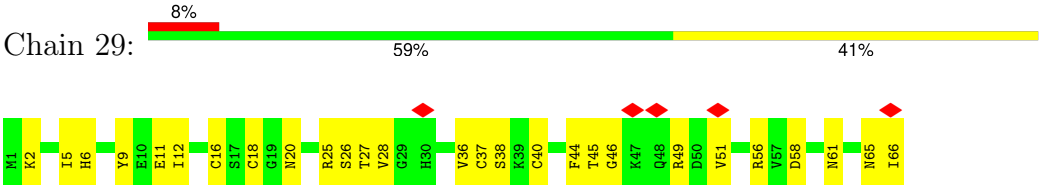
- Molecule 25: 50S ribosomal protein L30

Chain 28:



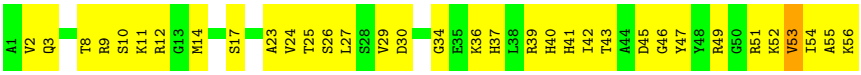
- Molecule 26: 50S ribosomal protein L31

Chain 29:



- Molecule 27: 50S ribosomal protein L32

Chain 30:

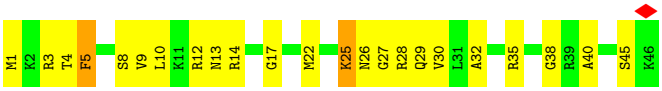


• Molecule 28: 50S ribosomal protein L33

Chain 31:

• Molecule 29: 50S ribosomal protein L34

Chain 32:

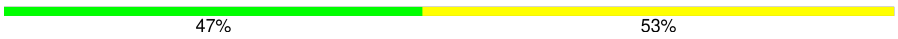


• Molecule 30: 50S ribosomal protein L35

Chain 33:

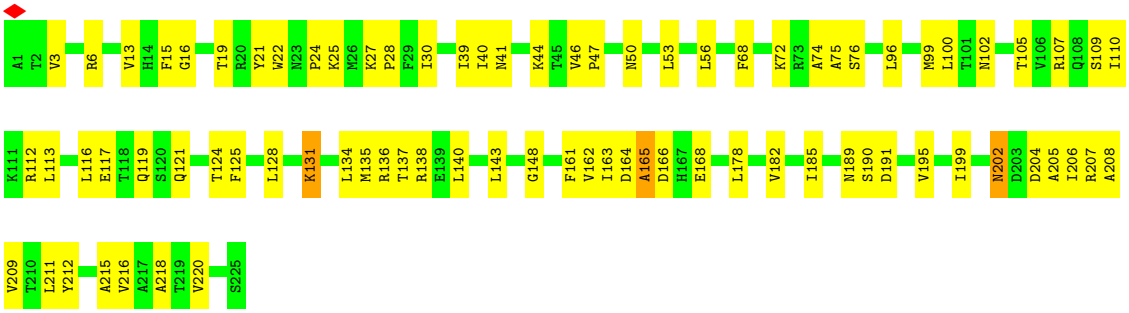
• Molecule 31: 50S ribosomal protein L36

Chain 34:



• Molecule 32: 30S ribosomal protein S2

Chain B:



• Molecule 33: 30S ribosomal protein S3

Chain C:

G1 Q2 K3 V4 H5 P6 N7 G8 I9 R10 I13 V14 N18 F22 A23 N24 F28 S34 D35 F36 K37 V38 R39 L42 K48 A49 I54 V55 I56 E57 R58 P59 A60 K61 S62 I63 T66 I67 H68 T69 A70 R71 P72 V75 I76 G77 K78 K79 G80 E81

D82 L86 V89 V90 I93 V96 P97 N101 I102 A103 E104 V105 R106 K107 P108 E109 L110 D111 A112 K113 L114 V115 A116 D117 S118 I119 T120 S121 Q122 R125 R126 V127 M128 F129 R130 R131 A132 M133 K134 R135 M141 R142 L143 G144 I148 K149 V150 E151 V152 S153 G154 R155

L156 I161 A162 R163 T164 E165 W166 Y167 R168 E169 L177 R178 A179 D180 I181 D182 Y183 N184 T185 S186 G196 V199 W200 I201 F202 K203 G204 E205 I206

- Molecule 34: 30S ribosomal protein S4

Chain D: 43% 51% 6%

A1 R2 Y3 L4 G5 P6 K7 L8 K9 L10 S11 R12 R13 L18 F19 L20 K21 S22 G23 V24 R25 A26 I27 D28 T29 K30 C31 K32 I33 E34 Q35 A36 P37 H40 G41 A42 R43 L47 S48 D49 Y50 G51 V52 E56 K57 Q58 K59 V60 R61 R62 V66 L67 E68 R69 Q70

F71 R72 N73 Y74 E77 A78 A79 R80 L81 T85 G86 E87 N88 L89 L90 L93 R96 L97 D98 N99 V100 M104 A108 T109 R110 V117 S118 H119 K120 A121 I122 M123 V124 N130 I131 A132 S133 V136 S137 P138 N139 D140 V141 V142 S143 I144 R145 E146 K147 A148 K149

K150 R153 L158 R164 E165 K166 P167 T168 W169 L170 E171 V172 D173 A174 G175 K176 M177 E178 G179 T180 F181 K182 E186 R187 S188 D189 L190 S191 A192 D193 I194 N195 E196 H197 L198 I199 L202 Y203 S204 K205

- Molecule 35: 30S ribosomal protein S5

Chain E: 40% 57%

E9 L10 Q11 E12 K13 L14 I15 K22 T23 V24 K25 G26 G27 R28 I29 L35 T36 V37 V38 G39 D40 G41 M42 V45 G46 F47 A52 R53 E54 V55 P56 A57 A58 I59 Q60 K61 A62 M63 R67 M70 V73 A74 L75 N76 T79 L80 Q81 H82 P83 V84 K85 G86

V87 H88 T89 G90 V93 F94 M95 Q96 P97 A98 T102 G103 I104 I105 A106 G107 G108 A109 M110 R111 A112 V113 L114 E115 V116 A117 V122 L123 A124 P132 I133 N134 V135 V136 R137 A138 T139 L143 M146 N147 S148 P149 V152 A153 A154 K155 R156 G157 K158 S159 V160 E161 E162

I163 L164 G165

- Molecule 36: 30S ribosomal protein S6

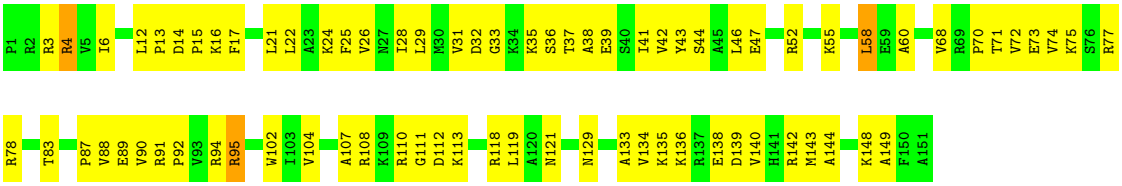
Chain F: 18% 55% 43%

M1 R2 H3 Y4 E5 T6 V7 P12 D13 Q14 S15 E16 Q17 V18 P19 G20 M21 I22 T26 I29 A32 E33 I36 H37 R38 L39 E40 D41 W42 Q46 L47 A48 Y49 P50 I51 L54 H55 K56 Y59 V60 L61 M62 M63 V64 E65 A66 P67 V70 T71 D72

E75 F78 R79 F80 R86 S87 M88 V89 M90 R91 T92 K93 H94 T97 E98 A99 S100 P101 M102 V103 K104 A105 K106 D107 E108 R109 R110 E111 R112 R113 D114 D115 F116 A117 N118 E119 T120 A121 D122 D123 A124 E125 A126

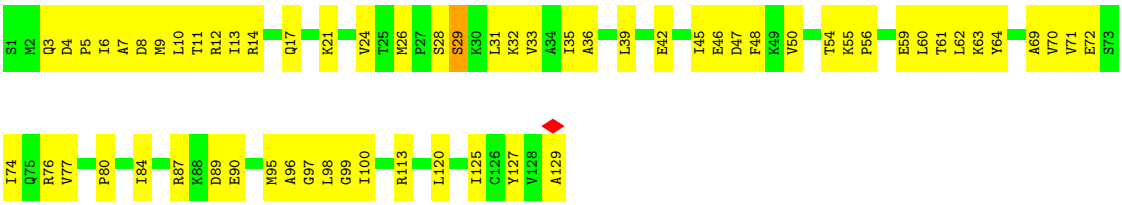
- Molecule 37: 30S ribosomal protein S7

Chain G: 50% 48%



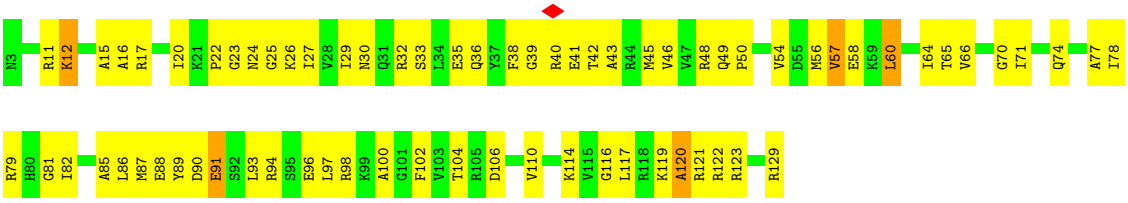
• Molecule 38: 30S ribosomal protein S8

Chain H:



• Molecule 39: 30S ribosomal protein S9

Chain I:

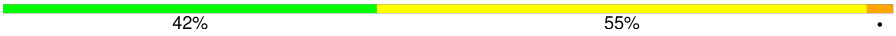


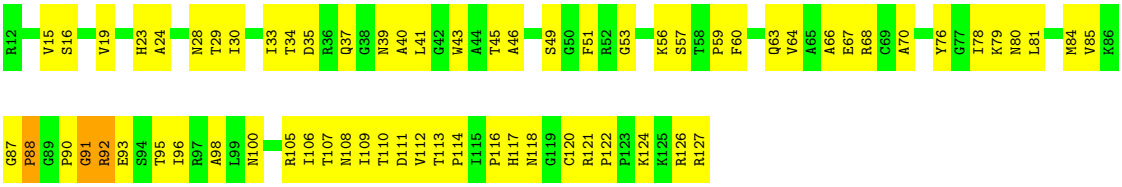
• Molecule 40: 30S ribosomal protein S10

Chain J:

• Molecule 41: 30S ribosomal protein S11

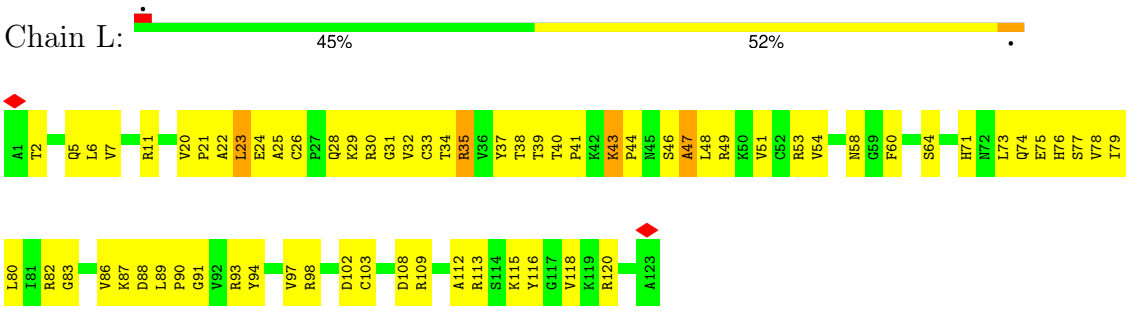
Chain K:





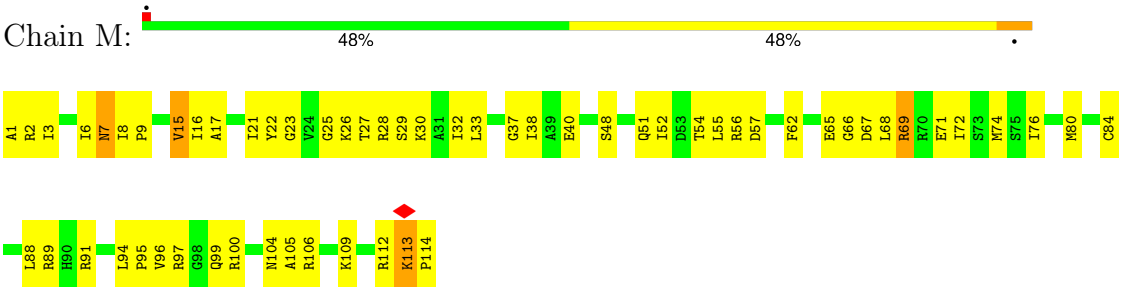
• Molecule 42: 30S ribosomal protein S12

Chain L:



- Molecule 43: 30S ribosomal protein S13

Chain M:

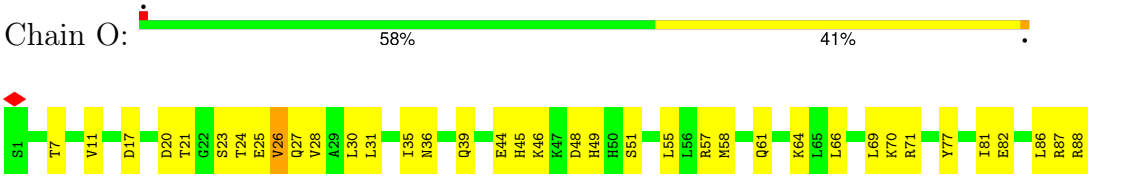


- Molecule 44: 30S ribosomal protein S14

Chain N:

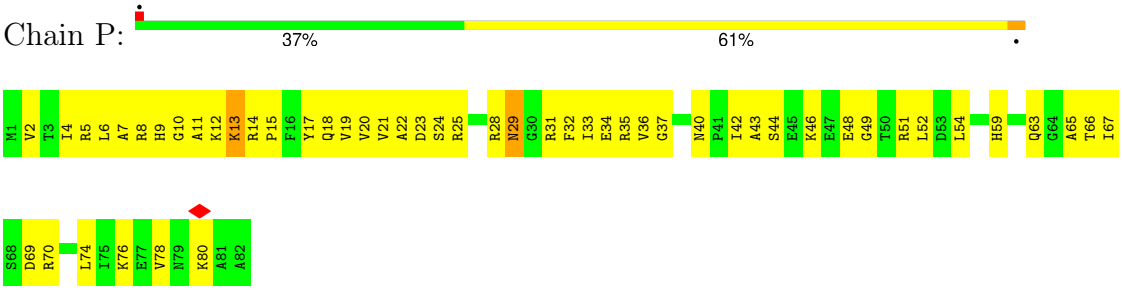
- Molecule 45: 30S ribosomal protein S15

Chain O:



- Molecule 46: 30S ribosomal protein S16

Chain P:



- Molecule 47: 30S ribosomal protein S17

Chain Q: 48% 51%

K3 I4 R5 T6 L7 V11 V12 S13 D14 K15 M16 E17 K18 S19 I20 V21 V22 A23 I24 V28 K29 F36 I37 K38 R39 T40 T41 K42 L43 H44 V45 H46 D47 E48 N49 N50 E51 D56 V57 V58 E59 I60 C63 R64 T69 K70 T73 L74 V77 V78 E79

V82

- Molecule 48: 30S ribosomal protein S18

Chain R: 42% 52% 6%

F9 C10 R11 F12 T13 A14 E15 G16 V17 Q18 E19 I20 D21 Y22 K23 D24 I25 A26 K29 I32 S35 I38 V39 P40 S41 R42 I43 T44 G45 A48 Q51 L54 A55 R56 A57 I58 K59 R60 A61 R62 Y63 L64 S65 P68 Y69 T70 D71 R72 H73

- Molecule 49: 30S ribosomal protein S19

Chain S: 52% 47%

R2 S3 L4 K5 K6 G7 P8 F9 I10 D11 L12 K17 V18 E19 K20 A21 V22 E23 S24 K27 K28 P29 L30 R31 T32 W33 S34 R35 R36 I48 A49 R54 V57 P58 T62 D63 E64 M65 H68 K69 L70 F73 A74 P75 T76 R77 R80

- Molecule 50: 30S ribosomal protein S20

Chain T: 49% 49%

N2 I3 K4 K8 I11 E14 K15 A16 R17 K18 H19 N20 R23 R28 T29 F30 K33 V34 Y35 I38 D42 K43 A44 A45 M53 Q54 P55 I56 V57 D58 R59 Q60 K63 H67 K68 N69 K70 A71 A72 R73 H74 K75 A76 N77 L78 T79 A80 Q81 I82

N83 K84 L85 A86

- Molecule 51: 30S ribosomal protein S21

Chain U: 5% 29% 66% 5%

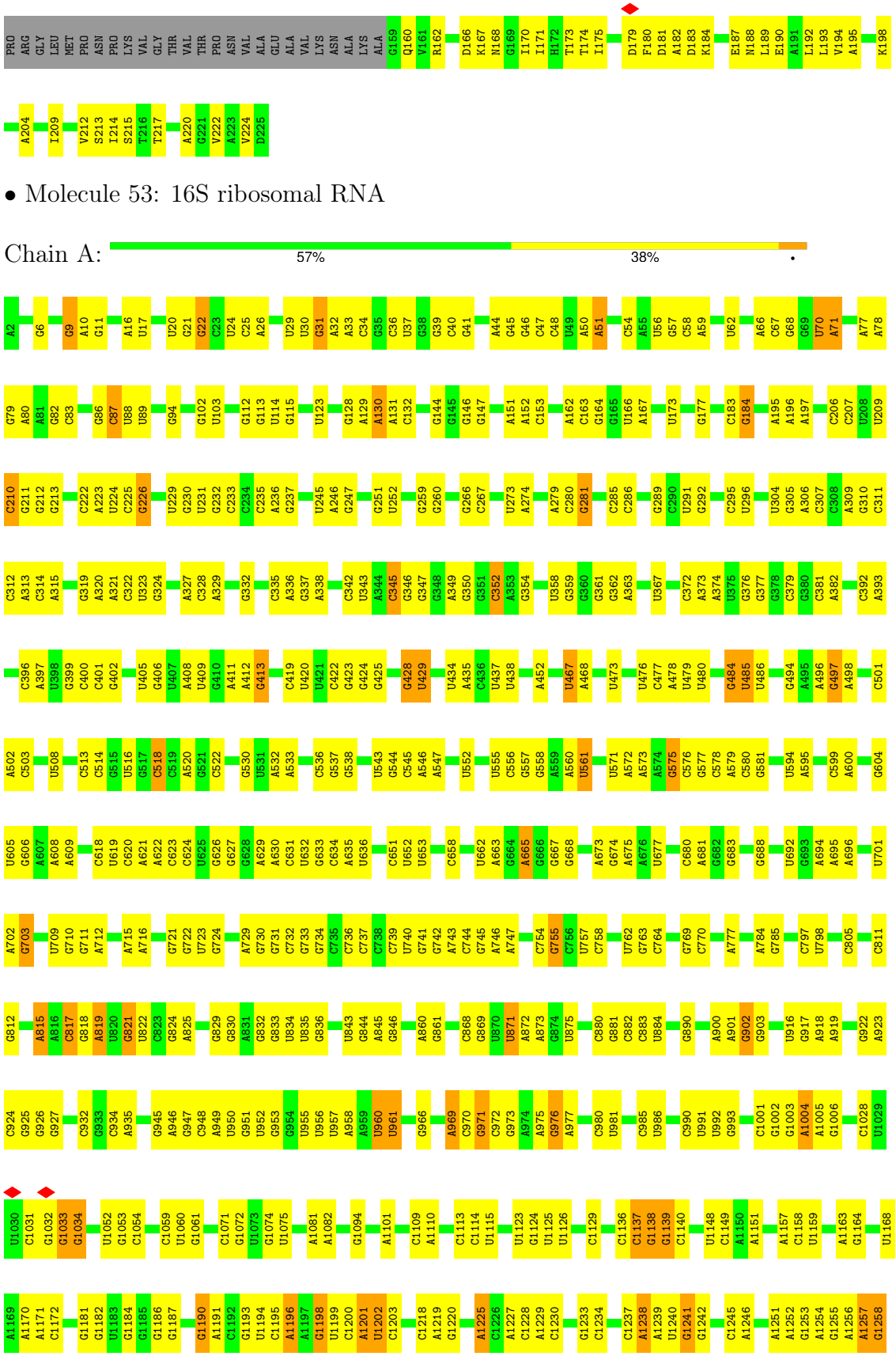
I3 K4 V5 R6 E7 N8 E9 P10 F11 D12 V13 A14 L15 R16 R17 F18 K19 R20 S21 C22 E23 K24 A25 G26 V27 L28 A29 E30 V31 R32 R33 R34 E35 F36 Y37 E38 K39 P40 R46 A47 K48 A49 S50 A51 V52 A56 K57 K58 L59 A60 R61 E62 N63 A64 R65 R66 T67

- Molecule 52: 50S ribosomal protein L1

Chain 03: 26% 34% 40%

K3 L4 T5 K6 R7 M8 R9 V10 I11 R12 E13 K14 V15 D16 A17 T18 K19 Q20 Y21 D22 I23 A26 I27 A28 L29 L30 K31 E32 L33 K37 F38 V39 D43 V44 A45 V46 I50 D51 A52 R53 K54 S55 D56 Q57 A62 T63 V64 L65 P66 H67 G68 T69 GLY ARG SER

VAL ARG VAL ALA VAL PHE THR GLN GLY ALA ASN ALA GLU ALA ALA LYS ALA ALA GLY ALA GLU LEU VAL GLY MET GLU ASP LEU ALA ASP GLN ILE LYS LYS GLY GLU MET ASN PHE ASP VAL VAL ILE ALA SER PRO ASP ALA MET ARG VAL VAL GLY GLN LEU GLY GLN VAL LEU GLY

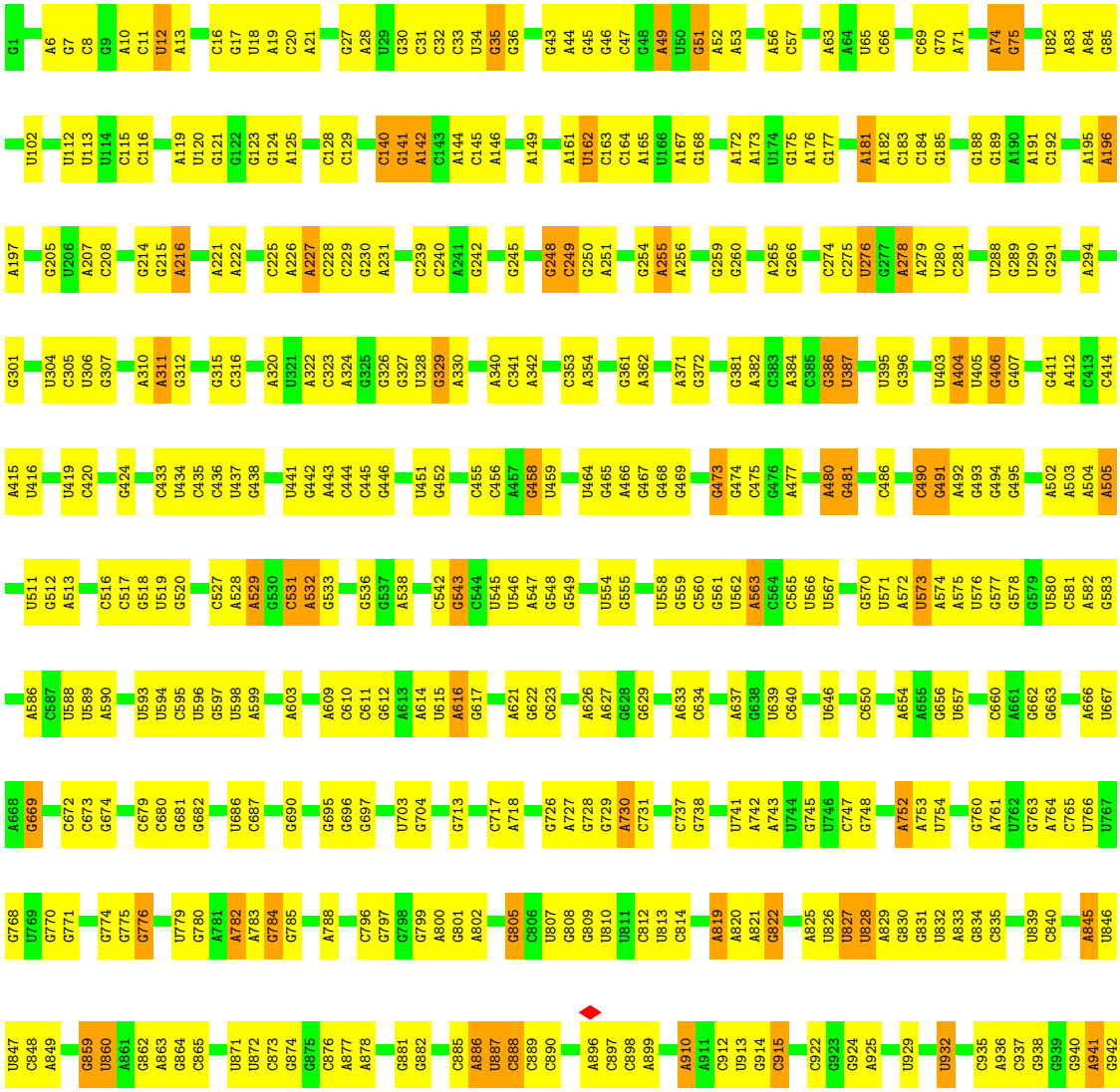


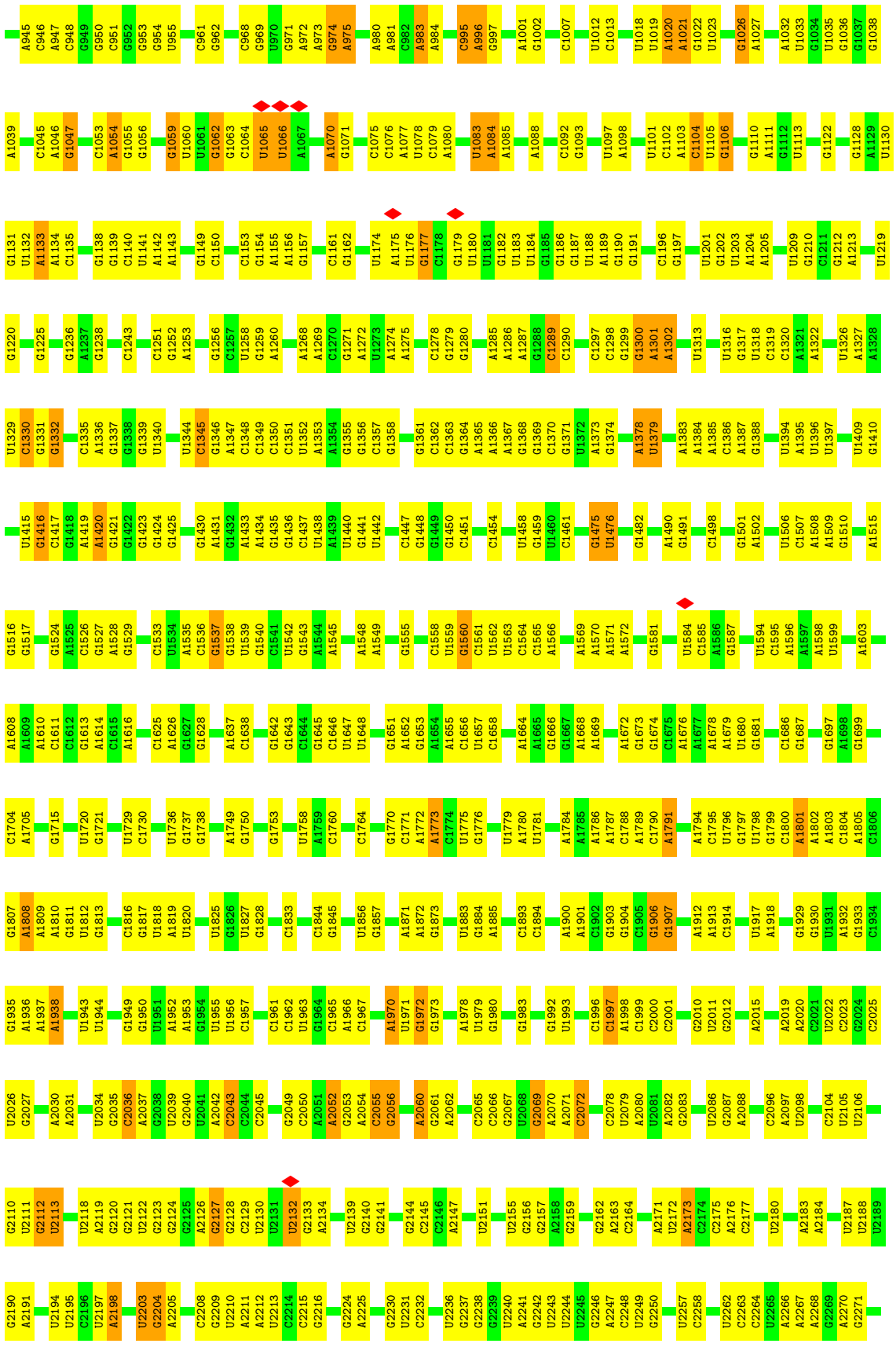
• Molecule 53: 16S ribosomal RNA

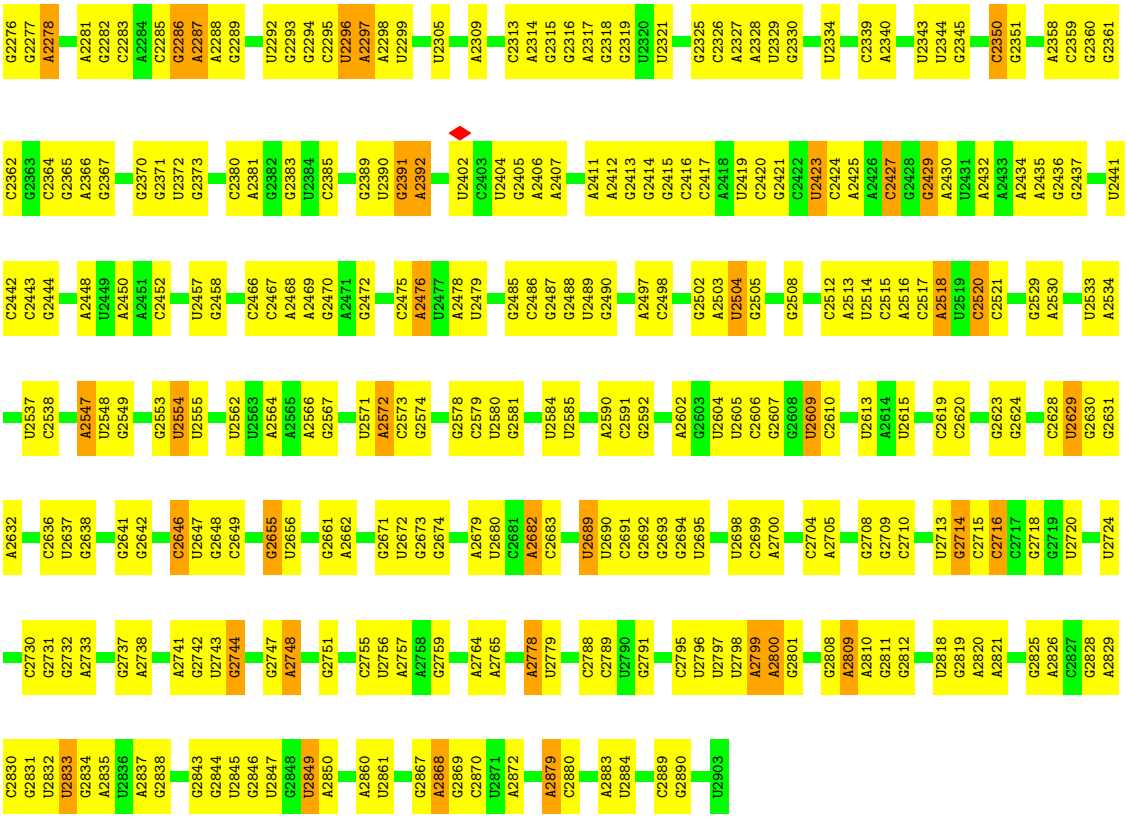
Chain A: 57% 38% •

• Molecule 54: 23S ribosomal RNA

Chain 01:

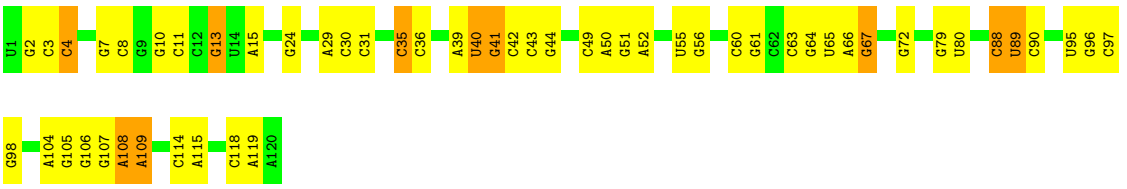



A945 C946 A947 C948 G949 G950 C951 G952 G953 G954 U955 C961 G962 C968 G969 U970 G971 A972 A973 G974 A975 A980 A981 C982 A983 A984 C995 A996 G997 A1001 G1002 C1007 U1012 C1013 U1018 U1019 A1020 A1021 G1022 U1023 G1026 A1027 A1032 U1033 G1034 U1035 G1036 G1037 G1038
A1039 C1045 A1046 G1047 C1053 A1054 G1055 G1056 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 A1070 G1071 C1075 C1076 A1077 U1078 C1079 A1080 U1083 A1084 A1085 A1088 C1092 G1093 U1097 A1098 U1101 C1102 A1103 C1104 U1105 G1106 G1110 A1111 G1112 U1113 G1122 G1128 A1129 U1130
G1131 U1132 A1133 A1134 C1135 G1138 G1139 C1140 U1141 A1142 A1143 G1149 C1150 C1153 G1154 A1155 A1156 G1157 C1161 G1162 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 G1190 G1191 C1196 G1197 U1201 G1202 U1203 A1204 A1205 U1209 G1210 C1211 G1212 A1213 U1219
G1220 G1225 G1236 A1237 G1238 C1243 C1251 G1252 A1253 G1256 C1257 U1258 G1259 A1260 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 C1278 G1279 G1280 A1285 A1286 A1287 G1288 C1289 C1290 C1297 C1298 G1299 G1300 A1301 A1302 U1313 U1316 G1317 U1318 C1319 C1320 A1321 A1322 U1326 A1327 A1328
U1329 C1330 G1331 G1332 C1335 A1336 G1337 G1338 G1339 U1340 U1344 C1345 G1346 A1347 C1348 C1349 C1350 C1351 U1352 A1353 A1354 G1355 G1356 C1357 G1358 G1361 C1362 C1363 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 G1374 A1378 U1379 A1383 A1384 A1385 C1386 A1387 G1388 U1394 A1395 U1396 U1397 U1409 G1410
U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1422 G1423 G1424 G1425 G1430 A1431 G1432 A1433 A1434 G1435 G1436 C1437 U1438 A1439 U1440 G1441 U1442 C1447 G1448 G1449 G1450 C1451 C1454 U1458 G1459 U1460 C1461 G1475 U1476 G1482 A1490 G1491 C1498 G1501 A1502 U1506 C1507 A1508 A1509 G1510 A1515
G1516 G1517 G1524 A1525 C1526 G1527 A1528 G1529 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1544 A1545 A1548 A1549 G1555 C1558 U1559 G1560 C1561 U1562 U1563 C1564 C1565 A1566 A1569 A1570 A1571 A1572 G1581 U1584 C1585 A1586 G1587 U1594 C1595 A1596 A1597 A1598 U1599 A1603
A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1625 A1626 G1627 G1628 A1637 C1638 G1642 G1643 C1644 G1645 G1646 C1647 U1648 G1651 A1652 G1653 A1654 A1655 C1656 U1657 C1658 A1664 A1665 G1666 G1667 A1668 A1669 A1672 G1673 G1674 C1675 A1676 A1677 A1678 A1679 U1680 G1681 C1686 G1687 G1697 A1698 G1699
C1704 A1705 G1715 U1720 G1721 U1729 C1730 U1736 G1737 G1738 A1749 G1750 G1753 U1758 A1759 C1760 C1764 G1770 C1771 A1772 A1773 C1774 U1775 G1776 U1779 A1780 U1781 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 C1804 A1805 C1806
G1807 A1808 A1809 A1810 G1811 U1812 G1813 C1816 G1817 U1818 A1819 U1820 U1825 G1826 U1827 G1828 C1833 C1844 G1845 U1856 G1857 A1871 A1872 G1873 U1883 G1884 A1885 C1893 C1894 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 A1912 A1913 C1914 U1917 A1918 G1929 G1930 U1931 A1932 G1933 C1934
G1935 A1936 A1937 A1938 U1943 U1944 G1949 G1950 U1951 A1952 A1953 G1954 U1955 U1956 C1957 C1961 C1962 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 G1973 A1978 U1979 G1980 G1983 G1992 U1993 C1996 C1997 A1998 C1999 C2000 C2001 G2010 U2011 G2012 A2015 A2019 A2020 C2021 U2022 C2023 G2024 C2025
U2026 G2027 A2030 A2031 U2034 G2035 C2036 A2037 G2038 U2039 G2040 U2041 A2042 C2043 C2044 C2045 G2049 C2050 A2051 A2052 G2053 A2054 C2055 G2056 A2060 G2061 A2062 C2065 C2066 G2067 U2068 G2069 A2070 A2071 C2072 C2078 U2079 A2080 U2081 A2082 G2083 U2086 G2087 A2088 C2096 A2097 U2098 C2104 U2105 U2106
G2110 U2111 G2112 U2113 U2118 A2119 G2120 G2121 U2122 U2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 U2139 G2140 G2141 G2144 C2145 C2146 A2147 U2151 U2155 G2156 G2157 A2158 G2159 G2162 A2163 C2164 A2171 U2172 A2173 C2174 C2175 A2176 C2177 U2180 A2183 A2184 U2187 U2188 U2189
G2190 A2191 U2194 U2195 C2196 U2197 A2198 U2203 G2204 A2205 C2208 G2209 U2210 A2211 A2212 U2213 C2214 C2215 G2216 G2224 A2225 G2230 U2231 C2232 U2236 G2237 G2238 G2239 U2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2250 U2257 C2258 U2262 C2263 C2264 U2265 A2266 A2267 A2268 G2269 A2270 G2271



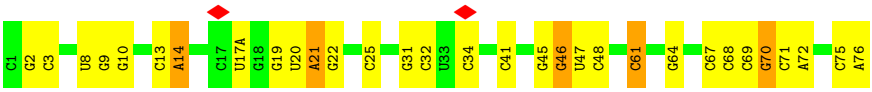
- Molecule 55: 5S ribosomal RNA

Chain 02:



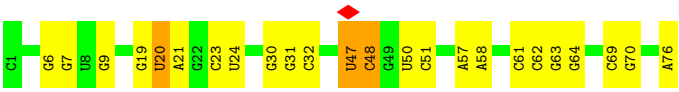
- Molecule 56: tRNAfMet

Chain X:



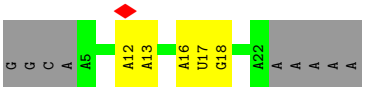
- Molecule 56: tRNAfMet

Chain W:



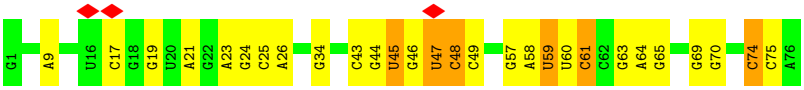
- Molecule 57: mRNA

Chain V: 48% 19% 33%



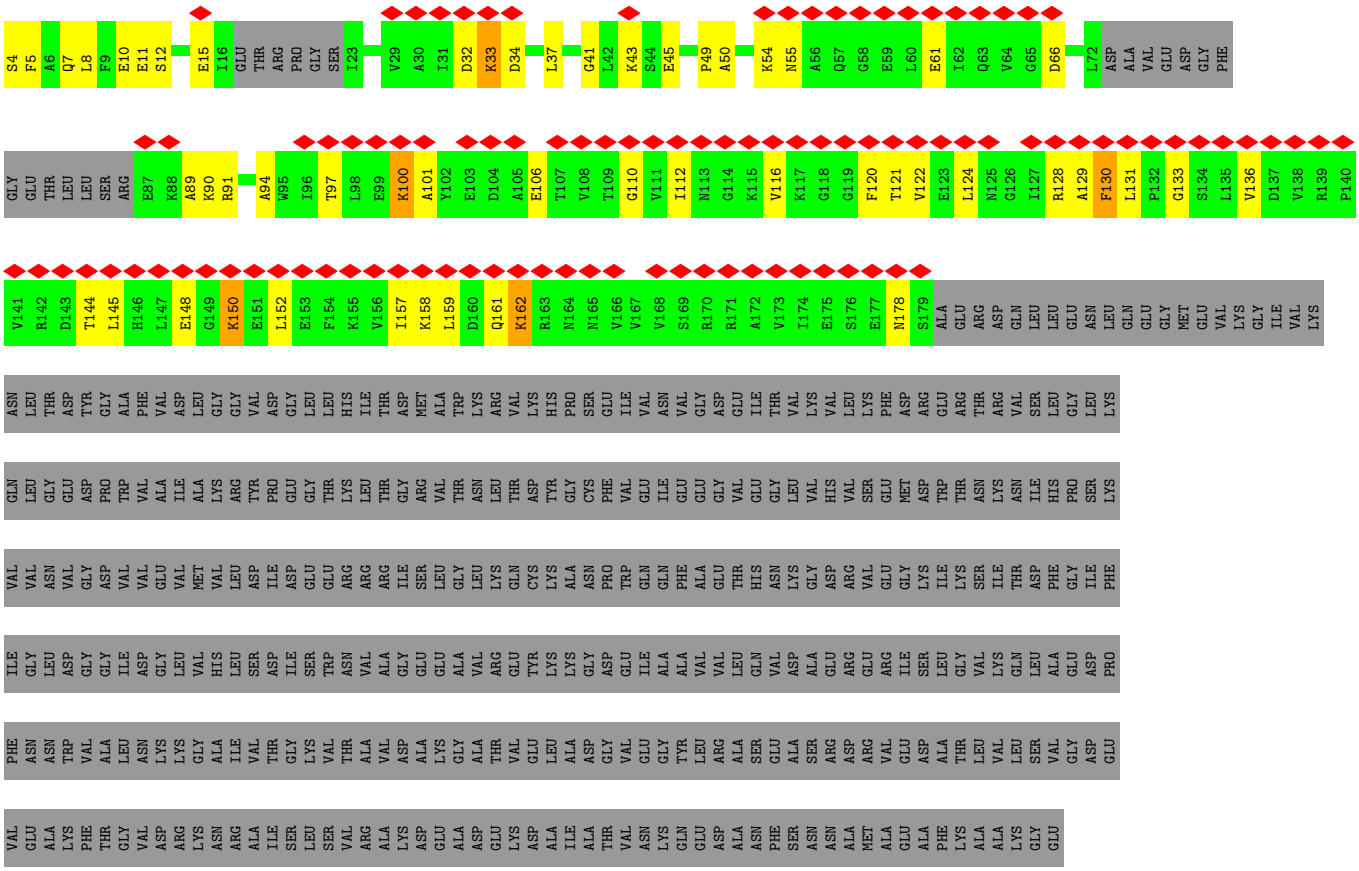
• Molecule 58: tRNAPhe

Chain Y: 63% 29% 8%



• Molecule 59: 30S ribosomal protein S1

Chain Z: 19% 19% 9% 72%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10289	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND3 was used to determine CTF values. FREALIGN applied CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	60976	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: FME

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	04	0.26	0/2122	0.56	0/2852
2	05	0.29	0/1586	0.51	0/2134
3	06	0.28	0/1571	0.51	0/2113
4	07	0.30	0/1435	0.53	0/1926
5	08	0.26	0/1343	0.51	0/1816
6	09	0.29	0/1122	0.55	0/1515
7	10	0.30	0/1002	0.58	0/1350
8	11	0.28	0/1046	0.53	0/1410
9	12	0.27	0/1152	0.51	0/1551
10	13	0.26	0/948	0.55	0/1268
11	14	0.27	0/1054	0.52	0/1403
12	15	0.30	0/1093	0.53	0/1460
13	16	0.29	0/974	0.51	0/1301
14	17	0.27	0/902	0.47	0/1209
15	18	0.29	0/929	0.54	0/1242
16	19	0.30	0/960	0.46	0/1278
17	20	0.31	0/829	0.59	1/1107 (0.1%)
18	21	0.25	0/864	0.53	0/1156
19	22	0.26	0/745	0.51	0/994
20	23	0.29	0/788	0.51	0/1051
21	24	0.29	0/766	0.50	0/1025
22	25	0.32	0/582	0.51	0/769
23	26	0.29	0/635	0.53	0/848
24	27	0.27	0/510	0.44	0/677
25	28	0.27	0/453	0.55	0/605
26	29	0.31	0/532	0.54	0/709
27	30	0.26	0/450	0.52	0/599
28	31	0.31	0/417	0.52	0/554
29	32	0.31	0/380	0.49	0/498
30	33	0.30	0/513	0.53	0/676
31	34	0.26	0/303	0.51	0/397
32	B	0.29	0/1788	0.53	0/2408

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	C	0.27	0/1652	0.52	0/2225
34	D	0.27	0/1665	0.50	0/2227
35	E	0.28	0/1170	0.53	0/1573
36	F	0.38	0/1048	0.53	0/1413
37	G	0.26	0/1196	0.51	0/1602
38	H	0.27	0/989	0.53	0/1326
39	I	0.28	0/1034	0.53	0/1375
40	J	0.26	0/797	0.56	0/1077
41	K	0.28	0/886	0.54	0/1195
42	L	0.27	0/969	0.61	0/1300
43	M	0.24	0/893	0.50	0/1193
44	N	0.28	0/817	0.46	0/1088
45	O	0.27	0/722	0.47	0/964
46	P	0.31	0/659	0.50	0/884
47	Q	0.28	0/658	0.59	0/881
48	R	0.29	0/545	0.51	0/731
49	S	0.31	0/653	0.52	0/877
50	T	0.27	0/671	0.44	0/888
51	U	0.30	0/551	0.53	0/728
52	03	0.26	0/1034	0.51	0/1387
53	A	0.30	0/36963	0.66	0/57662
54	01	0.29	0/69796	0.65	0/108888
55	02	0.28	0/2872	0.66	0/4479
56	W	0.28	0/1832	0.65	0/2855
56	X	0.30	0/1832	0.65	0/2855
57	V	0.28	0/436	0.63	0/679
58	Y	0.34	0/1812	0.67	0/2823
59	Z	0.44	0/1215	0.45	0/1635
All	All	0.29	0/165161	0.62	1/246711 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	20	50	GLY	N-CA-C	-5.75	98.73	113.10

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	04	2083	0	2157	128	0
2	05	1565	0	1616	78	0
3	06	1552	0	1619	97	0
4	07	1411	0	1447	100	0
5	08	1323	0	1374	69	0
6	09	1111	0	1148	72	0
7	10	989	0	1025	82	0
8	11	1032	0	1088	83	0
9	12	1129	0	1162	77	0
10	13	939	0	1012	56	0
11	14	1045	0	1117	69	0
12	15	1074	0	1157	64	0
13	16	961	0	1000	57	0
14	17	892	0	923	49	0
15	18	917	0	965	68	0
16	19	947	0	1022	66	0
17	20	816	0	839	51	0
18	21	857	0	922	64	0
19	22	739	0	807	36	0
20	23	780	0	834	37	0
21	24	753	0	780	31	0
22	25	575	0	592	23	0
23	26	625	0	655	22	0
24	27	509	0	543	26	0
25	28	449	0	491	28	0
26	29	523	0	524	24	0
27	30	444	0	461	43	0
28	31	410	0	440	21	0
29	32	377	0	418	19	0
30	33	504	0	574	20	0
31	34	302	0	343	22	0
32	B	1757	0	1787	81	0
33	C	1625	0	1699	89	0
34	D	1643	0	1710	120	0
35	E	1157	0	1199	98	0
36	F	1028	0	1002	61	0
37	G	1182	0	1240	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	979	0	1034	63	0
39	I	1022	0	1070	69	0
40	J	787	0	828	61	0
41	K	870	0	878	64	0
42	L	955	0	1019	72	0
43	M	884	0	944	66	0
44	N	805	0	847	57	0
45	O	714	0	737	28	0
46	P	649	0	666	64	0
47	Q	649	0	691	45	0
48	R	536	0	552	39	0
49	S	638	0	665	33	0
50	T	665	0	714	39	0
51	U	545	0	579	62	0
52	03	1027	0	1092	68	0
53	A	33012	0	16618	507	0
54	01	62317	0	31346	1010	0
55	02	2568	0	1303	47	0
56	W	1640	0	836	12	0
56	X	1640	0	837	19	0
57	V	388	0	196	3	0
58	Y	1622	0	821	16	0
59	Z	1204	0	1221	59	0
60	W	10	0	10	0	0
All	All	152151	0	103196	4269	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 17.

The worst 5 of 4269 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)
15:18:59:THR:HG22	15:18:72:VAL:HG12	1.33	1.10
54:01:45:G:H5”	54:01:46:G:H5’	1.22	1.09
14:17:29:HIS:HB3	14:17:36:TYR:HB2	1.37	1.04
52:03:174:THR:HG21	54:01:2124:G:H4’	1.39	1.04
43:M:97:ARG:HB2	43:M:99:GLN:HE22	1.23	1.03

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	04	269/271 (99%)	225 (84%)	33 (12%)	11 (4%)	2	20
2	05	207/209 (99%)	175 (84%)	31 (15%)	1 (0%)	25	59
3	06	199/201 (99%)	164 (82%)	29 (15%)	6 (3%)	3	26
4	07	175/177 (99%)	140 (80%)	31 (18%)	4 (2%)	5	31
5	08	174/176 (99%)	155 (89%)	17 (10%)	2 (1%)	12	45
6	09	147/149 (99%)	111 (76%)	27 (18%)	9 (6%)	1	13
7	10	129/131 (98%)	98 (76%)	25 (19%)	6 (5%)	2	17
8	11	139/141 (99%)	118 (85%)	18 (13%)	3 (2%)	5	31
9	12	140/142 (99%)	122 (87%)	13 (9%)	5 (4%)	3	22
10	13	120/122 (98%)	103 (86%)	15 (12%)	2 (2%)	7	36
11	14	141/143 (99%)	120 (85%)	19 (14%)	2 (1%)	9	40
12	15	134/136 (98%)	103 (77%)	26 (19%)	5 (4%)	2	22
13	16	118/120 (98%)	83 (70%)	30 (25%)	5 (4%)	2	19
14	17	114/116 (98%)	95 (83%)	14 (12%)	5 (4%)	2	18
15	18	112/114 (98%)	89 (80%)	18 (16%)	5 (4%)	2	18
16	19	115/117 (98%)	94 (82%)	17 (15%)	4 (4%)	3	24
17	20	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	2	20
18	21	108/110 (98%)	87 (81%)	17 (16%)	4 (4%)	2	22
19	22	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
20	23	100/102 (98%)	81 (81%)	15 (15%)	4 (4%)	2	20
21	24	92/94 (98%)	78 (85%)	11 (12%)	3 (3%)	3	25
22	25	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
23	26	75/77 (97%)	67 (89%)	7 (9%)	1 (1%)	10	41
24	27	61/63 (97%)	48 (79%)	10 (16%)	3 (5%)	2	16
25	28	56/58 (97%)	49 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	29	64/66 (97%)	53 (83%)	9 (14%)	2 (3%)	3	26
27	30	54/56 (96%)	46 (85%)	6 (11%)	2 (4%)	2	22
28	31	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
29	32	44/46 (96%)	29 (66%)	11 (25%)	4 (9%)	0	7
30	33	62/64 (97%)	50 (81%)	7 (11%)	5 (8%)	1	8
31	34	36/38 (95%)	29 (81%)	7 (19%)	0	100	100
32	B	223/225 (99%)	193 (86%)	26 (12%)	4 (2%)	7	35
33	C	204/206 (99%)	167 (82%)	29 (14%)	8 (4%)	2	21
34	D	203/205 (99%)	157 (77%)	32 (16%)	14 (7%)	1	10
35	E	155/157 (99%)	123 (79%)	24 (16%)	8 (5%)	1	15
36	F	124/126 (98%)	101 (82%)	17 (14%)	6 (5%)	2	17
37	G	149/151 (99%)	125 (84%)	21 (14%)	3 (2%)	6	33
38	H	127/129 (98%)	109 (86%)	16 (13%)	2 (2%)	8	38
39	I	125/127 (98%)	101 (81%)	16 (13%)	8 (6%)	1	12
40	J	96/98 (98%)	82 (85%)	11 (12%)	3 (3%)	3	26
41	K	114/116 (98%)	92 (81%)	19 (17%)	3 (3%)	4	28
42	L	121/123 (98%)	93 (77%)	20 (16%)	8 (7%)	1	11
43	M	112/114 (98%)	88 (79%)	20 (18%)	4 (4%)	3	22
44	N	98/100 (98%)	70 (71%)	24 (24%)	4 (4%)	2	20
45	O	86/88 (98%)	64 (74%)	20 (23%)	2 (2%)	5	31
46	P	80/82 (98%)	62 (78%)	17 (21%)	1 (1%)	10	41
47	Q	78/80 (98%)	61 (78%)	14 (18%)	3 (4%)	2	21
48	R	63/65 (97%)	50 (79%)	8 (13%)	5 (8%)	1	8
49	S	77/79 (98%)	63 (82%)	9 (12%)	5 (6%)	1	12
50	T	83/85 (98%)	74 (89%)	8 (10%)	1 (1%)	11	43
51	U	63/65 (97%)	42 (67%)	19 (30%)	2 (3%)	3	25
52	03	130/223 (58%)	114 (88%)	13 (10%)	3 (2%)	5	31
59	Z	150/554 (27%)	126 (84%)	21 (14%)	3 (2%)	6	33
All	All	6159/6758 (91%)	5040 (82%)	912 (15%)	207 (3%)	5	24

5 of 207 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	04	261	ARG
3	06	84	THR
4	07	175	PRO
6	09	10	ALA
7	10	58	THR

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	04	216/216 (100%)	215 (100%)	1 (0%)	86	93
2	05	164/164 (100%)	163 (99%)	1 (1%)	84	91
3	06	165/165 (100%)	165 (100%)	0	100	100
4	07	148/148 (100%)	147 (99%)	1 (1%)	81	89
5	08	137/137 (100%)	137 (100%)	0	100	100
6	09	114/114 (100%)	114 (100%)	0	100	100
7	10	100/100 (100%)	100 (100%)	0	100	100
8	11	109/109 (100%)	108 (99%)	1 (1%)	75	86
9	12	116/116 (100%)	116 (100%)	0	100	100
10	13	103/103 (100%)	103 (100%)	0	100	100
11	14	102/102 (100%)	101 (99%)	1 (1%)	73	84
12	15	109/109 (100%)	109 (100%)	0	100	100
13	16	100/100 (100%)	100 (100%)	0	100	100
14	17	86/86 (100%)	86 (100%)	0	100	100
15	18	99/99 (100%)	99 (100%)	0	100	100
16	19	89/89 (100%)	89 (100%)	0	100	100
17	20	84/84 (100%)	84 (100%)	0	100	100
18	21	93/93 (100%)	92 (99%)	1 (1%)	70	83
19	22	80/80 (100%)	80 (100%)	0	100	100
20	23	83/83 (100%)	82 (99%)	1 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	24	78/78 (100%)	77 (99%)	1 (1%)	65	81
22	25	57/57 (100%)	57 (100%)	0	100	100
23	26	67/67 (100%)	66 (98%)	1 (2%)	60	77
24	27	55/55 (100%)	55 (100%)	0	100	100
25	28	48/48 (100%)	48 (100%)	0	100	100
26	29	59/59 (100%)	59 (100%)	0	100	100
27	30	47/47 (100%)	47 (100%)	0	100	100
28	31	45/45 (100%)	45 (100%)	0	100	100
29	32	38/38 (100%)	38 (100%)	0	100	100
30	33	51/51 (100%)	51 (100%)	0	100	100
31	34	34/34 (100%)	34 (100%)	0	100	100
32	B	186/186 (100%)	185 (100%)	1 (0%)	86	93
33	C	170/170 (100%)	170 (100%)	0	100	100
34	D	172/172 (100%)	169 (98%)	3 (2%)	56	75
35	E	119/119 (100%)	119 (100%)	0	100	100
36	F	108/108 (100%)	107 (99%)	1 (1%)	75	86
37	G	124/124 (100%)	124 (100%)	0	100	100
38	H	104/104 (100%)	104 (100%)	0	100	100
39	I	105/105 (100%)	104 (99%)	1 (1%)	73	84
40	J	86/86 (100%)	85 (99%)	1 (1%)	67	82
41	K	89/89 (100%)	89 (100%)	0	100	100
42	L	103/103 (100%)	103 (100%)	0	100	100
43	M	92/92 (100%)	92 (100%)	0	100	100
44	N	83/83 (100%)	83 (100%)	0	100	100
45	O	76/76 (100%)	76 (100%)	0	100	100
46	P	65/65 (100%)	64 (98%)	1 (2%)	60	77
47	Q	74/74 (100%)	74 (100%)	0	100	100
48	R	56/56 (100%)	56 (100%)	0	100	100
49	S	70/70 (100%)	70 (100%)	0	100	100
50	T	65/65 (100%)	65 (100%)	0	100	100
51	U	55/55 (100%)	54 (98%)	1 (2%)	54	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	03	110/174 (63%)	110 (100%)	0	100	100
59	Z	129/458 (28%)	120 (93%)	9 (7%)	12	38
All	All	5117/5510 (93%)	5090 (100%)	27 (0%)	85	93

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	I	60	LEU
51	U	62	GLU
59	Z	150	LYS
46	P	29	ASN
59	Z	66	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
18	21	40	ASN
44	N	42	ASN
32	B	17	HIS
43	M	7	ASN
48	R	53	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	135 (8%)	4 (0%)
54	01	2902/2903 (99%)	345 (11%)	10 (0%)
55	02	119/120 (99%)	12 (10%)	1 (0%)
56	W	76/77 (98%)	7 (9%)	0
56	X	76/77 (98%)	15 (19%)	0
57	V	17/27 (62%)	3 (17%)	0
58	Y	75/76 (98%)	14 (18%)	1 (1%)
All	All	4803/4819 (99%)	531 (11%)	16 (0%)

5 of 531 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	G
53	A	9	G

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Mol	Chain	Res	Type
53	A	22	G
53	A	31	G
53	A	32	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	02	88	C
54	01	2391	G
54	01	1130	U
54	01	2326	C
54	01	1020	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	FME	W	101	56	8,9,10	0.67	0	8,9,11	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	FME	W	101	56	-	1/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	W	101	FME	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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.

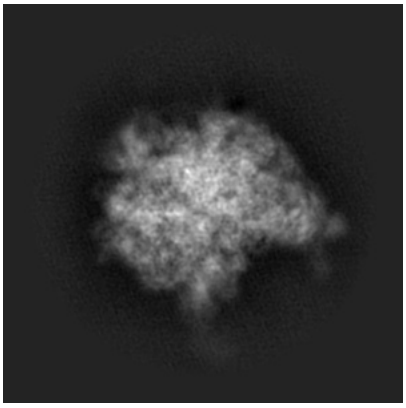
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7289. These allow visual inspection of the internal detail of the map and identification of artifacts.

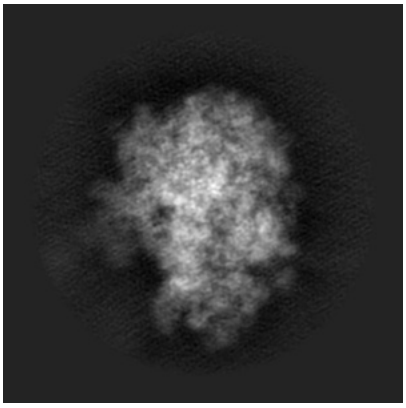
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

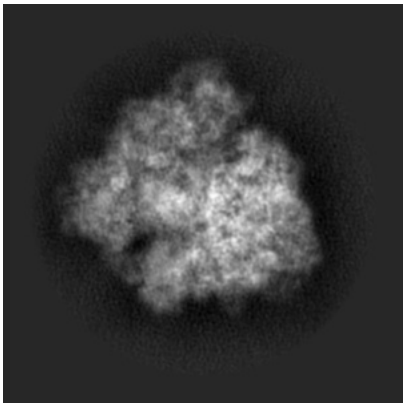
6.1.1 Primary map



X



Y

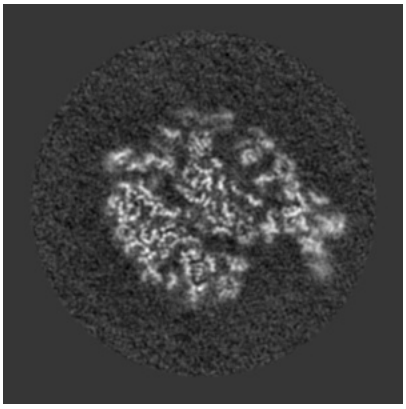


Z

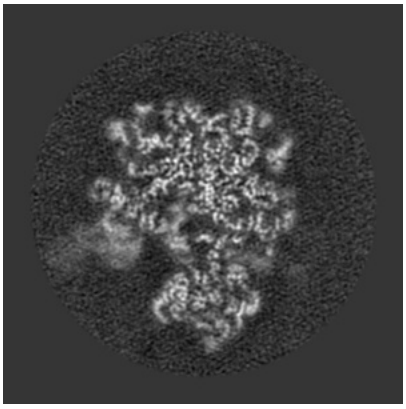
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

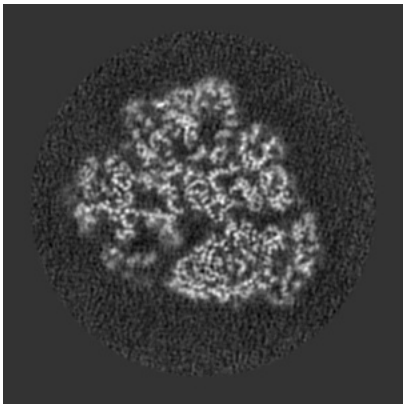
6.2.1 Primary map



X Index: 240



Y Index: 240

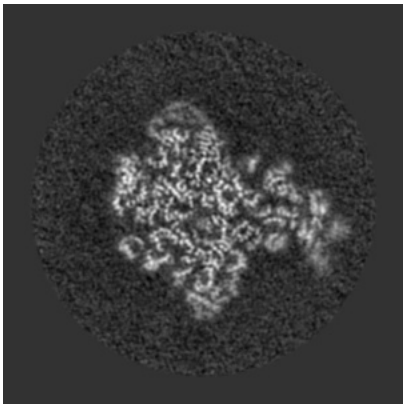


Z Index: 240

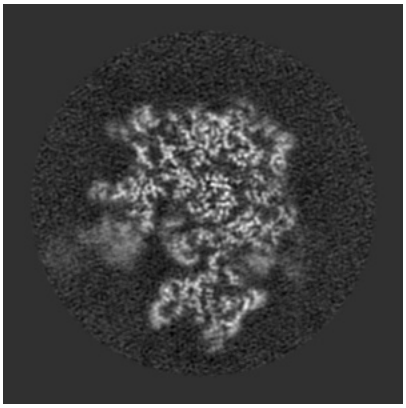
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

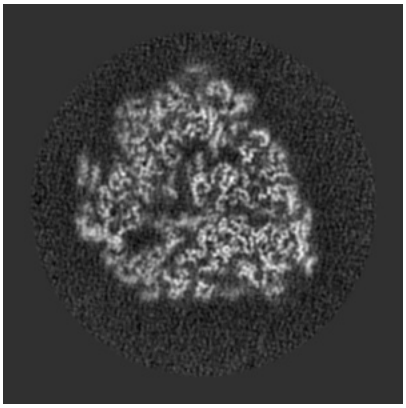
6.3.1 Primary map



X Index: 252



Y Index: 247

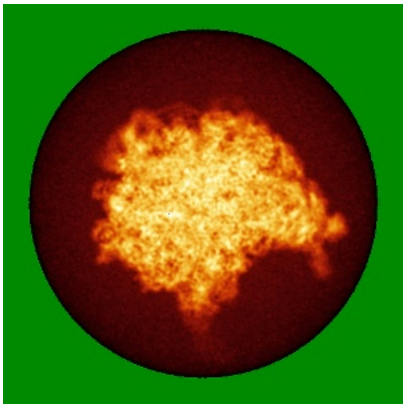


Z Index: 228

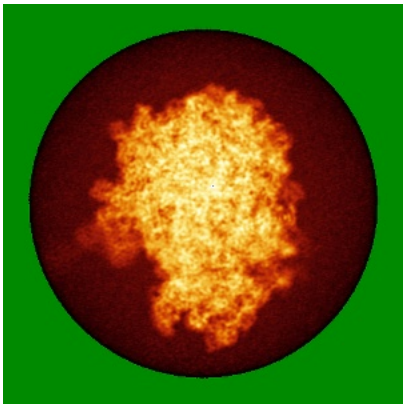
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

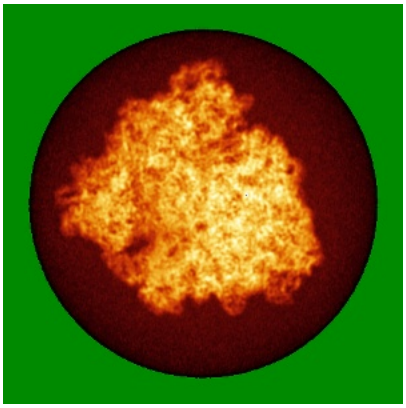
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

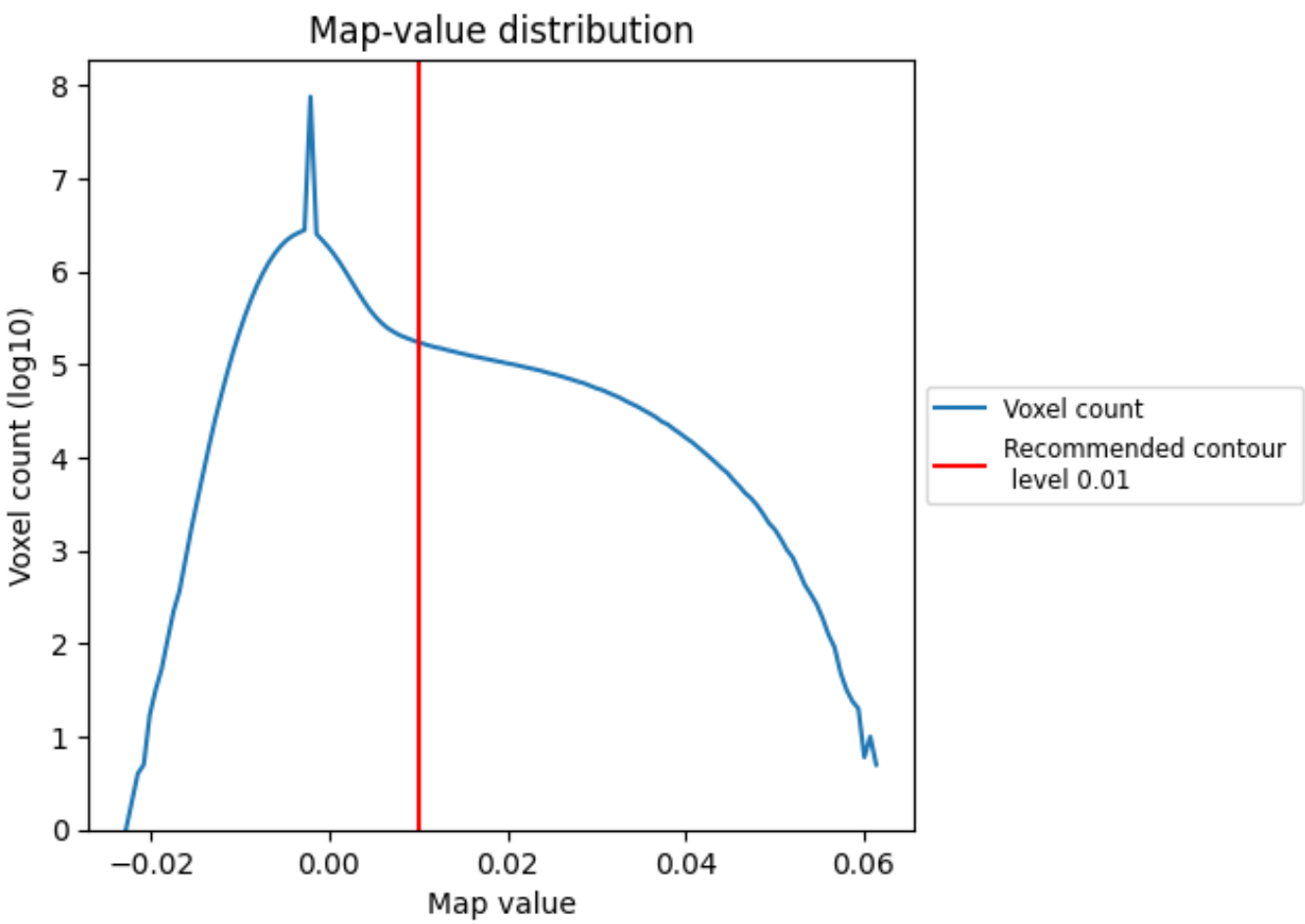
6.6 Mask visualisation (i)

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

7 Map analysis (i)

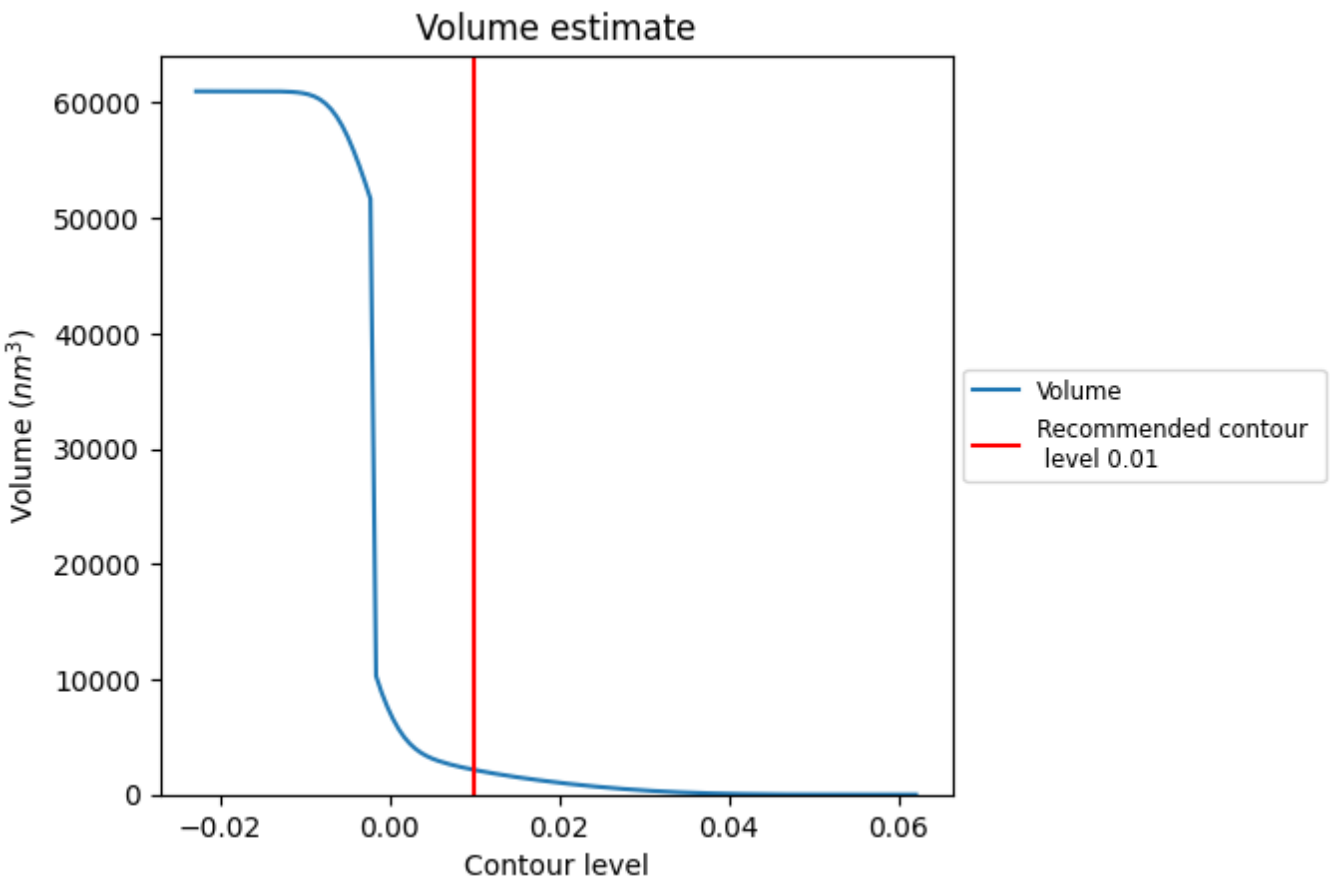
This section contains the results of statistical analysis of the map.

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.

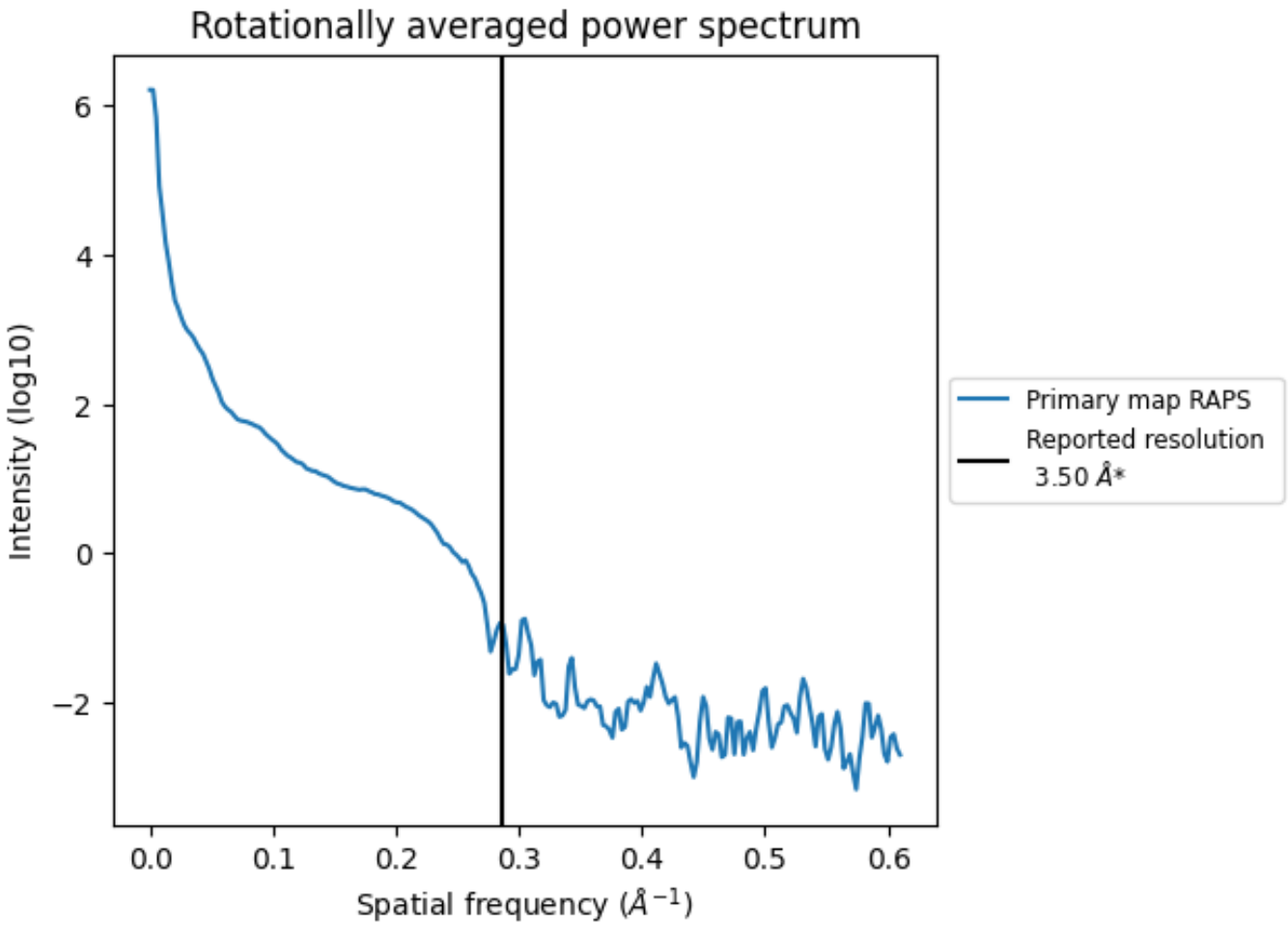
7.2 Volume estimate (i)



The volume at the recommended contour level is 2139 nm^3; this corresponds to an approximate mass of 1932 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 0.286 Å^{-1}

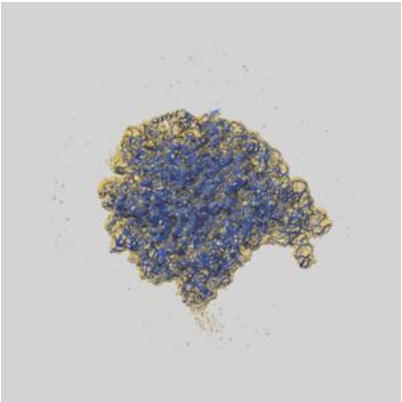
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

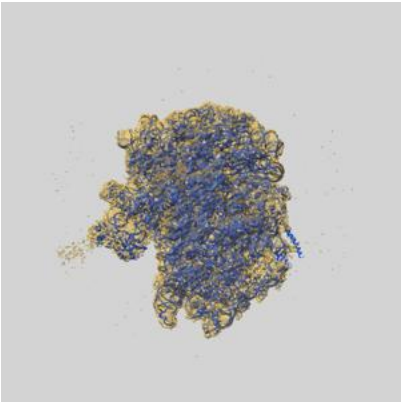
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7289 and PDB model 6BU8. Per-residue inclusion information can be found in section 3 on page 16.

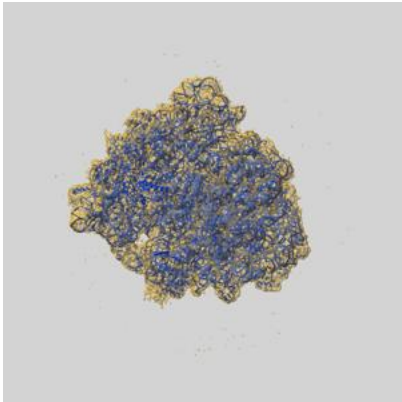
9.1 Map-model overlay (i)



X



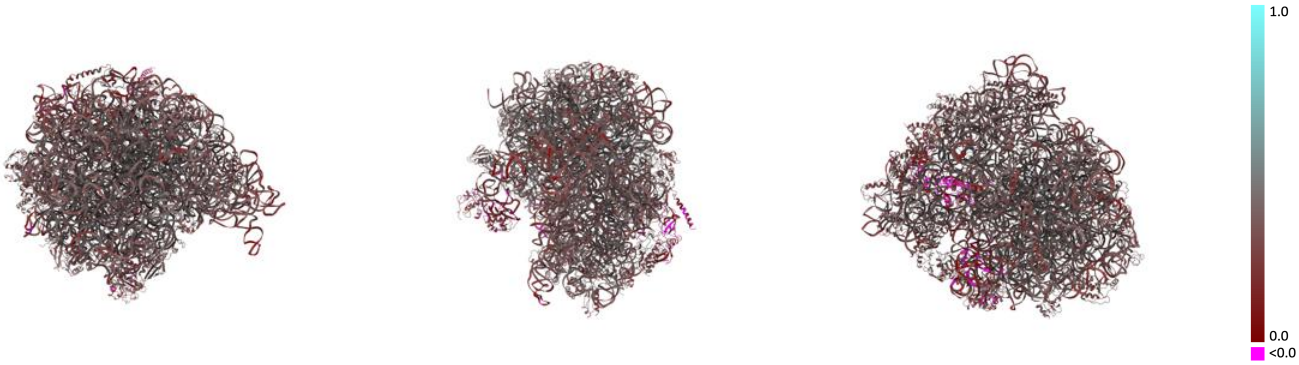
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

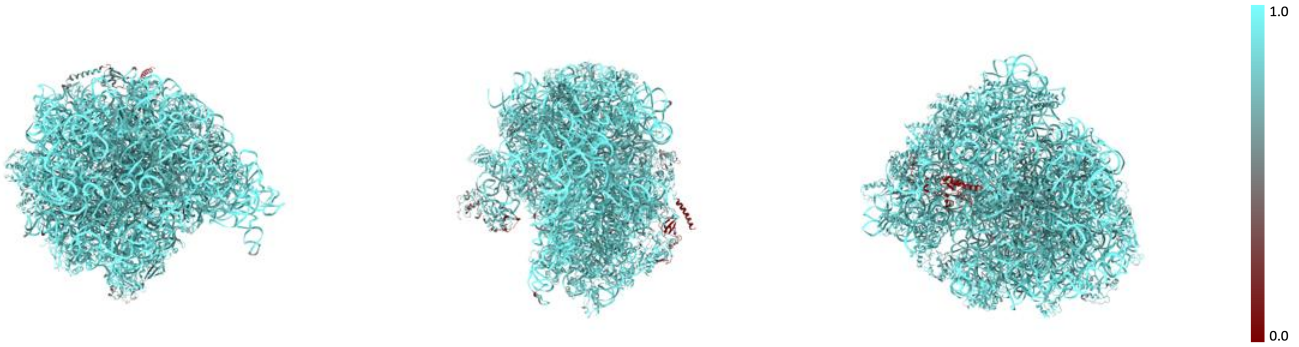
9.2 Q-score mapped to coordinate model (i)



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.

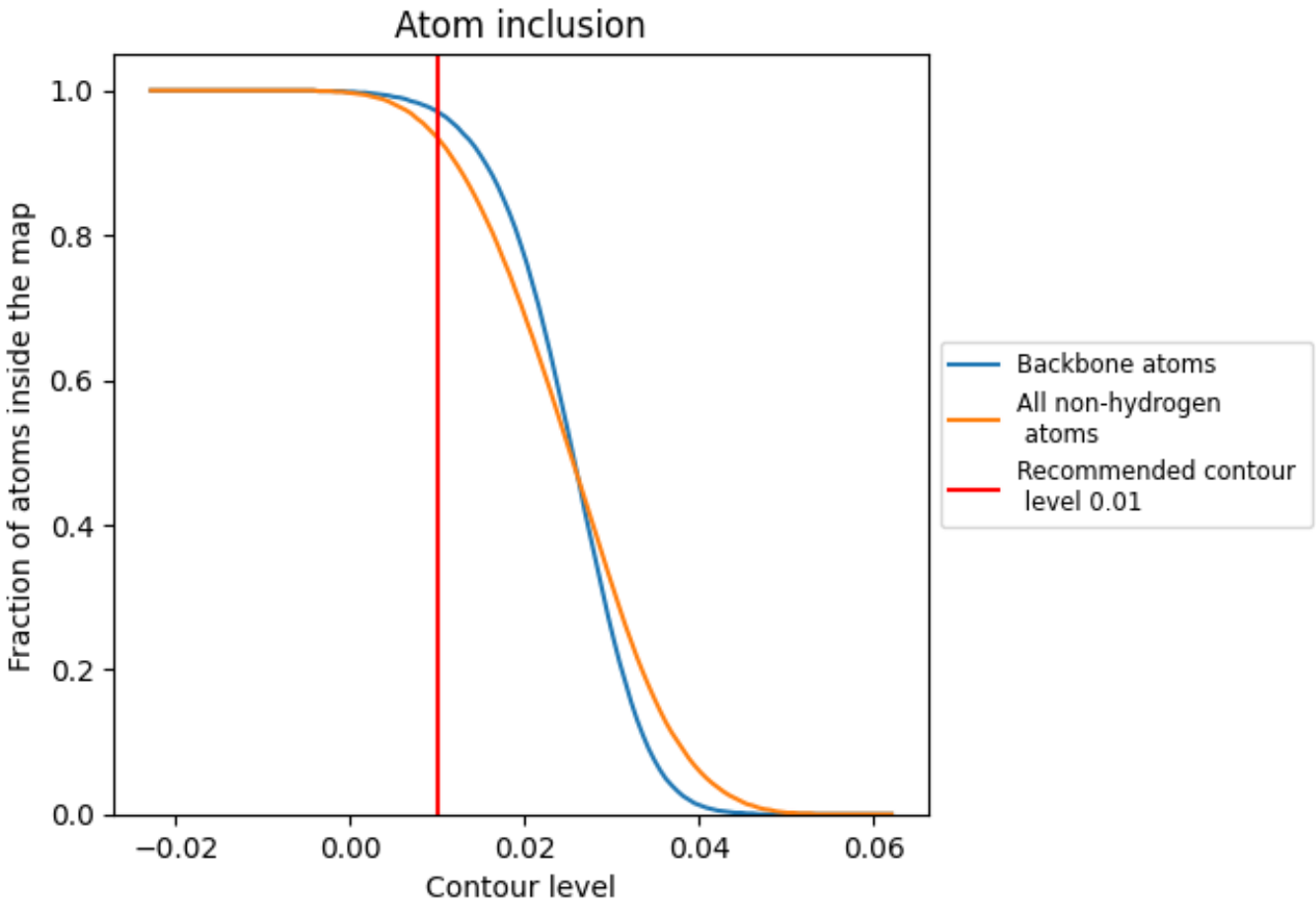
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.3600
01	0.9790	0.3740
02	0.9820	0.3500
03	0.8570	0.2350
04	0.8820	0.4170
05	0.8780	0.4050
06	0.8660	0.3690
07	0.8890	0.3370
08	0.8990	0.3530
09	0.7050	0.2910
10	0.5810	0.1830
11	0.6310	0.2060
12	0.8820	0.3750
13	0.8490	0.4110
14	0.8860	0.3910
15	0.8460	0.4040
16	0.9010	0.3760
17	0.9080	0.3530
18	0.8580	0.3900
19	0.8960	0.3830
20	0.8810	0.3820
21	0.8410	0.3890
22	0.8660	0.3670
23	0.9080	0.3540
24	0.8900	0.3790
25	0.9140	0.4020
26	0.8830	0.3980
27	0.8510	0.3030
28	0.9150	0.3890
29	0.8340	0.3230
30	0.9090	0.3970
31	0.8510	0.3810
32	0.8620	0.4010
33	0.8900	0.4120
34	0.9110	0.4000

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Chain	Atom inclusion	Q-score
A	0.9820	0.3640
B	0.8730	0.3330
C	0.8630	0.3740
D	0.8850	0.3370
E	0.8950	0.3830
F	0.7180	0.2920
G	0.8690	0.3430
H	0.8820	0.3850
I	0.8850	0.3570
J	0.8410	0.3470
K	0.8740	0.3790
L	0.8680	0.3790
M	0.9000	0.3420
N	0.8880	0.3710
O	0.8970	0.3520
P	0.9200	0.3550
Q	0.8770	0.3460
R	0.9070	0.3730
S	0.9160	0.3500
T	0.8950	0.3300
U	0.7740	0.3060
V	0.8220	0.2680
W	0.9350	0.3480
X	0.8650	0.1800
Y	0.9010	0.2770
Z	0.3090	0.0490