wwPDB EM Validation Summary Report (i)

Mar 2, 2024 – 01:16 PM EST

PDB ID	:	5UYM
EMDB ID	:	EMD-8617
Title	:	70S ribosome bound with cognate ternary complex base-paired to A site codon, closed 30S (Structure III)
Authors	:	Loveland, A.B.; Demo, G.; Grigorieff, N.; Korostelev, A.A.
Deposited on	:	2017-02-24
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

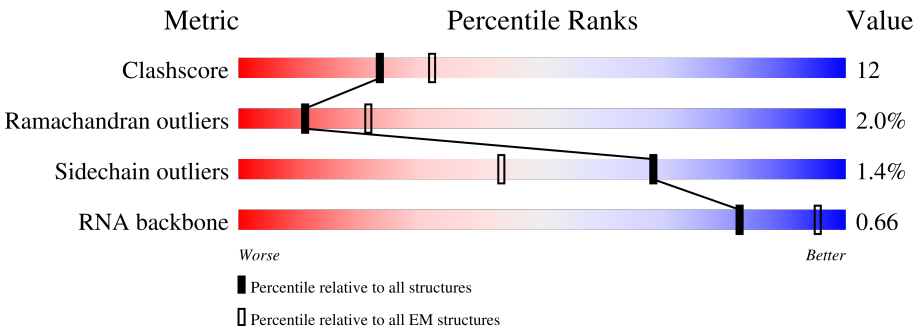
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	68% 32%
2	05	209	• 70% 30%
3	06	201	• 70% 29% •
4	07	177	• 63% 36% •
5	08	176	• 73% 26% •
6	09	149	38% 62% 38%
7	10	131	34% 46% 52% • •

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Mol	Chain	Length	Quality of chain
8	11	141	17% 57% 40%
9	12	142	64% 35%
10	13	122	65% 34%
11	14	143	65% 32%
12	15	136	71% 26%
13	16	120	70% 28%
14	17	116	54% 46%
15	18	114	68% 31%
16	19	117	74% 26%
17	20	103	76% 23%
18	21	110	59% 39%
19	22	93	70% 29%
20	23	102	71% 25%
21	24	94	70% 30%
22	25	75	75% 25%
23	26	77	78% 22%
24	27	63	63% 37%
25	28	58	67% 33%
26	29	66	17% 71% 27%
27	30	56	70% 30%
28	31	50	70% 26%
29	32	46	70% 30%
30	33	64	67% 33%
31	34	38	50% 42% 8%
32	B	218	63% 35%

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Mol	Chain	Length	Quality of chain
33	C	206	58% 42%
34	D	205	59% 39%
35	E	157	60% 36%
36	F	100	57% 42%
37	G	151	68% 30%
38	H	129	63% 36%
39	I	127	57% 39%
40	J	98	58% 39%
41	K	116	56% 40%
42	L	123	68% 30%
43	M	114	64% 35%
44	N	100	63% 37%
45	O	88	73% 26%
46	P	82	5% 55% 40% 5%
47	Q	80	58% 41%
48	R	65	62% 34% 5%
49	S	79	61% 38%
50	T	85	71% 28%
51	U	65	12% 57% 38% 5%
52	03	223	13% 12% 47% 40%
53	A	1539	66% 30%
54	01	2903	62% 33% 5%
55	02	120	62% 30% 8%
56	W	77	5% 86% 12%
56	X	77	9% 39% 49% 12%

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Mol	Chain	Length	Quality of chain
57	V	18	11% 56% 44%
58	Y	76	61% 36%
59	Z	392	37% 57% 5%

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 154139 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	218	1705	1081	305	312	7	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	100	818	515	148	149	6	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	conflict	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

- 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 Phe-tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	Y	76	1619	723	290	531	75	0	0

- Molecule 59 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	Z	392	3029	1915	521	580	13	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	12	1	1	1	0
60	25	1	1	1	0
60	N	1	1	1	0
60	A	107	107	107	0
60	01	263	263	263	0

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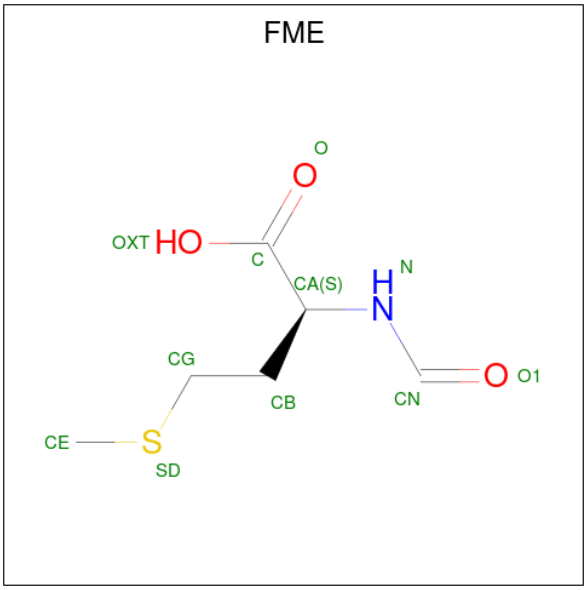
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	02	6	6	6	0
60	V	2	2	2	0
60	W	1	1	1	0
60	Z	1	1	1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

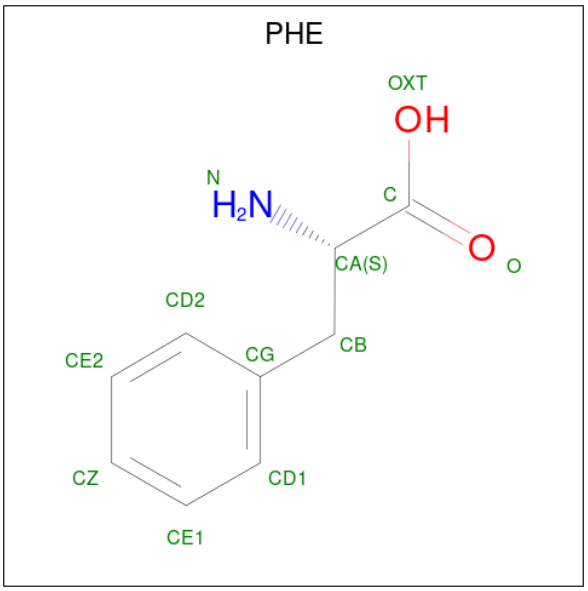
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
61	29	1	1	1	0
61	34	1	1	1	0

- Molecule 62 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



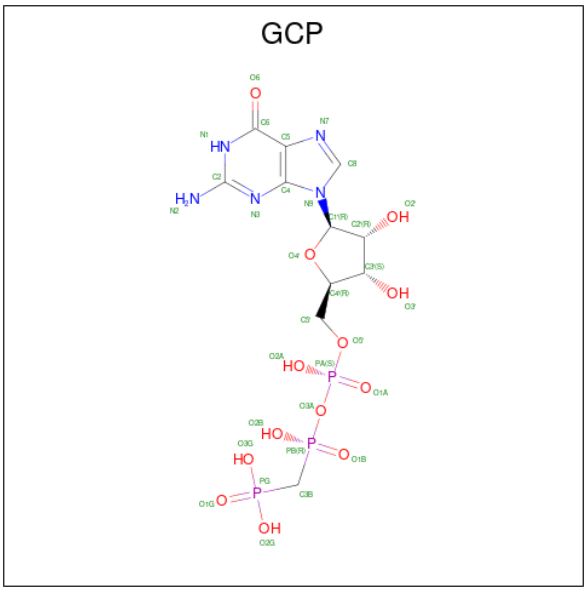
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
62	W	1	10	6	1	2	1	0

- Molecule 63 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
63	Y	1	11	9	1	1	0

- Molecule 64 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	Z	1	32	11	5	13	3	0

3 Residue-property plots (i)

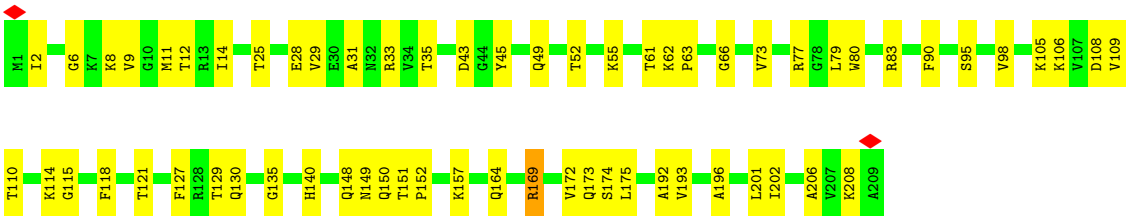
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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:

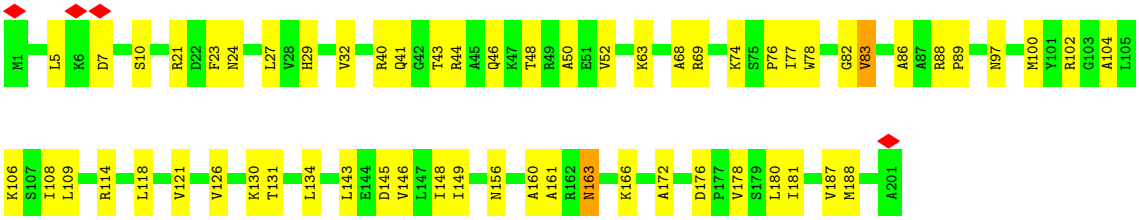
• Molecule 2: 50S ribosomal protein L3

Chain 05:



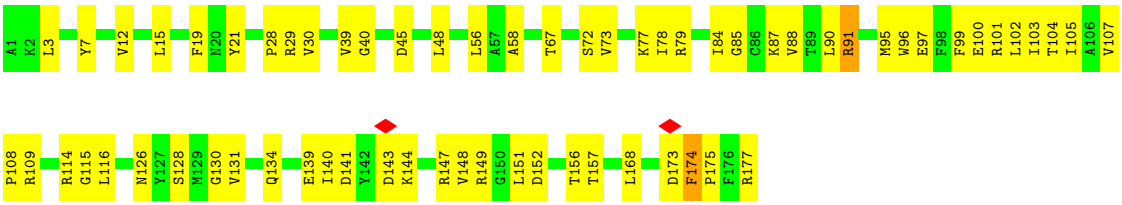
• Molecule 3: 50S ribosomal protein L4

Chain 06:



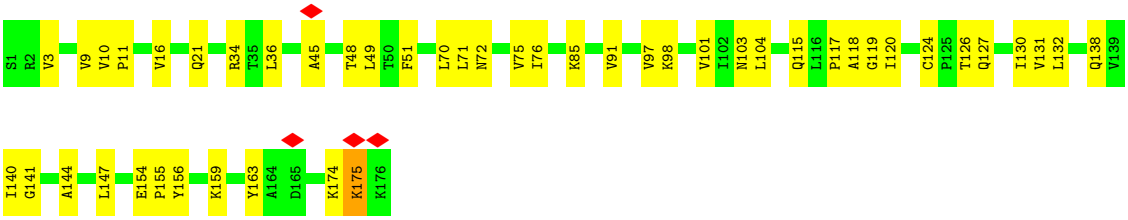
• Molecule 4: 50S ribosomal protein L5

Chain 07:



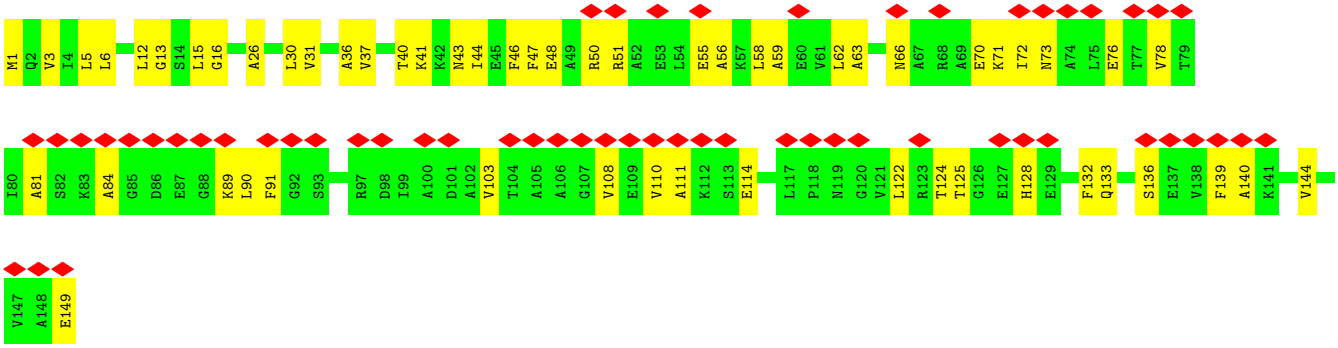
- Molecule 5: 50S ribosomal protein L6

Chain 08:



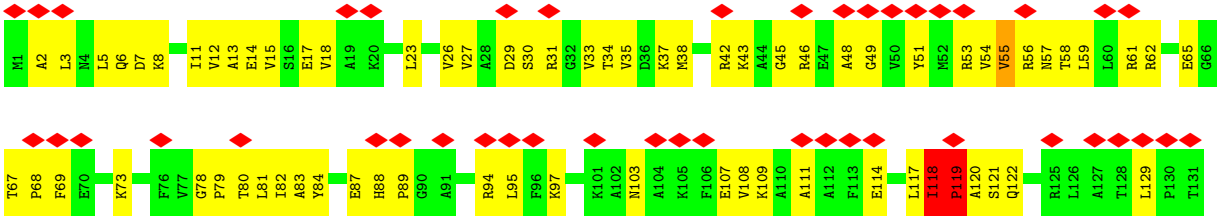
- Molecule 6: 50S ribosomal protein L9

Chain 09:



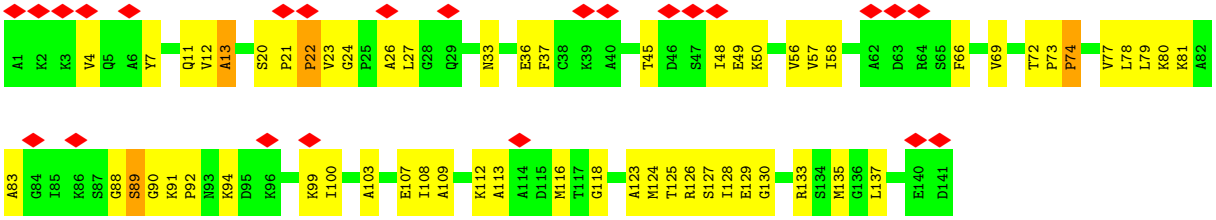
- Molecule 7: 50S ribosomal protein L10

Chain 10:



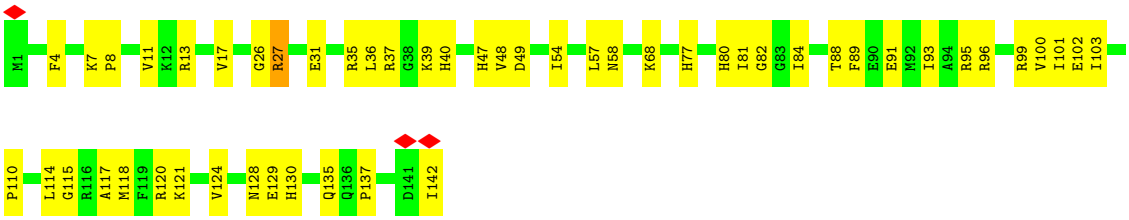
- Molecule 8: 50S ribosomal protein L11

Chain 11:



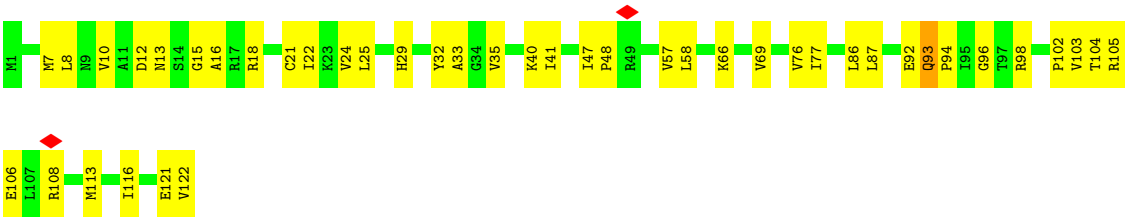
• Molecule 9: 50S ribosomal protein L13

Chain 12:



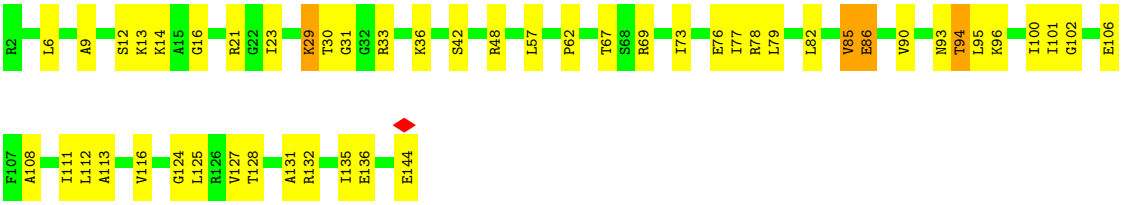
• Molecule 10: 50S ribosomal protein L14

Chain 13:



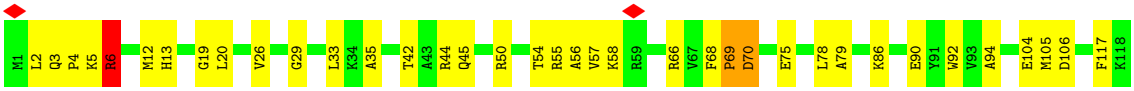
• Molecule 11: 50S ribosomal protein L15

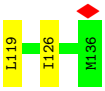
Chain 14:



• Molecule 12: 50S ribosomal protein L16

Chain 15:



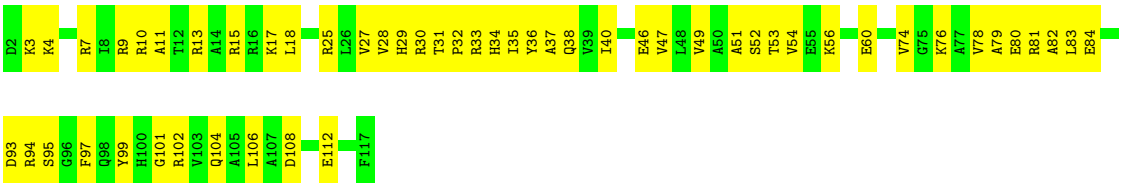


• Molecule 13: 50S ribosomal protein L17

Chain 16:

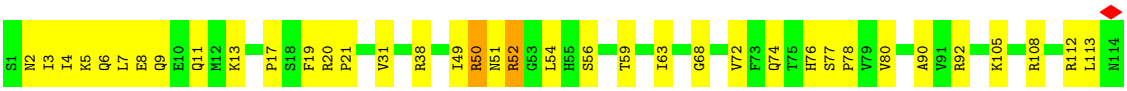
• Molecule 14: 50S ribosomal protein L18

Chain 17:



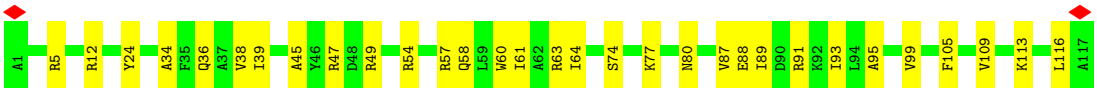
• Molecule 15: 50S ribosomal protein L19

Chain 18:



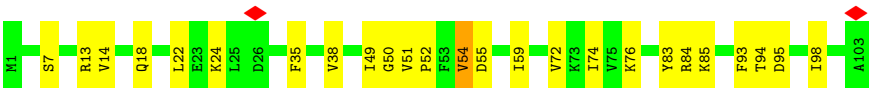
• Molecule 16: 50S ribosomal protein L20

Chain 19:



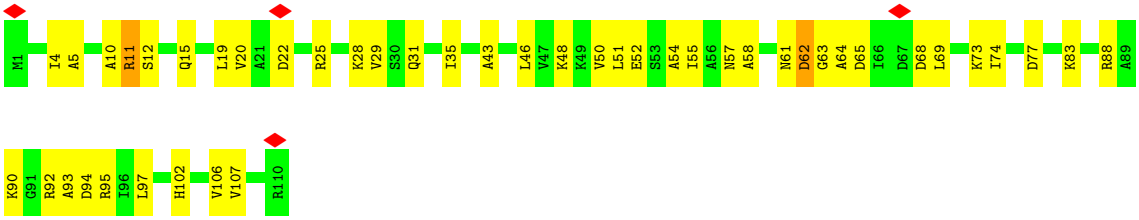
• Molecule 17: 50S ribosomal protein L21

Chain 20:



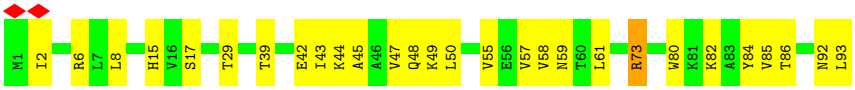
• Molecule 18: 50S ribosomal protein L22

Chain 21:



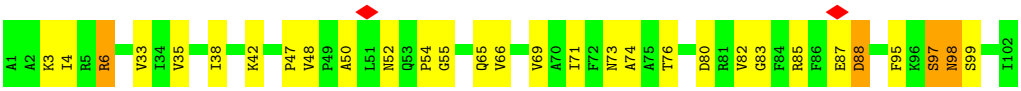
• Molecule 19: 50S ribosomal protein L23

Chain 22:



• Molecule 20: 50S ribosomal protein L24

Chain 23:

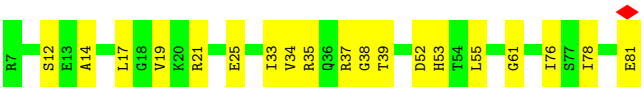


• Molecule 21: 50S ribosomal protein L25

Chain 24:

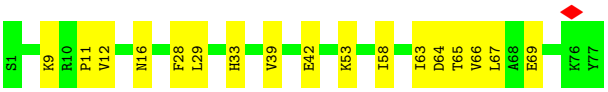
• Molecule 22: 50S ribosomal protein L27

Chain 25:



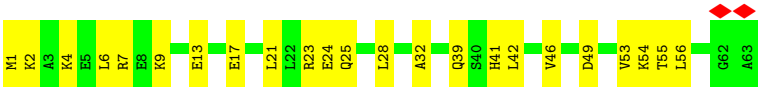
• Molecule 23: 50S ribosomal protein L28

Chain 26:



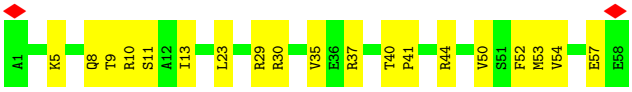
• Molecule 24: 50S ribosomal protein L29

Chain 27:



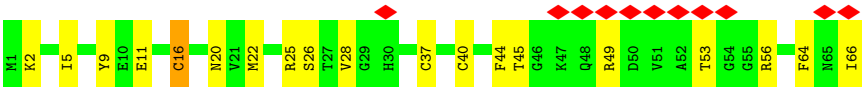
• Molecule 25: 50S ribosomal protein L30

Chain 28:



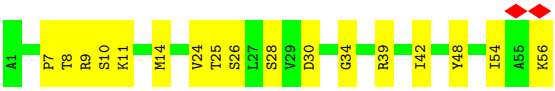
• Molecule 26: 50S ribosomal protein L31

Chain 29:



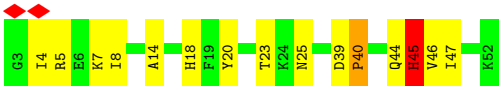
• Molecule 27: 50S ribosomal protein L32

Chain 30:



• Molecule 28: 50S ribosomal protein L33

Chain 31:

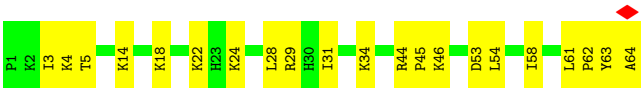


• Molecule 29: 50S ribosomal protein L34

Chain 32:

• Molecule 30: 50S ribosomal protein L35

Chain 33:



• Molecule 31: 50S ribosomal protein L36

Chain 34: 50% 42% 8%

M1 K2 V3 R4 K8 G11 R12 K15 I16 R19 I23 R24 V25 I26 C27 S28 A29 E30 P31 K32 Q35 R36 Q37 G38

- Molecule 32: 30S ribosomal protein S2

Chain B: 63% 35%

M8 G12 V13 G16 H17 Q18 T19 R20 K27 P28 F31 R34 N35 K36 V37 H38 I39 I40 N41 L42 E43 K44 T45 V46 P47 M48 F49 N50 E51 A52 L53 A54 E55 L56 I59 A60 K63 L67 T71 K72 R73 A74 A75 V79 K80 C86 D87 D88 F89

F90 V91 R94 W95 L96 G97 G98 N102 T105 E117 T118 Q119 S120 Q121 T124 K127 L128 T129 K130 G149 I150 M153 L160 F161 V162 I163 D164 A165 D166 H169 I170 A171 I172 N176 F183 A184 D187 S190 D193 F197 N202 D203 D204

A205 I206 V209 T210 L211 Y212 L213 V216 G223 R224 S225

- Molecule 33: 30S ribosomal protein S3

Chain C: 58% 42%

G1 Q2 K3 V4 H5 P6 G12 I13 V14 S19 T20 W21 V38 R39 Q40 Y41 L42 E45 L46 A49 I54 V55 K61 S62 I63 R64 V65 T66 I67 H68 T69 A70 R71 P72 G73 I74 V75 I76 G77 K78 K79 G80 V83 E84 K85 L86 R87 K88 V89 V90 I93

V96 P97 A98 I102 A103 E104 V105 R106 K107 L110 D111 V115 A116 D117 S118 I119 T120 S121 Q122 L123 R126 V127 K134 R135 A136 V137 Q138 M141 R142 L143 G144 A145 I148 E151 V152 S153 L156 I161 T164 E165 W166 Y167 R168 E169 P173 L174

I181 D182 Y183 S186 E187 A188 H189 T190 I195 K198 I206

- Molecule 34: 30S ribosomal protein S4

Chain D: 59% 39%

A1 P6 K7 L8 K9 L10 E14 G15 T16 D17 L18 K21 S22 G23 V24 R25 A26 I27 D28 T29 K30 C31 K32 I33 E34 P37 G41 R46 E56 K57 Q58 K59 V60 R61 R62 I63 Y64 G65 V66 L67 E68 R69 R72 R80 L81 K82 L93 E94 G95 R96

L97 D98 N99 V100 V101 Y102 R103 M104 G105 F106 A113 V117 K120 V124 R127 V128 V129 N130 I131 A132 S133 Y134 I144 R145 E146 K149 S152 L158 R164 E165 K166 P167 T168 W169 L170 E171 V172 M177 E178 G179 K182 R183 K184 P185 E186 R187 L190

S191 A192 D193 I194 L198 I199 V200 E201 L202 Y203 S204 K205

- Molecule 35: 30S ribosomal protein S5

Chain E: 60% 36%

E9 L10 Q11 L14 I15 K22 T23 V24 K25 R28 I29 T36 V37 V38 G39 D40 C41 N42 G50 E54 V55 P56 A57 A58 I59 Q60 M63 E64 K65 A66 R67 N76 T79 L80 Q81 T89 G90 S91 R92 Q96 P97 A98 S99 I104 I105 A106 G107 G108

A109 M110 R111 A112 V113 L114 E115 V119 H120 N121 V122 L123 Y127 I133 N134 V135 V136 T139 S148 P149 V152 R156 S159 E162 I163 L164 G165

- Molecule 36: 30S ribosomal protein S6

Chain F: 57% 42%

M1 R2 H3 Y4 E5 M9 V10 H11 V18 P19 I22 E23 T26 I29 A32 I36 H37 R38 L39 E40 Q46 L47 A48 Y49 P50 I51 N52 K53 L54 H55 K56 A57 H58 N63 V64 E65 A66 P67 Q68 E69 V70 I71 D72 E73 L74 T77 F78 R86

R91 T92 K93 T97 E98 A99 S100

- Molecule 37: 30S ribosomal protein S7

Chain G: 68% 30%

P1 R2 R3 R4 V5 I6 D14 P15 K16 F17 V26 N27 I28 A38 E39 S40 I41 V42 Y43 S56 E57 L58 E59 V63 E66 N67 V68 R69 P70 S76 V79 G80 G81 S82 T83 Y84 Q85 V86 P87 R95 L98 A99 M100 I103 V104 G111 D112 K113

A116 L117 R118 L119 E128 N129 K130 V134 K135 K136 D139 V140 H141 R142 M143 N147 K148 A151

- Molecule 38: 30S ribosomal protein S8

Chain H: 63% 36%

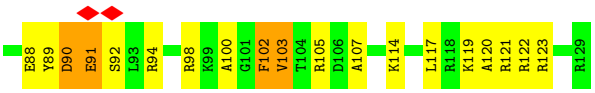
S1 D4 P5 I6 A7 D8 M9 L10 T11 R12 I13 R14 M26 P27 S28 S29 K30 L31 K32 V33 A34 V38 L39 K40 I45 E46 D47 F48 K49 V50 K55 P56 E57 L58 E59 L60 T61 L62 K63 I74 Q75 R76 V77 S78 R79 P80 I84 Y85 K86 E90 M95

L98 G99 I100 S104 T105 R113 L120 E123 I124 I125 A129

- Molecule 39: 30S ribosomal protein S9

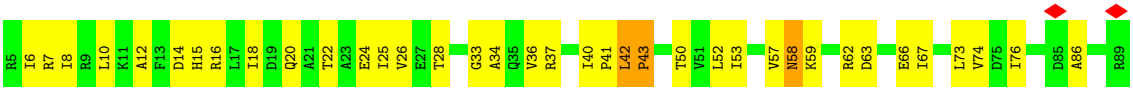
Chain I: 57% 39%

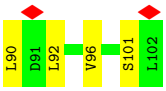
N3 Q4 Y5 Y6 R17 I20 K21 N24 G25 K26 I27 N30 Q31 R32 S33 L34 E35 Q36 Y37 F38 G39 R40 E41 T42 A43 R44 M45 V46 V47 R48 Q49 P50 L51 E52 L53 V54 D55 M56 V57 E58 K59 L60 D61 L62 T65 G70 Q74 I78 R79 I82 T83



• Molecule 40: 30S ribosomal protein S10

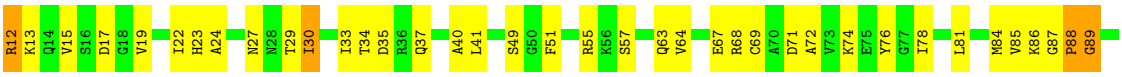
Chain J:

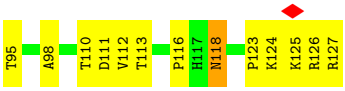




• Molecule 41: 30S ribosomal protein S11

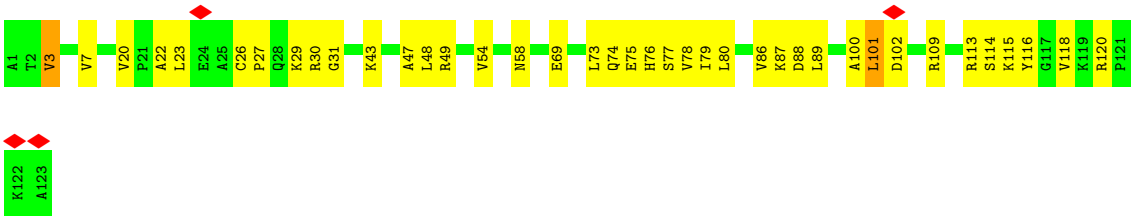
Chain K:





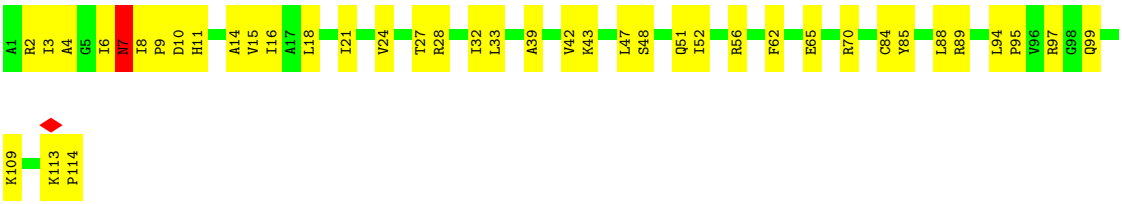
• Molecule 42: 30S ribosomal protein S12

Chain L:



• Molecule 43: 30S ribosomal protein S13

Chain M:



• Molecule 44: 30S ribosomal protein S14

Chain N: 63% 37%

A1 K2 Q3 S4 M5 K6 A7 R8 E9 V10 K11 R12 V13 F20 A21 K22 R23 A24 E25 L26 K27 A28 I29 I30 V33 S36 R40 A43 V44 L45 K46 L47 L50 D53 S54 R62 P69 R80 V83 R84 E85 A86 E91 I92 A98 S99 W100

- Molecule 45: 30S ribosomal protein S15

Chain O: 73% 26%

S1 T7 V11 D17 A18 N19 D20 T21 G22 S23 T24 E25 V26 Q27 V28 H41 E44 H45 K46 K47 R53 G54 L55 L56 R57 R62 R63 L66 L69 K70 R71 R87 R88

- Molecule 46: 30S ribosomal protein S16

Chain P: 5% 55% 40% 5%

M1 V2 T3 I4 R5 L6 A7 R8 R14 Y17 Q18 V19 V20 V21 R25 R28 R31 F32 I33 E34 R35 V36 I42 A43 S44 E45 K46 E47 E48 G49 T50 R51 L52 D53 I57 A58 H59 W60 V61 G62 Q63 G64 A65 T66 I67 S68 D69 R70 V71 V78 N79 K80

A81 A82

- Molecule 47: 30S ribosomal protein S17

Chain Q: 58% 41%

K3 I4 R5 T6 L7 Q8 V11 V12 S13 D14 K15 M16 E17 K18 S19 I20 V21 V28 K29 H30 P31 R39 V45 H46 N49 V58 E59 I60 R64 S67 K68 T69 K70 S71 W72 T73 L74 E79 V82

- Molecule 48: 30S ribosomal protein S18

Chain R: 62% 34% 5%

F9 C10 R11 F12 T13 A14 E15 G16 V17 I20 I25 L28 T33 E34 S35 P40 S41 R42 I43 Y50 Q51 L54 A55 R56 A57 I58 K59 R60 Y63 L64 S65 L66 L67 P68 R72 H73

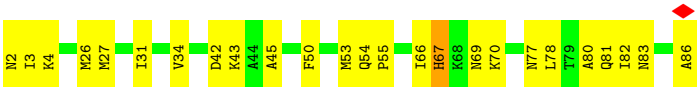
- Molecule 49: 30S ribosomal protein S19

Chain S: 61% 38%

R2 S3 L4 K5 K6 F9 I10 D11 L12 H13 L14 K17 V18 E19 V22 E23 K27 K28 P29 L30 R35 F40 I48 A49 V50 H51 N52 G53 R54 Q55 H56 V59 T62 D63 H68 E72 Y79 R80

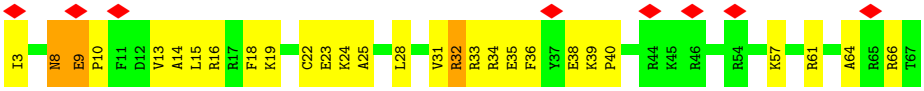
- Molecule 50: 30S ribosomal protein S20

Chain T: 71% 28%



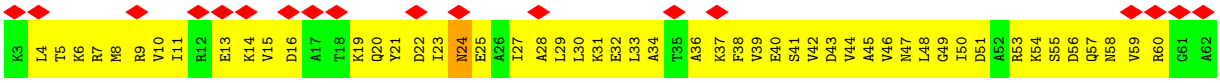
• Molecule 51: 30S ribosomal protein S21

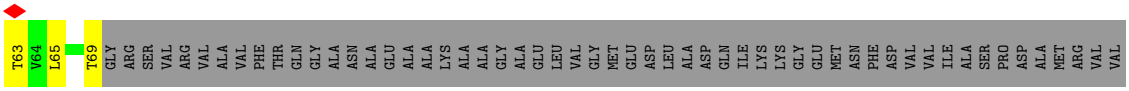
Chain U:

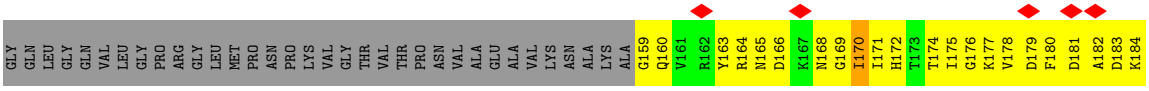


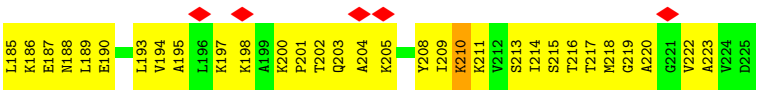
• Molecule 52: 50S ribosomal protein L1

Chain 03:



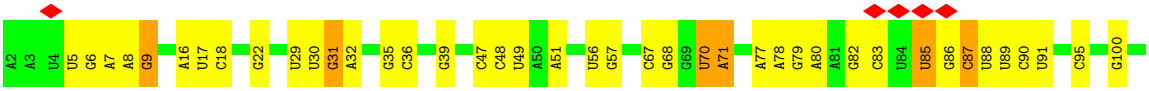


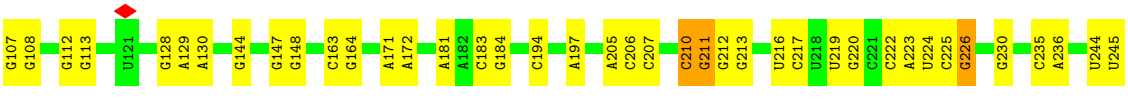


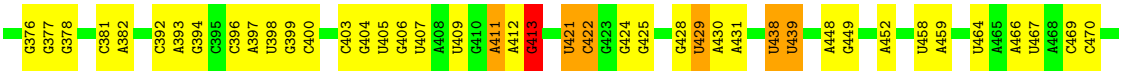


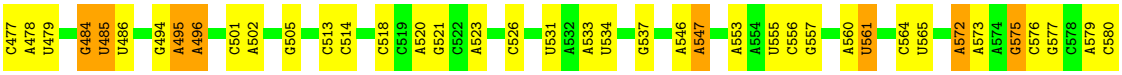
• Molecule 53: 16S ribosomal RNA

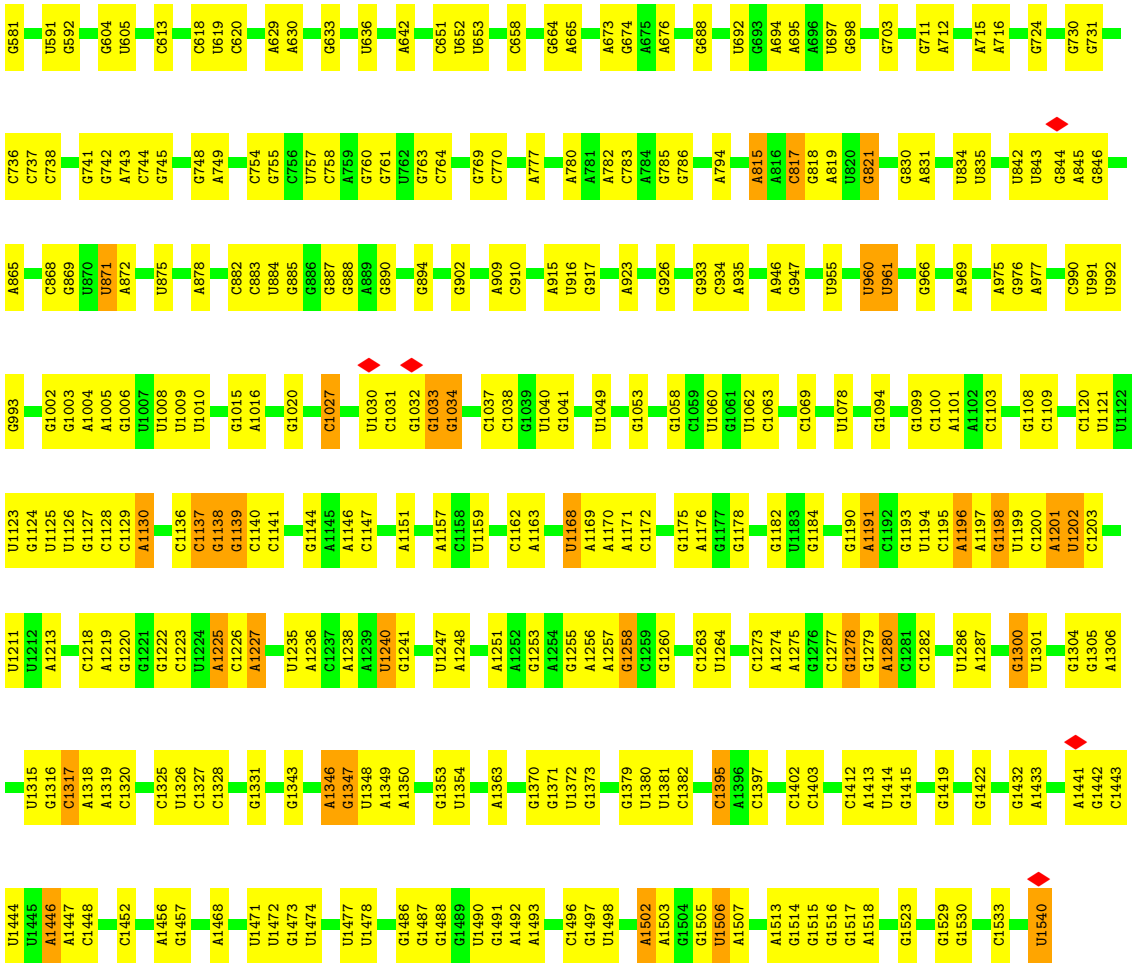
Chain A:





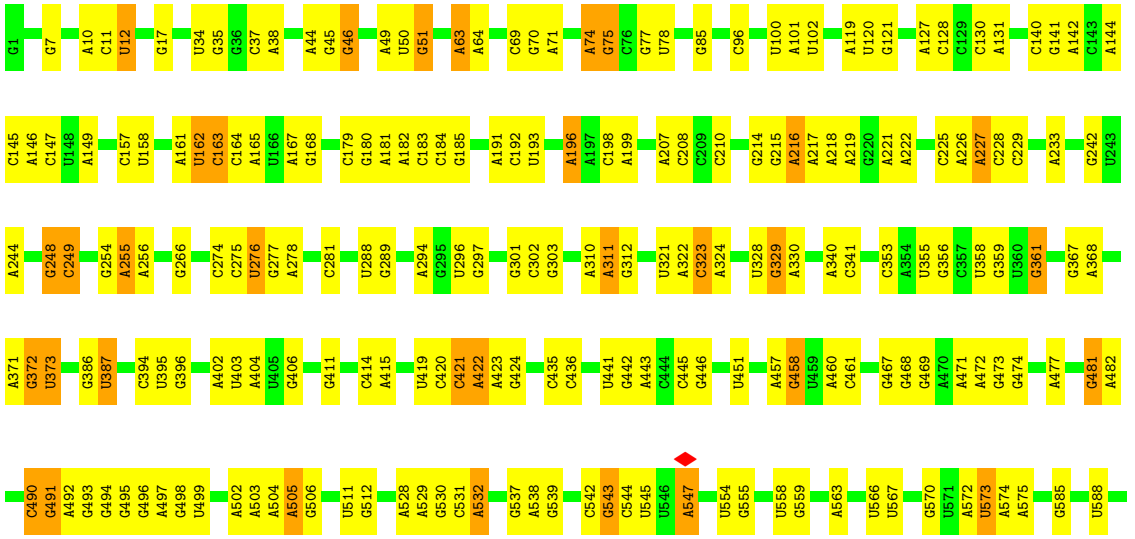


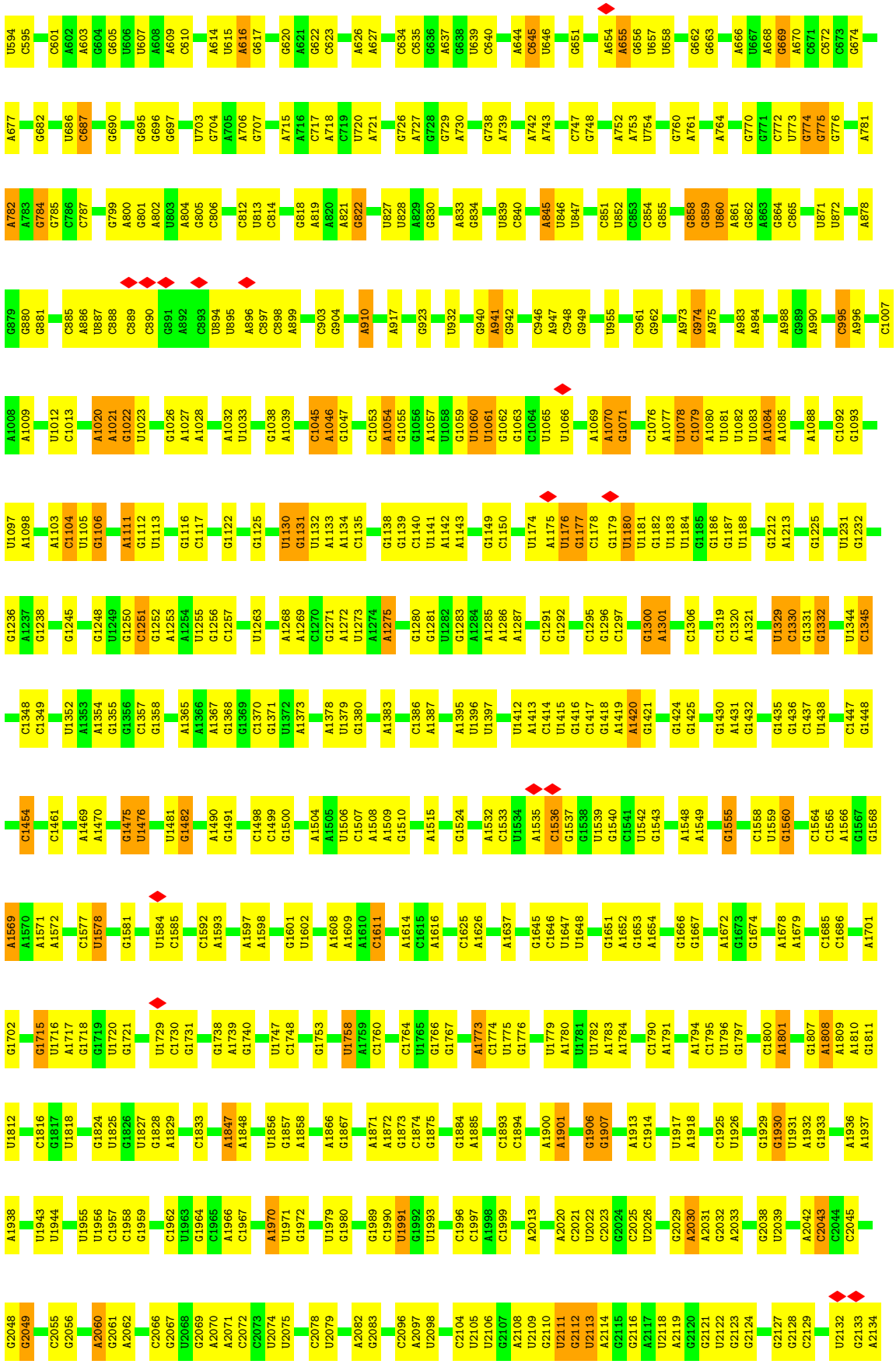


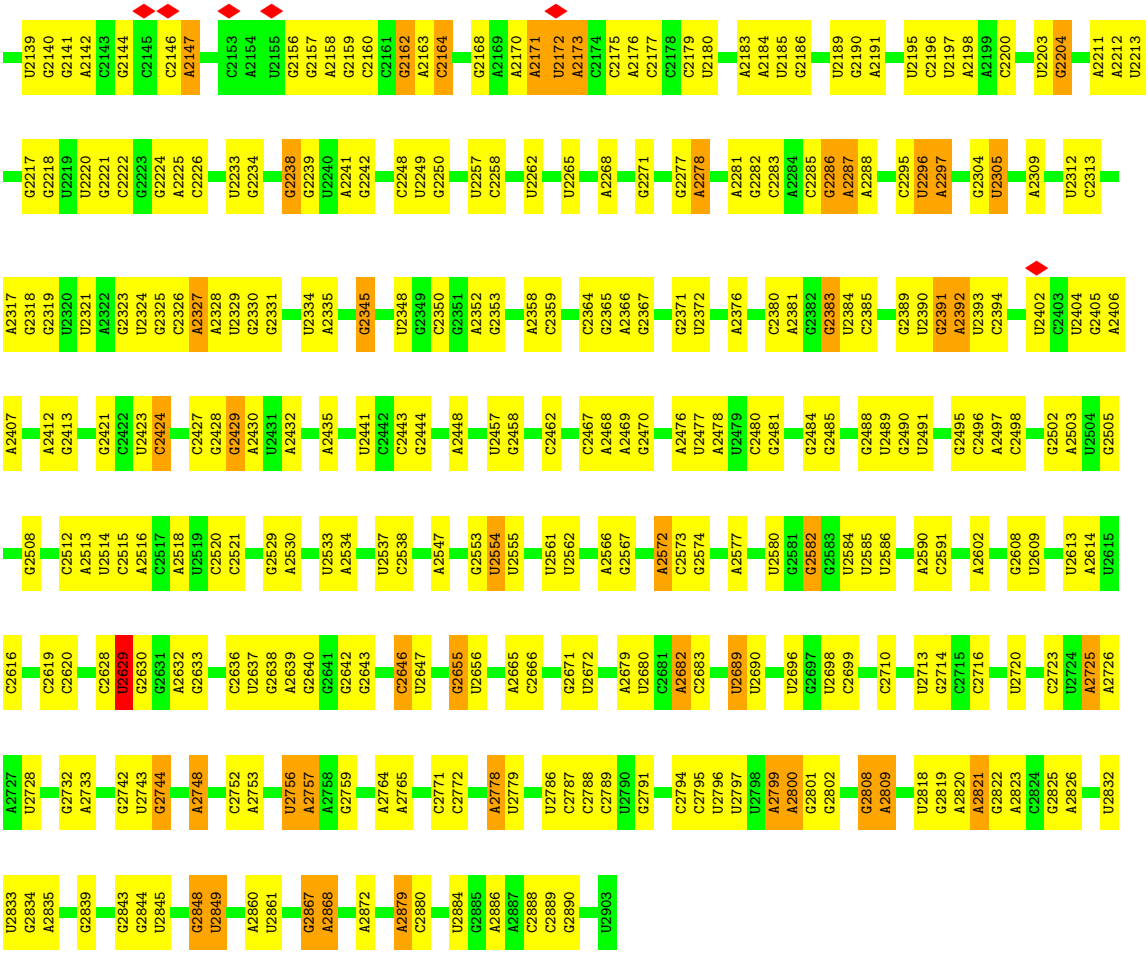


- Molecule 54: 23S ribosomal RNA

Chain 01:

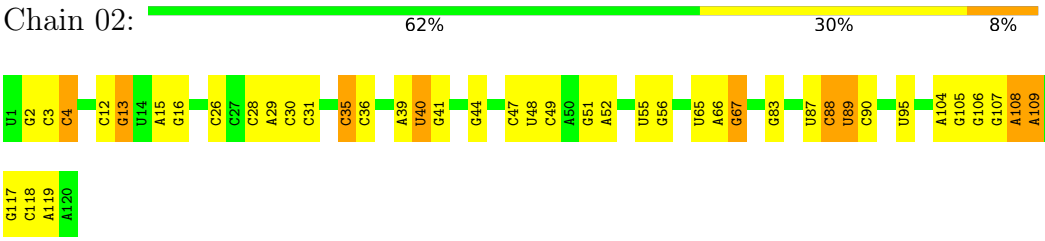



U594 C595 C601 A602 A603 G604 G605 U606 U607 A608 A609 C610 A614 U615 A616 G617 G620 A621 G622 C623 A626 A627 C634 C635 G636 A637 G638 U639 C640 A644 C645 U646 G651 A654 A655 G656 U657 U658 G662 G663 A666 U667 A668 G669 A670 C671 C672 C673 G674
A677 G682 U686 C687 G690 G695 G696 G697 U703 G704 A705 A706 G707 A715 A716 C717 A718 C719 U720 A721 G726 A727 G728 G729 A730 G738 A739 A742 A743 C747 G748 A752 A753 U754 G760 A761 A764 G770 G771 C772 U773 G774 G775 G776 A781
A782 A783 G784 G785 C786 C787 G799 A800 G801 A802 U803 A804 G805 C806 C812 U813 C814 G818 A819 A820 A821 G822 U827 U828 A829 G830 A833 G834 U839 C840 A845 U846 U847 C851 U852 C853 C854 G855 G858 G859 U860 A861 G862 A863 G864 C865 U871 U872 A878
G879 G880 G881 C885 A886 U887 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 C903 G904 A910 A917 G923 U932 G940 A941 G942 C946 A947 C948 G949 U955 C961 G962 A973 G974 A975 A983 A984 A988 G989 A990 C995 A996 C1007
A1008 A1009 U1012 C1013 A1020 A1021 G1022 U1023 G1026 A1027 A1028 A1032 U1033 G1038 A1039 C1045 A1046 G1047 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1069 A1070 G1071 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1088 C1092 G1093
U1097 A1098 A1103 C1104 U1105 G1106 A1111 G1112 U1113 G1116 C1117 G1122 G1125 U1130 G1131 U1132 A1133 A1134 C1135 G1138 G1139 C1140 U1141 A1142 A1143 G1149 C1150 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 G1212 A1213 G1225 U1231 G1232
G1236 A1237 G1238 G1245 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 U1263 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 G1280 G1281 U1282 G1283 A1284 A1285 A1286 A1287 C1291 G1292 C1295 G1296 C1297 G1300 A1301 C1306 C1319 C1320 A1321 U1329 C1330 G1331 G1332 U1344 C1345
C1348 C1349 U1352 A1353 A1354 G1355 G1356 C1357 G1358 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 A1378 G1379 G1380 A1383 C1386 A1387 A1395 U1396 U1397 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1424 G1425 G1430 A1431 G1432 G1435 G1436 C1437 U1438 C1447 G1448
C1454 C1461 A1469 A1470 G1475 U1476 U1481 G1482 A1490 G1491 C1498 C1499 G1500 A1504 A1505 U1506 C1507 A1508 A1509 G1510 A1515 G1524 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1548 A1549 G1555 C1558 U1559 G1560 C1564 C1565 A1566 G1567 G1568
A1569 A1570 A1571 A1572 C1577 U1578 G1581 U1584 C1585 C1592 A1593 A1597 A1598 G1601 U1602 A1608 A1609 A1610 C1611 A1614 C1615 A1616 C1625 A1626 A1637 G1645 C1646 U1647 U1648 G1651 A1652 G1653 A1654 G1666 G1667 A1672 G1673 G1674 A1678 A1679 C1685 C1686 A1701
G1702 G1715 U1716 A1717 G1718 G1719 U1720 G1721 U1729 C1730 G1731 G1738 A1739 G1740 U1747 C1748 G1753 U1758 A1759 C1760 C1764 U1765 G1766 G1767 A1773 C1774 U1775 G1776 U1779 A1780 U1781 U1782 A1783 A1784 C1790 A1791 A1794 C1795 U1796 G1797 C1800 A1801 G1807 A1808 A1809 A1810 G1811
U1812 C1816 G1817 U1818 G1824 U1825 G1826 U1827 G1828 A1829 C1833 A1847 A1848 U1856 G1857 A1858 A1866 G1867 A1871 A1872 G1873 C1874 G1875 G1884 A1885 C1893 C1894 A1900 A1901 G1906 G1907 A1913 C1914 U1917 A1918 C1925 U1926 G1929 G1930 U1931 A1932 G1933 A1936 A1937
A1938 U1943 U1944 U1955 U1956 C1957 C1958 G1959 C1962 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 U1979 G1980 G1989 C1990 U1991 G1992 U1993 C1996 C1997 A1998 C1999 A2013 A2020 C2021 U2022 C2023 G2024 C2025 U2026 G2029 A2030 A2031 G2032 A2033 G2038 U2039 A2042 C2043 C2044 C2045
G2048 G2049 C2055 G2056 A2060 G2061 A2062 C2066 G2067 U2068 G2069 A2070 A2071 C2072 C2073 U2074 U2075 C2078 U2079 A2082 G2083 C2096 A2097 U2098 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2127 G2128 C2129 U2132 G2133 A2134



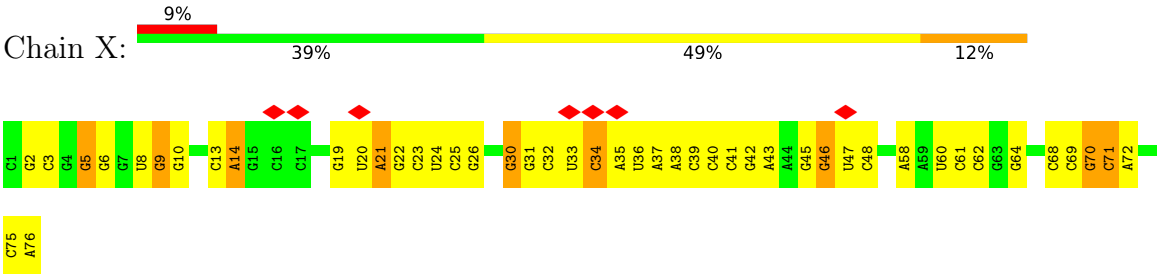
- Molecule 55: 5S ribosomal RNA

Chain 02:



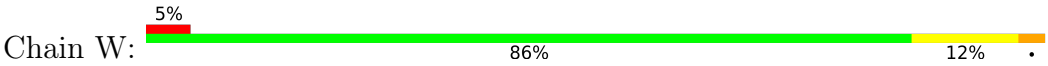
- Molecule 56: tRNAfMet

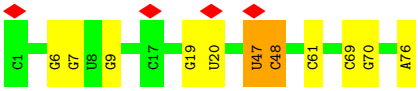
Chain X:



- Molecule 56: tRNAfMet

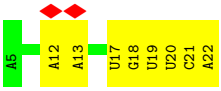
Chain W:





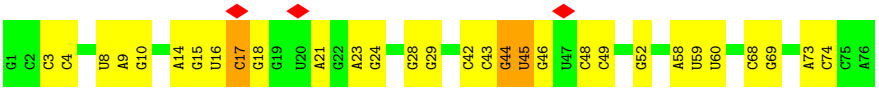
- Molecule 57: mRNA

Chain V:



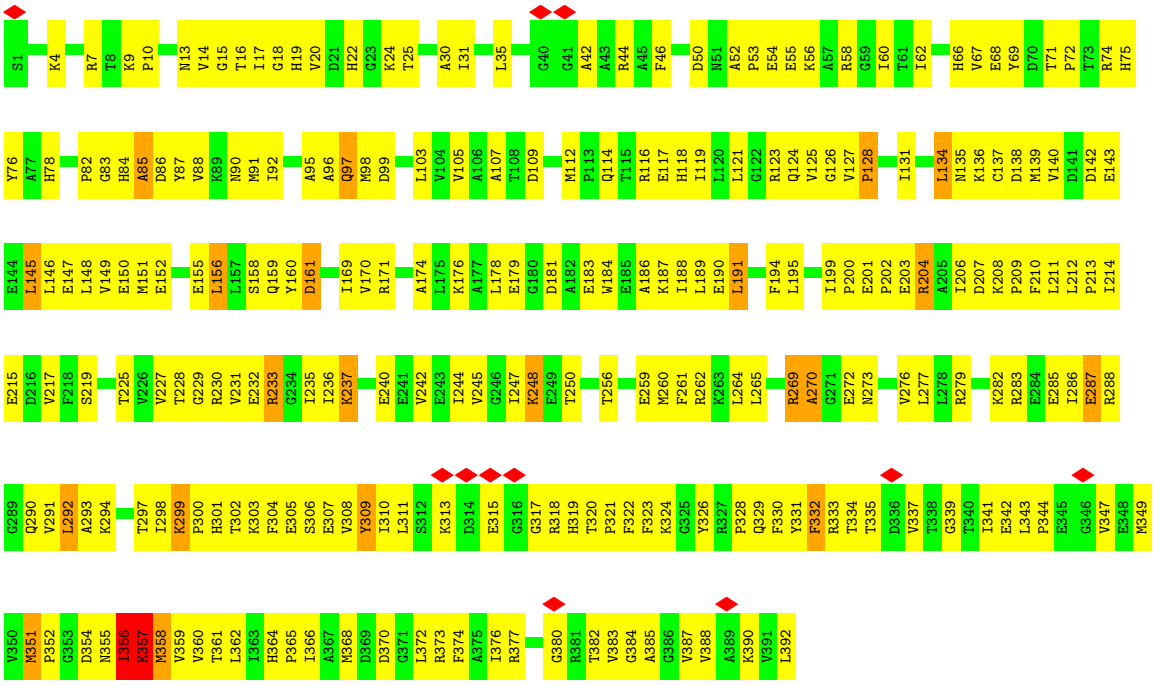
- Molecule 58: Phe-tRNAPhe

Chain Y:



- Molecule 59: Elongation factor Tu 2

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153597	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	17.168	Depositor
Minimum map value	-4.064	Depositor
Average map value	-0.393	Depositor
Map value standard deviation	1.187	Depositor
Recommended contour level	3.17	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: ZN, FME, GCP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	04	0.26	0/2122	0.58	0/2852
2	05	0.27	0/1586	0.55	0/2134
3	06	0.26	0/1571	0.55	0/2113
4	07	0.29	0/1435	0.55	0/1926
5	08	0.27	0/1343	0.52	0/1816
6	09	0.29	0/1122	0.63	0/1515
7	10	0.32	0/1002	0.68	0/1350
8	11	0.31	0/1046	0.58	0/1410
9	12	0.27	0/1152	0.54	0/1551
10	13	0.26	0/948	0.59	0/1268
11	14	0.26	0/1054	0.61	0/1403
12	15	0.28	0/1093	0.57	0/1460
13	16	0.26	0/974	0.56	0/1301
14	17	0.25	0/902	0.55	0/1209
15	18	0.27	0/929	0.56	0/1242
16	19	0.28	0/960	0.48	0/1278
17	20	0.28	0/829	0.63	1/1107 (0.1%)
18	21	0.25	0/864	0.58	0/1156
19	22	0.27	0/745	0.54	0/994
20	23	0.28	0/788	0.62	0/1051
21	24	0.29	0/766	0.56	0/1025
22	25	0.28	0/582	0.51	0/769
23	26	0.27	0/635	0.54	0/848
24	27	0.27	0/510	0.51	0/677
25	28	0.25	0/453	0.51	0/605
26	29	0.30	0/532	0.54	0/709
27	30	0.26	0/450	0.56	0/599
28	31	0.30	0/417	0.57	0/554
29	32	0.29	0/380	0.53	0/498
30	33	0.26	0/513	0.60	0/676
31	34	0.26	0/303	0.54	0/397
32	B	0.29	0/1736	0.58	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	C	0.28	0/1652	0.52	0/2225
34	D	0.26	0/1665	0.55	0/2227
35	E	0.28	0/1170	0.59	0/1573
36	F	0.29	0/836	0.61	0/1128
37	G	0.25	0/1196	0.53	0/1602
38	H	0.26	0/989	0.57	0/1326
39	I	0.28	0/1034	0.61	0/1375
40	J	0.27	0/797	0.65	0/1077
41	K	0.28	0/886	0.60	0/1195
42	L	0.28	0/969	0.68	1/1300 (0.1%)
43	M	0.25	0/893	0.57	0/1193
44	N	0.26	0/817	0.54	0/1088
45	O	0.26	0/722	0.54	0/964
46	P	0.28	0/659	0.59	0/884
47	Q	0.28	0/658	0.62	0/881
48	R	0.30	0/545	0.55	0/731
49	S	0.28	0/653	0.57	0/877
50	T	0.26	0/671	0.49	0/888
51	U	0.33	0/551	0.61	0/728
52	03	1.37	0/1034	0.73	0/1387
53	A	0.31	0/36963	0.68	1/57662 (0.0%)
54	01	0.32	0/69796	0.67	2/108888 (0.0%)
55	02	0.31	0/2872	0.67	0/4479
56	W	0.31	0/1832	0.67	0/2855
56	X	0.47	0/1832	0.67	0/2855
57	V	0.32	0/436	0.67	0/679
58	Y	0.36	0/1809	0.67	0/2819
59	Z	1.18	0/3085	0.73	1/4173 (0.0%)
All	All	0.36	0/166764	0.65	6/248890 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
54	01	0	3
59	Z	0	1
All	All	0	4

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	20	50	GLY	N-CA-C	-6.04	98.01	113.10
59	Z	71	THR	N-CA-C	-5.68	95.66	111.00
42	L	43	LYS	N-CA-C	5.29	125.29	111.00
54	01	458	G	C1'-O4'-C4'	-5.24	105.71	109.90
53	A	413	G	N9-C1'-C2'	5.11	120.64	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	01	2629	U	Sidechain
54	01	2725	A	Sidechain
54	01	775	G	Sidechain
59	Z	309	TYR	Sidechain

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	90	0
2	05	1565	0	1616	52	0
3	06	1552	0	1619	50	0
4	07	1411	0	1447	55	0
5	08	1323	0	1374	31	0
6	09	1111	0	1148	45	0
7	10	989	0	1025	75	0
8	11	1032	0	1088	60	0
9	12	1129	0	1162	51	0
10	13	939	0	1012	37	0
11	14	1045	0	1117	46	0
12	15	1074	0	1157	32	0
13	16	961	0	1000	30	0
14	17	892	0	923	45	0
15	18	917	0	965	45	0
16	19	947	0	1022	28	0
17	20	816	0	839	22	0
18	21	857	0	922	28	0
19	22	739	0	807	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	23	780	0	834	26	0
21	24	753	0	780	22	0
22	25	575	0	592	14	0
23	26	625	0	655	9	0
24	27	509	0	543	17	0
25	28	449	0	491	14	0
26	29	523	0	524	13	0
27	30	444	0	461	15	0
28	31	410	0	440	12	0
29	32	377	0	418	15	0
30	33	504	0	574	16	0
31	34	302	0	343	21	0
32	B	1705	0	1732	67	0
33	C	1625	0	1699	64	0
34	D	1643	0	1710	77	0
35	E	1157	0	1199	53	0
36	F	818	0	808	43	0
37	G	1182	0	1240	42	0
38	H	979	0	1034	46	0
39	I	1022	0	1070	47	0
40	J	787	0	828	47	0
41	K	870	0	878	46	0
42	L	955	0	1019	44	0
43	M	884	0	944	41	0
44	N	805	0	847	33	0
45	O	714	0	737	20	0
46	P	649	0	666	42	0
47	Q	649	0	691	34	0
48	R	536	0	552	23	0
49	S	638	0	665	31	0
50	T	665	0	714	16	0
51	U	545	0	579	36	0
52	03	1027	0	1092	155	0
53	A	33012	0	16618	357	0
54	01	62317	0	31346	697	0
55	02	2568	0	1303	38	0
56	W	1640	0	836	4	0
56	X	1640	0	837	33	0
57	V	388	0	196	4	0
58	Y	1619	0	821	12	0
59	Z	3029	0	3043	319	0
60	01	263	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	02	6	0	0	0	0
60	12	1	0	0	0	0
60	25	1	0	0	0	0
60	A	107	0	0	0	0
60	N	1	0	0	0	0
60	V	2	0	0	0	0
60	W	1	0	0	0	0
60	Z	1	0	0	0	0
61	29	1	0	0	0	0
61	34	1	0	0	0	0
62	W	10	0	10	0	0
63	Y	11	0	8	2	0
64	Z	32	0	14	1	0
All	All	154139	0	104791	3196	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 12.

The worst 5 of 3196 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)
59:Z:151:MET:CE	59:Z:151:MET:SD	2.01	1.46
52:03:181:ASP:HB2	52:03:184:LYS:HD3	1.19	1.19
59:Z:212:LEU:HD11	59:Z:229:GLY:HA3	1.32	1.08
35:E:80:LEU:HD13	35:E:122:VAL:HG11	1.31	1.08
59:Z:344:PRO:HG2	59:Z:347:VAL:HG21	1.36	1.06

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%)	241 (90%)	24 (9%)	4 (2%)	10	44
2	05	207/209 (99%)	191 (92%)	15 (7%)	1 (0%)	29	67
3	06	199/201 (99%)	179 (90%)	19 (10%)	1 (0%)	29	67
4	07	175/177 (99%)	156 (89%)	18 (10%)	1 (1%)	25	64
5	08	174/176 (99%)	155 (89%)	15 (9%)	4 (2%)	6	34
6	09	147/149 (99%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	10	129/131 (98%)	90 (70%)	32 (25%)	7 (5%)	2	14
8	11	139/141 (99%)	113 (81%)	19 (14%)	7 (5%)	2	16
9	12	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
10	13	120/122 (98%)	99 (82%)	19 (16%)	2 (2%)	9	42
11	14	141/143 (99%)	120 (85%)	14 (10%)	7 (5%)	2	16
12	15	134/136 (98%)	118 (88%)	13 (10%)	3 (2%)	6	35
13	16	118/120 (98%)	104 (88%)	12 (10%)	2 (2%)	9	42
14	17	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
15	18	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	56
16	19	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
17	20	101/103 (98%)	87 (86%)	13 (13%)	1 (1%)	15	54
18	21	108/110 (98%)	97 (90%)	8 (7%)	3 (3%)	5	29
19	22	91/93 (98%)	76 (84%)	15 (16%)	0	100	100
20	23	100/102 (98%)	79 (79%)	17 (17%)	4 (4%)	3	21
21	24	92/94 (98%)	84 (91%)	8 (9%)	0	100	100
22	25	73/75 (97%)	62 (85%)	11 (15%)	0	100	100
23	26	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
24	27	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	9	43
25	28	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
26	29	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
27	30	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	31	48/50 (96%)	43 (90%)	3 (6%)	2 (4%)	3	20
29	32	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
30	33	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	9	43
31	34	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	5	29
32	B	216/218 (99%)	181 (84%)	30 (14%)	5 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	C	204/206 (99%)	188 (92%)	15 (7%)	1 (0%)	29	67
34	D	203/205 (99%)	172 (85%)	26 (13%)	5 (2%)	5	32
35	E	155/157 (99%)	122 (79%)	26 (17%)	7 (4%)	2	18
36	F	98/100 (98%)	77 (79%)	18 (18%)	3 (3%)	4	26
37	G	149/151 (99%)	131 (88%)	18 (12%)	0	100	100
38	H	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	58
39	I	125/127 (98%)	102 (82%)	17 (14%)	6 (5%)	2	17
40	J	96/98 (98%)	76 (79%)	14 (15%)	6 (6%)	1	10
41	K	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	3	24
42	L	121/123 (98%)	98 (81%)	18 (15%)	5 (4%)	3	21
43	M	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	5	30
44	N	98/100 (98%)	78 (80%)	18 (18%)	2 (2%)	7	38
45	O	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13	49
46	P	80/82 (98%)	67 (84%)	9 (11%)	4 (5%)	2	16
47	Q	78/80 (98%)	63 (81%)	11 (14%)	4 (5%)	2	15
48	R	63/65 (97%)	54 (86%)	7 (11%)	2 (3%)	4	26
49	S	77/79 (98%)	65 (84%)	10 (13%)	2 (3%)	5	31
50	T	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	13	49
51	U	63/65 (97%)	43 (68%)	17 (27%)	3 (5%)	2	17
52	03	130/223 (58%)	114 (88%)	14 (11%)	2 (2%)	10	44
59	Z	390/392 (100%)	328 (84%)	54 (14%)	8 (2%)	7	37
All	All	6366/6563 (97%)	5507 (86%)	729 (12%)	130 (2%)	11	38

5 of 130 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	04	232	GLY
3	06	83	VAL
5	08	45	ALA
5	08	119	GLY
7	10	81	LEU

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%)	213 (99%)	3 (1%)	67	86
2	05	164/164 (100%)	163 (99%)	1 (1%)	86	94
3	06	165/165 (100%)	163 (99%)	2 (1%)	71	88
4	07	148/148 (100%)	147 (99%)	1 (1%)	84	94
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%)	98 (98%)	2 (2%)	55	80
8	11	109/109 (100%)	109 (100%)	0	100	100
9	12	116/116 (100%)	115 (99%)	1 (1%)	78	91
10	13	103/103 (100%)	103 (100%)	0	100	100
11	14	102/102 (100%)	102 (100%)	0	100	100
12	15	109/109 (100%)	107 (98%)	2 (2%)	59	82
13	16	100/100 (100%)	99 (99%)	1 (1%)	76	90
14	17	86/86 (100%)	86 (100%)	0	100	100
15	18	99/99 (100%)	97 (98%)	2 (2%)	55	80
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%)	91 (98%)	2 (2%)	52	79
19	22	80/80 (100%)	78 (98%)	2 (2%)	47	77
20	23	83/83 (100%)	83 (100%)	0	100	100
21	24	78/78 (100%)	78 (100%)	0	100	100
22	25	57/57 (100%)	57 (100%)	0	100	100
23	26	67/67 (100%)	66 (98%)	1 (2%)	65	85
24	27	55/55 (100%)	55 (100%)	0	100	100
25	28	48/48 (100%)	47 (98%)	1 (2%)	53	79
26	29	59/59 (100%)	57 (97%)	2 (3%)	37	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	30	47/47 (100%)	47 (100%)	0	100	100
28	31	45/45 (100%)	44 (98%)	1 (2%)	52	79
29	32	38/38 (100%)	37 (97%)	1 (3%)	46	76
30	33	51/51 (100%)	51 (100%)	0	100	100
31	34	34/34 (100%)	32 (94%)	2 (6%)	19	54
32	B	180/180 (100%)	175 (97%)	5 (3%)	43	74
33	C	170/170 (100%)	170 (100%)	0	100	100
34	D	172/172 (100%)	169 (98%)	3 (2%)	60	83
35	E	119/119 (100%)	117 (98%)	2 (2%)	60	83
36	F	87/87 (100%)	87 (100%)	0	100	100
37	G	124/124 (100%)	122 (98%)	2 (2%)	62	84
38	H	104/104 (100%)	104 (100%)	0	100	100
39	I	105/105 (100%)	102 (97%)	3 (3%)	42	74
40	J	86/86 (100%)	86 (100%)	0	100	100
41	K	89/89 (100%)	86 (97%)	3 (3%)	37	70
42	L	103/103 (100%)	103 (100%)	0	100	100
43	M	92/92 (100%)	91 (99%)	1 (1%)	73	88
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%)	65 (100%)	0	100	100
47	Q	74/74 (100%)	74 (100%)	0	100	100
48	R	56/56 (100%)	55 (98%)	1 (2%)	59	82
49	S	70/70 (100%)	70 (100%)	0	100	100
50	T	65/65 (100%)	64 (98%)	1 (2%)	65	85
51	U	55/55 (100%)	53 (96%)	2 (4%)	35	69
52	03	110/174 (63%)	108 (98%)	2 (2%)	59	82
59	Z	324/325 (100%)	303 (94%)	21 (6%)	17	51
All	All	5285/5350 (99%)	5212 (99%)	73 (1%)	68	86

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	Z	156	LEU

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Mol	Chain	Res	Type
59	Z	357	LYS
59	Z	191	LEU
59	Z	287	GLU
29	32	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
30	33	27	ASN
37	G	129	ASN
59	Z	364	HIS
32	B	176	ASN
34	D	35	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	147 (9%)	8 (0%)
54	01	2902/2903 (99%)	359 (12%)	22 (0%)
55	02	119/120 (99%)	11 (9%)	1 (0%)
56	W	76/77 (98%)	7 (9%)	0
56	X	76/77 (98%)	18 (23%)	0
57	V	17/18 (94%)	2 (11%)	0
58	Y	75/76 (98%)	12 (16%)	1 (1%)
All	All	4803/4810 (99%)	556 (11%)	32 (0%)

5 of 556 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	G
53	A	9	G
53	A	22	G
53	A	31	G
53	A	32	A

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	01	2808	G
54	01	2848	G

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Mol	Chain	Res	Type
54	01	774	G
54	01	490	C
55	02	88	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 388 ligands modelled in this entry, 385 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
63	PHE	Y	101	58	10,11,12	0.66	0	10,13,15	0.52	0
64	GCP	Z	402	60	27,34,34	2.53	11 (40%)	34,54,54	3.84	18 (52%)
62	FME	W	101	-	8,9,10	0.89	0	7,9,11	1.17	1 (14%)

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
63	PHE	Y	101	58	-	0/5/6/8	0/1/1/1
64	GCP	Z	402	60	-	9/15/38/38	0/3/3/3
62	FME	W	101	-	-	3/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	Z	402	GCP	PB-O3A	-5.85	1.51	1.58
64	Z	402	GCP	O4'-C1'	5.16	1.48	1.41
64	Z	402	GCP	C6-N1	4.33	1.40	1.33
64	Z	402	GCP	C5-C6	4.10	1.48	1.41
64	Z	402	GCP	C2'-C1'	4.05	1.59	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	Z	402	GCP	C1'-N9-C4	12.82	149.17	126.64
64	Z	402	GCP	C5-C6-N1	-8.85	111.32	123.43
64	Z	402	GCP	O1G-PG-C3B	-7.44	95.20	111.24
64	Z	402	GCP	C2-N1-C6	6.89	126.88	115.93
64	Z	402	GCP	O4'-C1'-C2'	-4.88	99.79	106.93

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	W	101	FME	O1-CN-N-CA
62	W	101	FME	O-C-CA-CB
64	Z	402	GCP	PB-C3B-PG-O1G
64	Z	402	GCP	PB-C3B-PG-O2G
64	Z	402	GCP	PG-C3B-PB-O1B

There are no ring outliers.

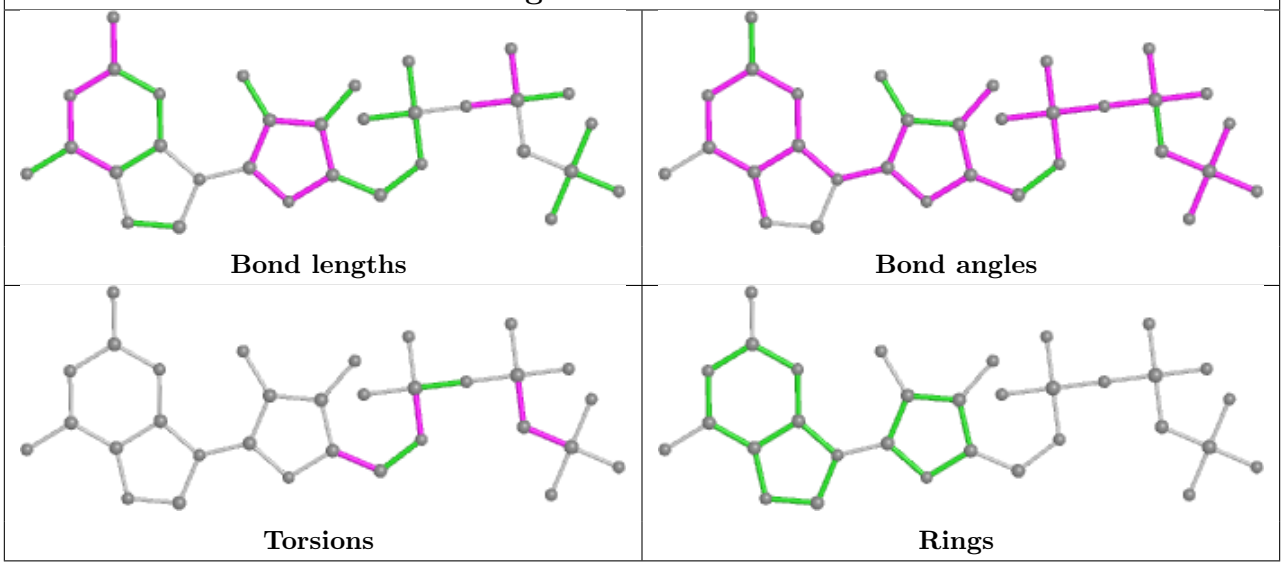
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	Y	101	PHE	2	0
64	Z	402	GCP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GCP Z 402



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.

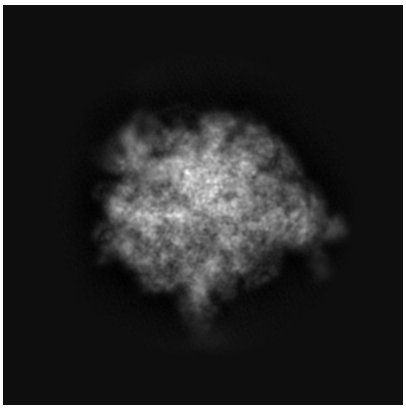
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8617. These allow visual inspection of the internal detail of the map and identification of artifacts.

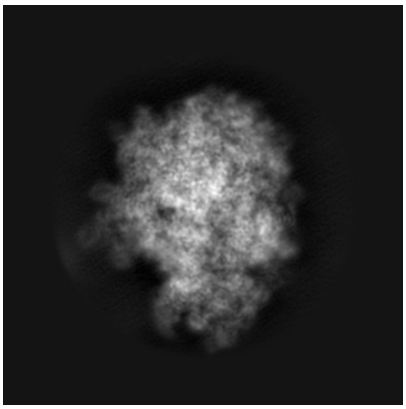
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

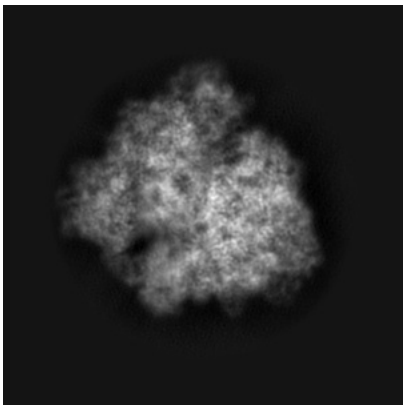
6.1.1 Primary map



X

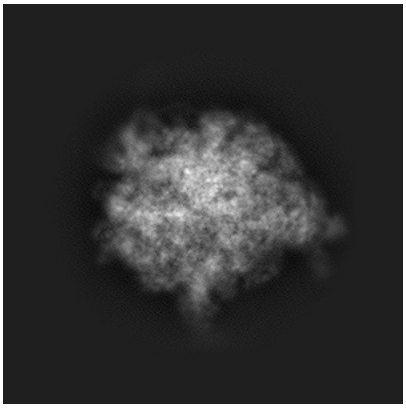


Y

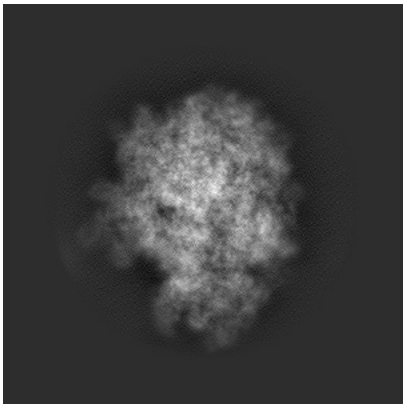


Z

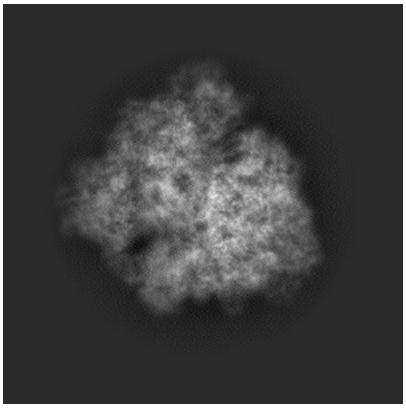
6.1.2 Raw map



X



Y

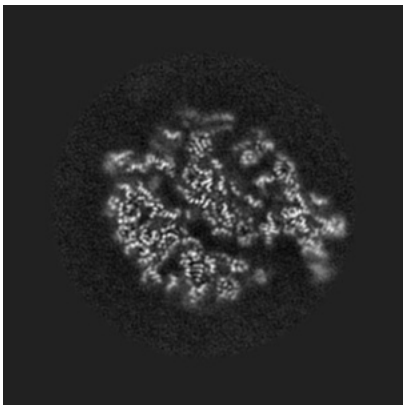


Z

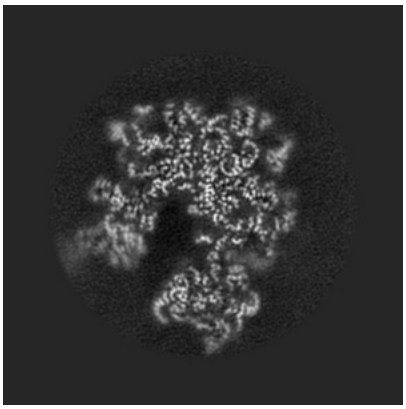
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

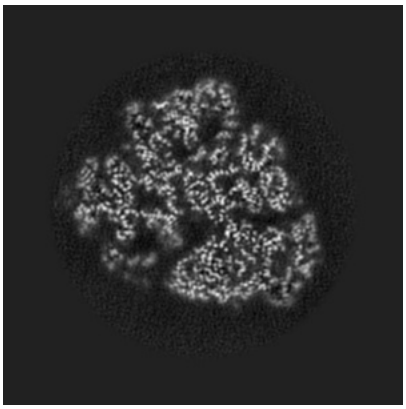
6.2.1 Primary map



X Index: 240

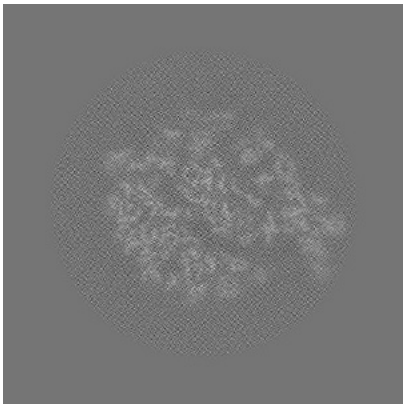


Y Index: 240

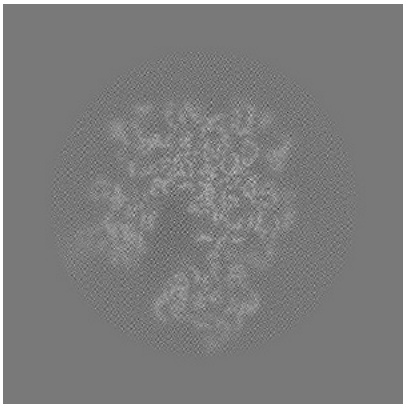


Z Index: 240

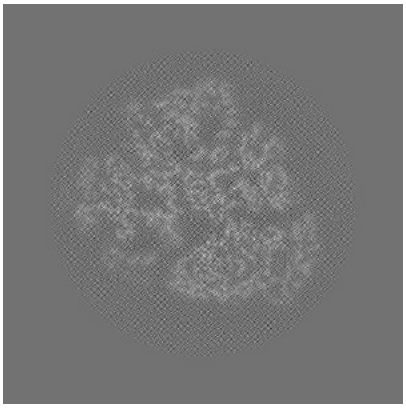
6.2.2 Raw map



X Index: 240



Y Index: 240

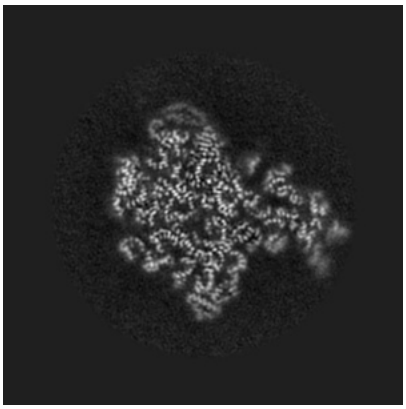


Z Index: 240

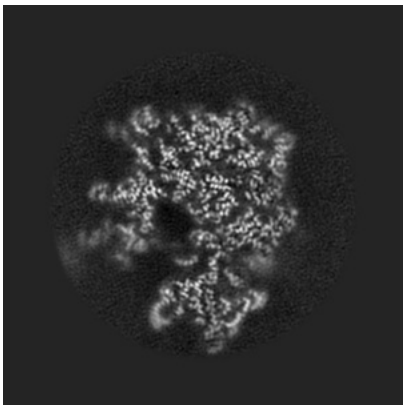
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

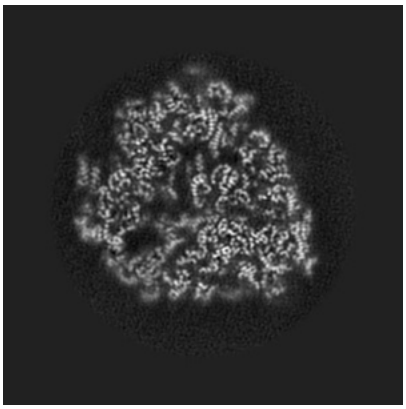
6.3.1 Primary map



X Index: 252

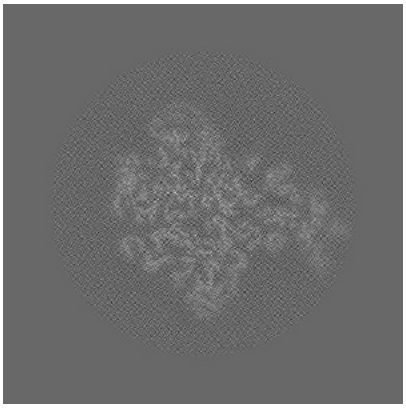


Y Index: 248

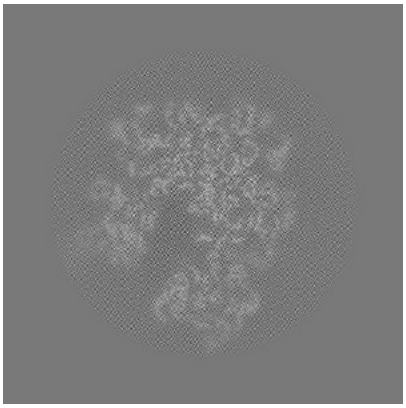


Z Index: 228

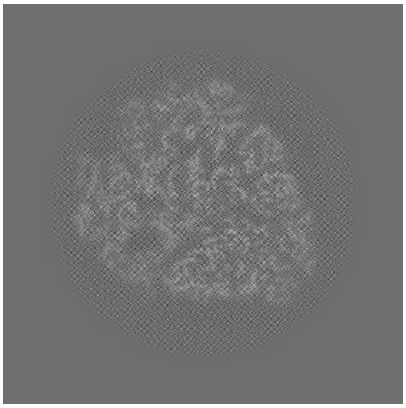
6.3.2 Raw map



X Index: 251



Y Index: 240

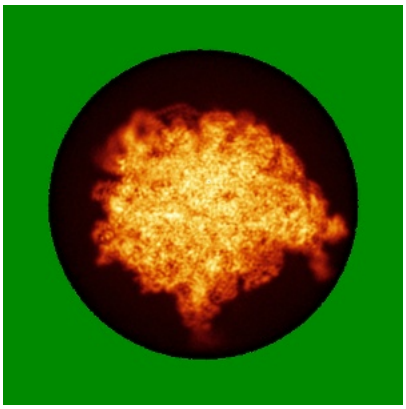


Z Index: 233

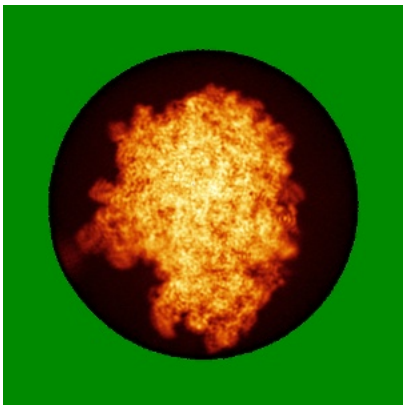
The images above show the largest variance slices of the map in three orthogonal directions.

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

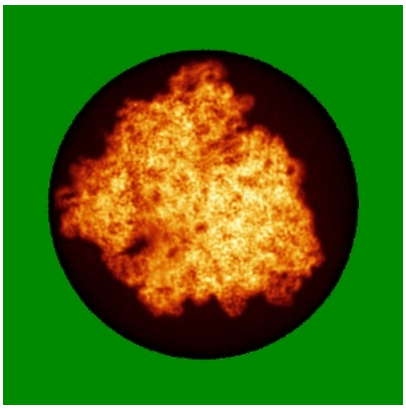
6.4.1 Primary map



X

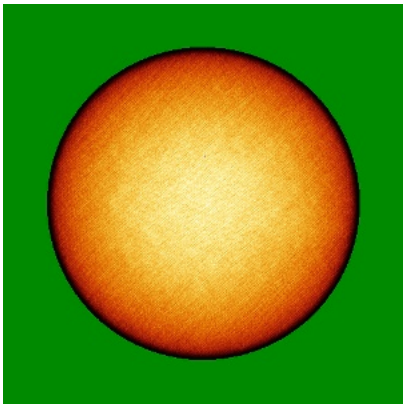


Y

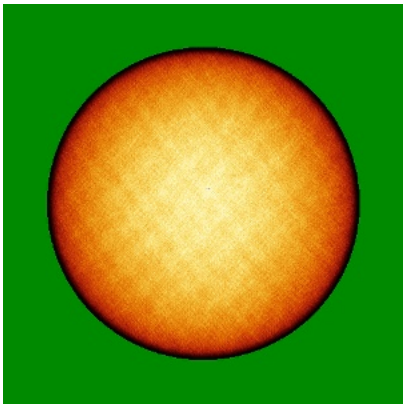


Z

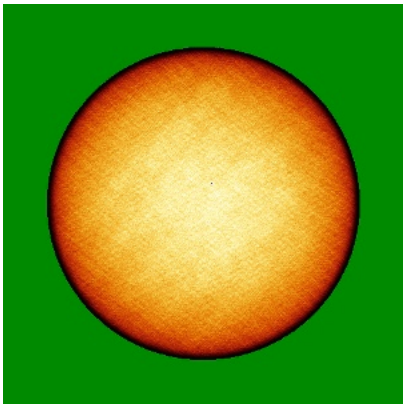
6.4.2 Raw map



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.

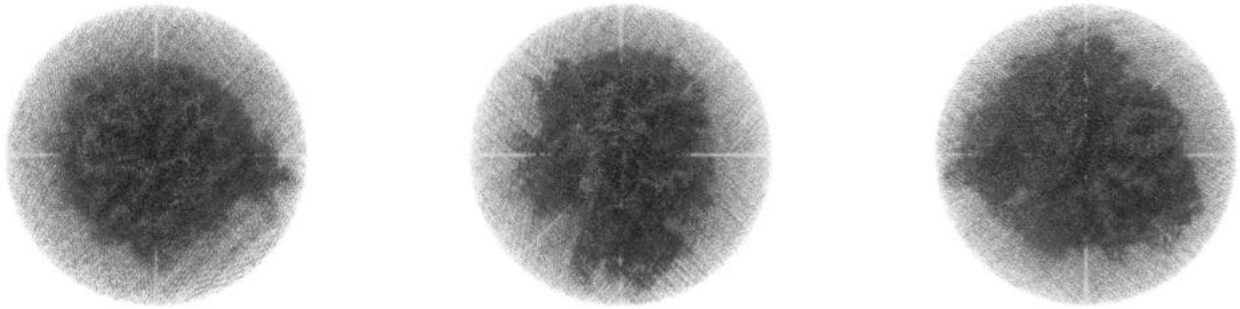
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

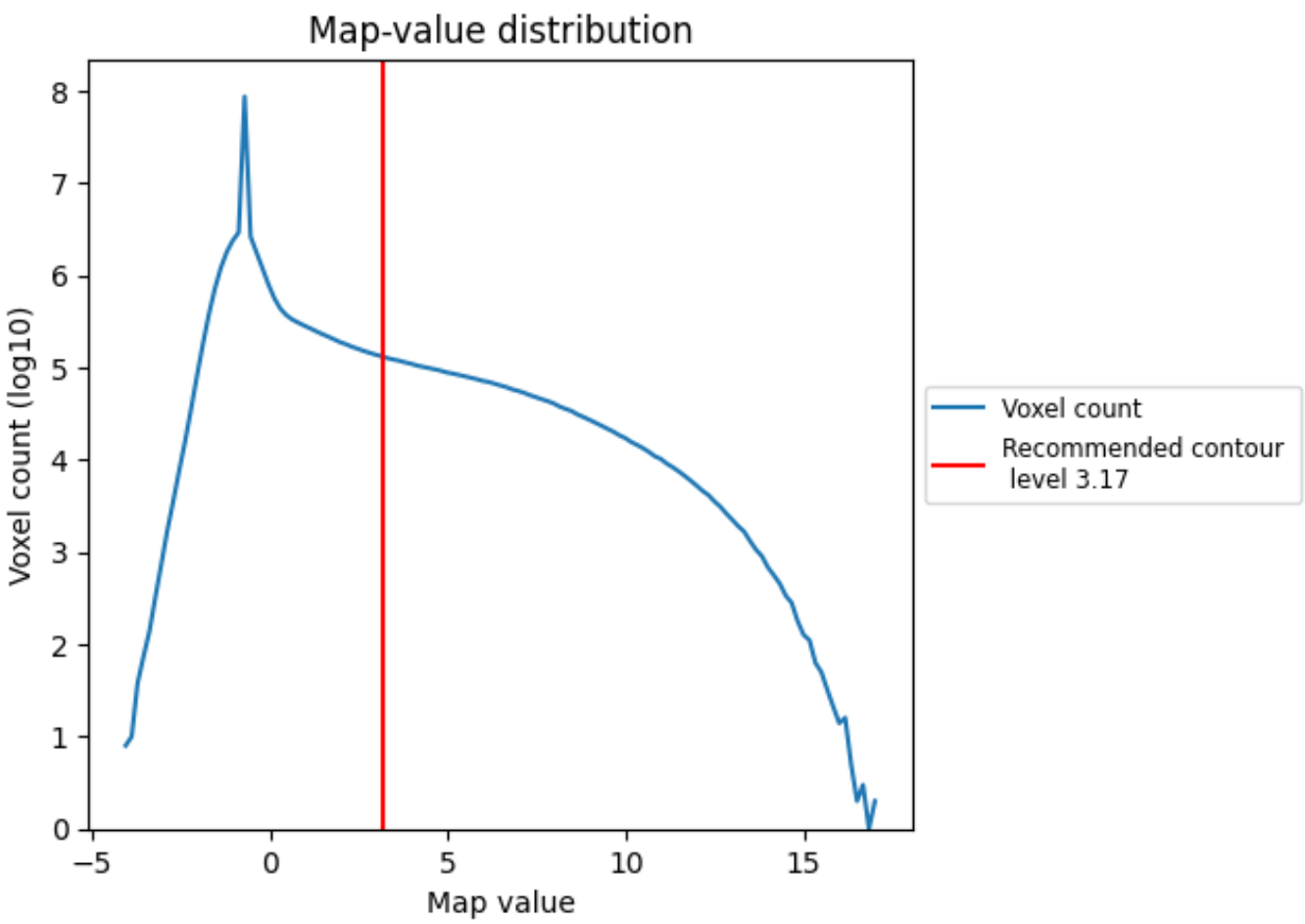
6.6 Mask visualisation (i)

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

7 Map analysis (i)

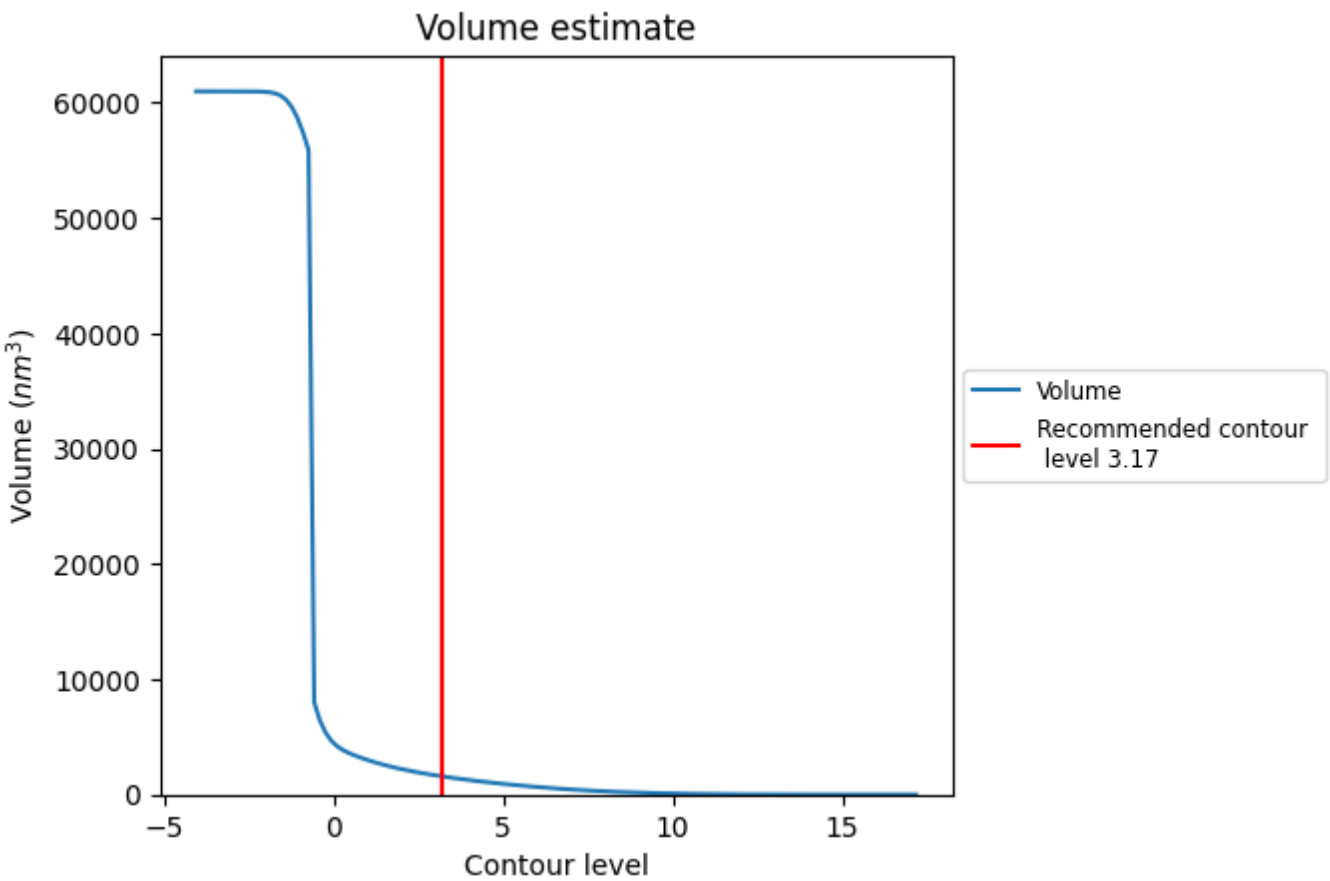
This section contains the results of statistical analysis of the map.

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.

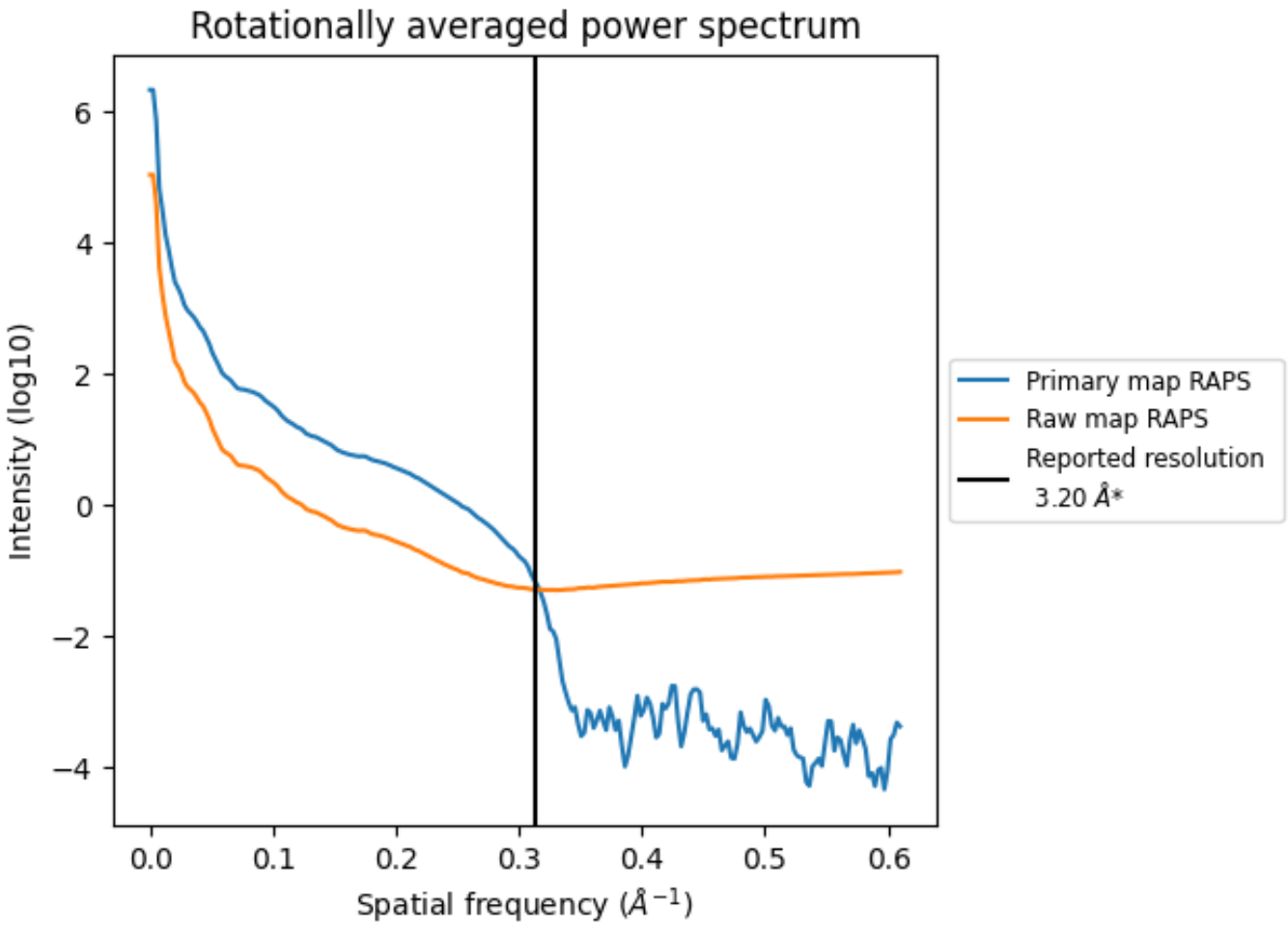
7.2 Volume estimate (i)



The volume at the recommended contour level is 1587 nm^3; this corresponds to an approximate mass of 1433 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

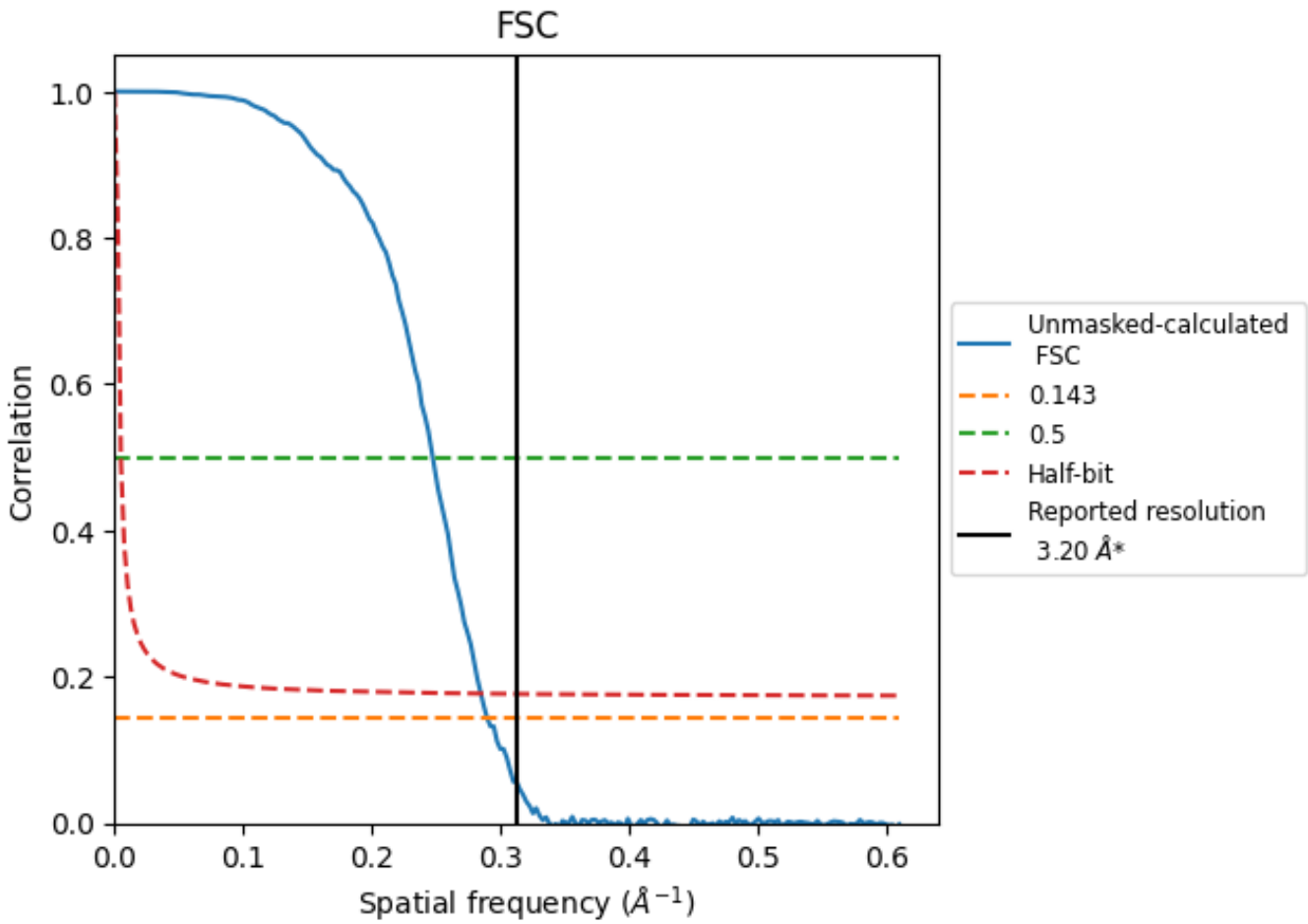


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates (i)

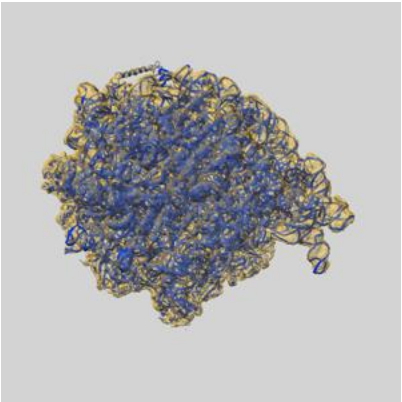
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	4.05	3.51

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

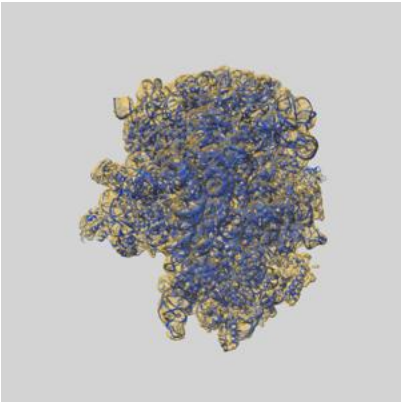
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8617 and PDB model 5UYM. Per-residue inclusion information can be found in section 3 on page 17.

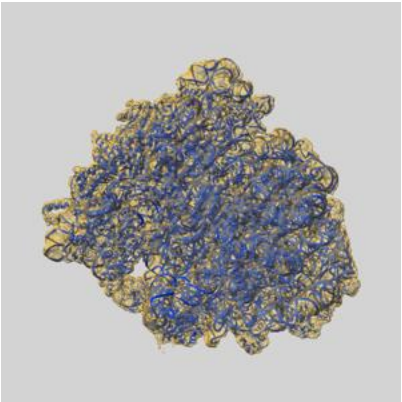
9.1 Map-model overlay (i)



X



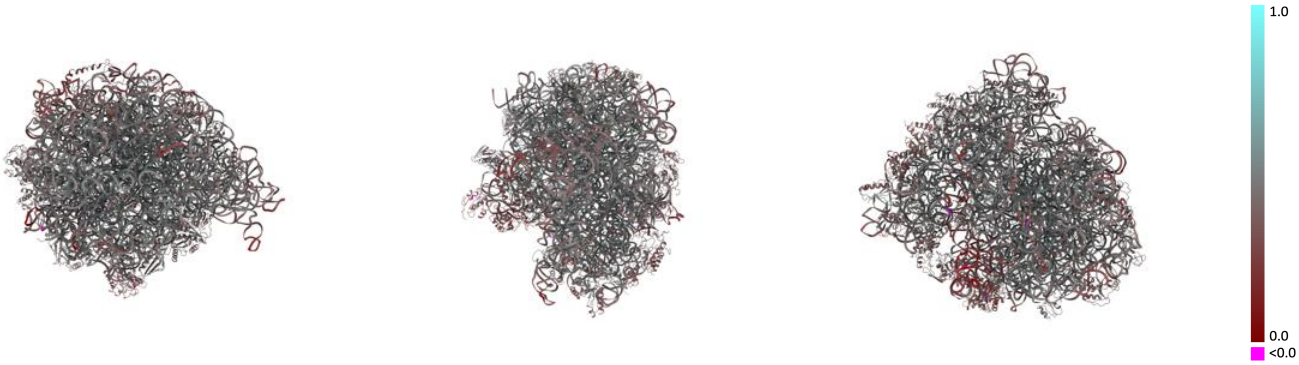
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.17 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.

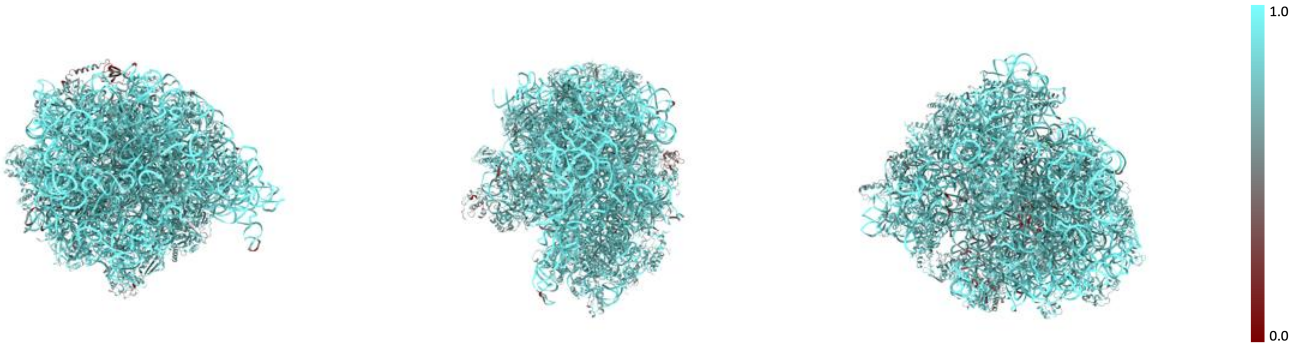
9.2 Q-score mapped to coordinate model (i)



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.

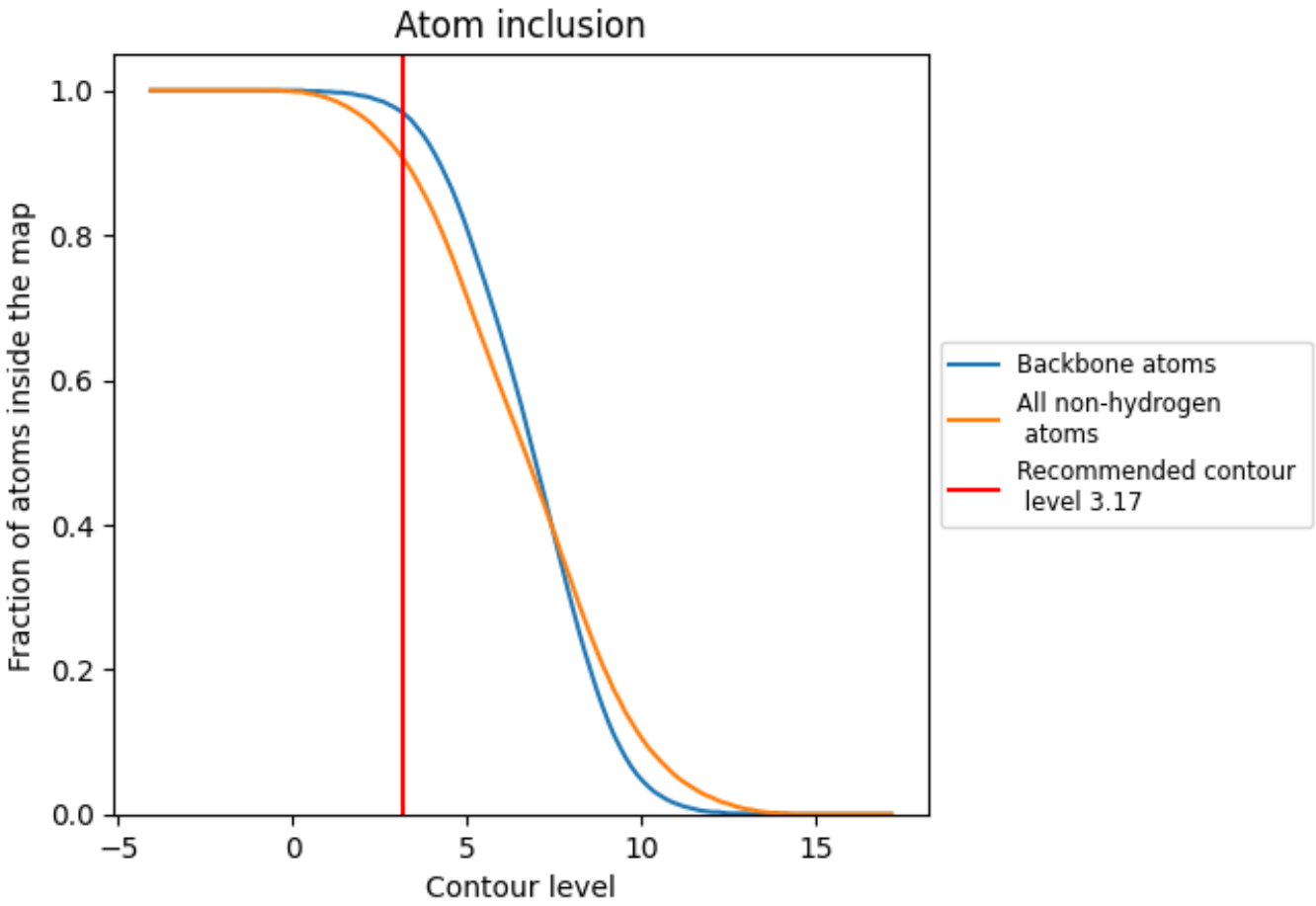
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.17).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (3.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9050	0.4440
01	0.9670	0.4590
02	0.9660	0.4320
03	0.6340	0.2870
04	0.8560	0.4910
05	0.8240	0.4790
06	0.8040	0.4450
07	0.8060	0.4040
08	0.8060	0.4290
09	0.4960	0.3490
10	0.4920	0.2500
11	0.6400	0.2700
12	0.8130	0.4530
13	0.7640	0.4680
14	0.8350	0.4640
15	0.7730	0.4700
16	0.8670	0.4670
17	0.8400	0.4260
18	0.7900	0.4550
19	0.8480	0.4680
20	0.8160	0.4560
21	0.7830	0.4570
22	0.7830	0.4360
23	0.8020	0.4340
24	0.7990	0.4440
25	0.8360	0.4800
26	0.8100	0.4670
27	0.7730	0.3830
28	0.8030	0.4470
29	0.7270	0.3660
30	0.8130	0.4570
31	0.7590	0.4570
32	0.8450	0.4800
33	0.8680	0.5030
34	0.8260	0.4810

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Chain	Atom inclusion	Q-score
A	0.9730	0.4590
B	0.7480	0.3790
C	0.7930	0.4380
D	0.7910	0.4180
E	0.8110	0.4510
F	0.7930	0.3980
G	0.7870	0.4010
H	0.8150	0.4450
I	0.8130	0.4210
J	0.7400	0.4080
K	0.8180	0.4400
L	0.8100	0.4810
M	0.8040	0.4130
N	0.8220	0.4340
O	0.8220	0.4150
P	0.8410	0.4480
Q	0.8090	0.4500
R	0.8140	0.4280
S	0.8340	0.4270
T	0.8140	0.4140
U	0.6580	0.2960
V	0.7590	0.3690
W	0.9110	0.4410
X	0.7250	0.2460
Y	0.9080	0.4100
Z	0.7900	0.4140