wwPDB EM Validation Summary Report (i)

Sep 16, 2026 – 09:04 AM EDT

PDB ID	:	8FTO / pdb_00008fto
EMDB ID	:	EMD-29449
Title	:	E. coli 70S ribosome with an improved MS2 tag inserted in H98
Authors	:	Nissley, A.J.; Cate, J.H.D.
Deposited on	:	2023-01-12
Resolution	:	1.85 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:

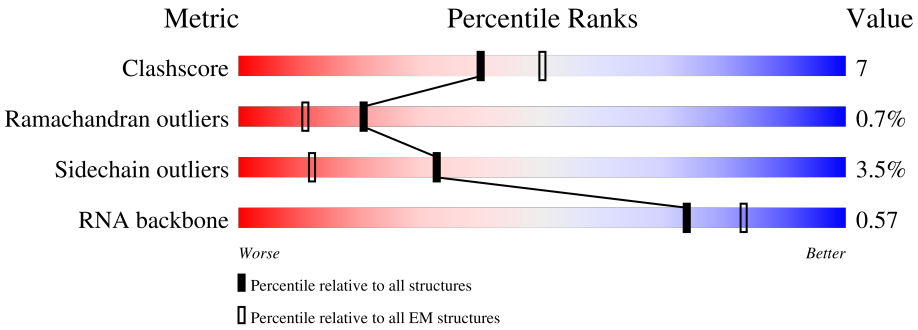
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

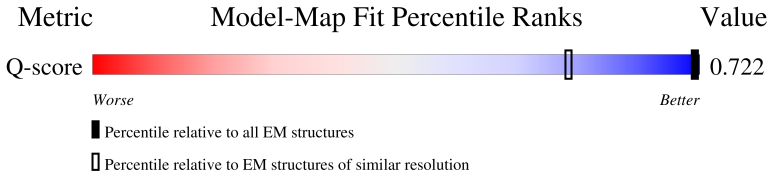
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	944 (1.35 - 2.35)

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	0	55	7%, 82%, 11%, 7%
2	1	46	89%, 11%
3	2	65	86%, 11%

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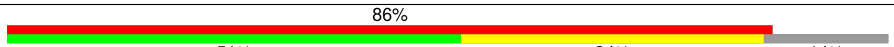
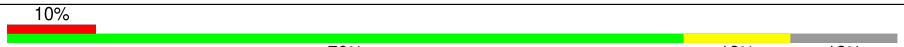
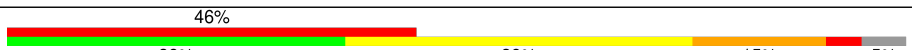
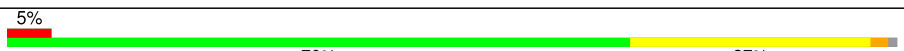
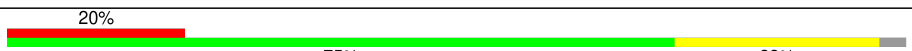
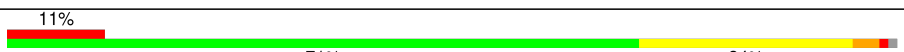
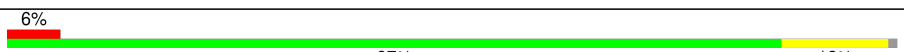
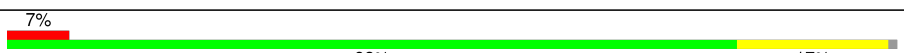
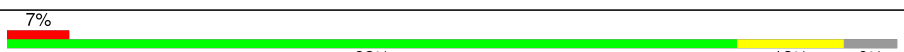
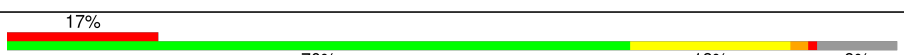
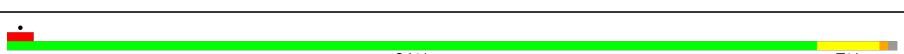
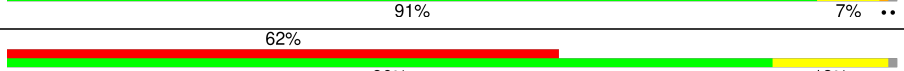
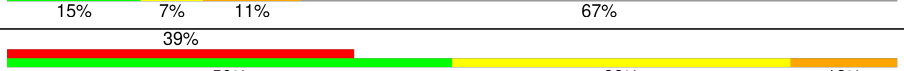
Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	27	
28	Z	76	

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Mol	Chain	Length	Quality of chain
29	a	2937	7% 65% 25% 6%
30	b	120	9% 71% 27%
31	c	273	90% 9%
32	d	209	91% 9%
33	e	201	19% 86% 14%
34	f	179	51% 53% 35% 11%
35	g	177	45% 72% 22% 5%
36	h	149	15% 10% 15% 72%
37	i	142	89% 11%
38	j	123	92% 8%
39	k	144	92% 8%
40	l	136	85% 15%
41	m	127	82% 9% 7%
42	n	117	16% 84% 15%
43	o	115	85% 12%
44	p	118	91% 8%
45	q	103	10% 94% 6%
46	r	110	5% 91% 9%
47	s	100	11% 77% 15% 7%
48	t	104	21% 75% 21%
49	u	94	18% 83% 16%
50	v	85	79% 11% 11%
51	w	78	92% 6%
52	x	63	32% 83% 16%
53	y	59	5% 92% 7%

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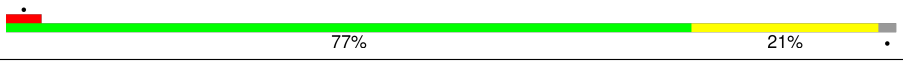
Mol	Chain	Length	Quality of chain
54	z	57	

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 146561 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 L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called 30S ribosomal protein S3.

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

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

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total 643	C 403	N 127	O 112	S 1	0	0

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total 641	C 406	N 120	O 112	S 3	0	0

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total 544	C 345	N 102	O 96	S 1	0	0

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total 668	C 427	N 127	O 112	S 2	0	0

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	70	Total 589	C 366	N 125	O 97	S 1	0	0

- Molecule 27 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	9	Total	C	N	O	P	0	0
			189	85	31	64	9		

- Molecule 28 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	76	Total	C	N	O	P	0	0
			1623	723	295	529	76		

- Molecule 29 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2767	Total	C	N	O	P	0	0
			59422	26515	10942	19198	2767		

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 31 is a protein called 50S ribosomal protein L2.

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

- Molecule 32 is a protein called 50S ribosomal protein L3.

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

- Molecule 33 is a protein called 50S ribosomal protein L4.

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

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

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

- Molecule 35 is a protein called 50S ribosomal protein L6.

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

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A0A0H3EMH6

- Molecule 41 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called Ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	76	Total	C	N	O	S	0	0
			576	357	114	104	1		

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

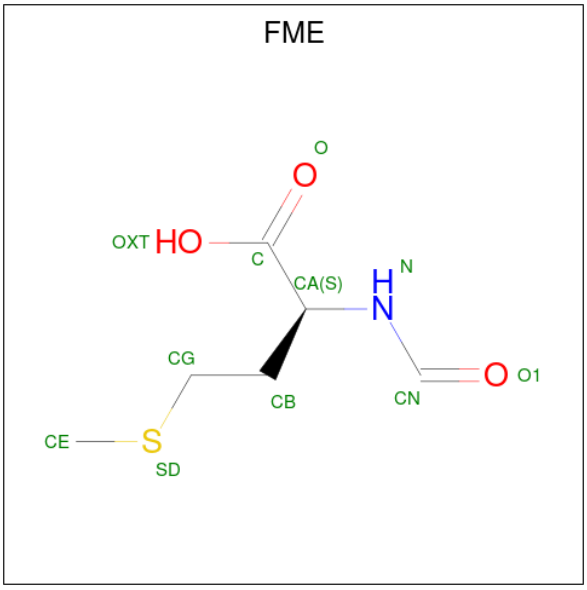
- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	81	Total	Mg	0
			81	81	
55	a	195	Total	Mg	0
			195	195	
55	b	5	Total	Mg	0
			5	5	
55	c	1	Total	Mg	0
			1	1	
55	d	1	Total	Mg	0
			1	1	
55	z	1	Total	Mg	0
			1	1	

- Molecule 56 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
56	a	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	AltConf
57	0	7	Total O 7 7	0
57	1	24	Total O 24 24	0
57	2	19	Total O 19 19	0
57	3	2	Total O 2 2	0
57	A	1650	Total O 1650 1650	0
57	B	1	Total O 1 1	0
57	C	39	Total O 39 39	0
57	D	3	Total O 3 3	0
57	E	12	Total O 12 12	0
57	G	4	Total O 4 4	0
57	H	29	Total O 29 29	0
57	I	20	Total O 20 20	0
57	J	14	Total O 14 14	0
57	K	12	Total O 12 12	0
57	L	18	Total O 18 18	0
57	M	12	Total O 12 12	0
57	N	27	Total O 27 27	0
57	O	11	Total O 11 11	0
57	P	8	Total O 8 8	0
57	Q	4	Total O 4 4	0
57	R	2	Total O 2 2	0
57	S	10	Total O 10 10	0

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Mol	Chain	Residues	Atoms	AltConf
57	T	2	Total O 2 2	0
57	U	4	Total O 4 4	0
57	X	6	Total O 6 6	0
57	Z	21	Total O 21 21	0
57	a	3559	Total O 3559 3559	0
57	b	93	Total O 93 93	0
57	c	90	Total O 90 90	0
57	d	40	Total O 40 40	0
57	e	44	Total O 44 44	0
57	f	9	Total O 9 9	0
57	h	3	Total O 3 3	0
57	i	16	Total O 16 16	0
57	j	14	Total O 14 14	0
57	k	42	Total O 42 42	0
57	l	27	Total O 27 27	0
57	m	26	Total O 26 26	0
57	n	23	Total O 23 23	0
57	o	12	Total O 12 12	0
57	p	28	Total O 28 28	0
57	q	20	Total O 20 20	0
57	r	21	Total O 21 21	0

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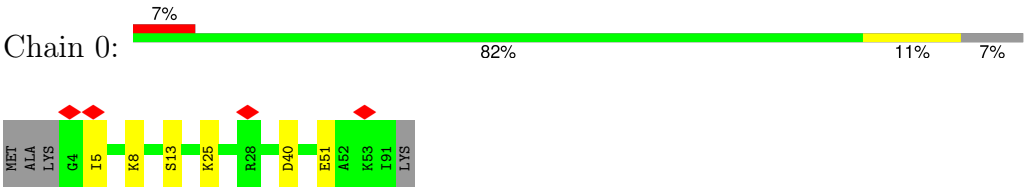
Mol	Chain	Residues	Atoms	AltConf
57	s	12	Total O 12 12	0
57	t	2	Total O 2 2	0
57	u	4	Total O 4 4	0
57	v	15	Total O 15 15	0
57	w	18	Total O 18 18	0
57	x	2	Total O 2 2	0
57	y	5	Total O 5 5	0
57	z	28	Total O 28 28	0

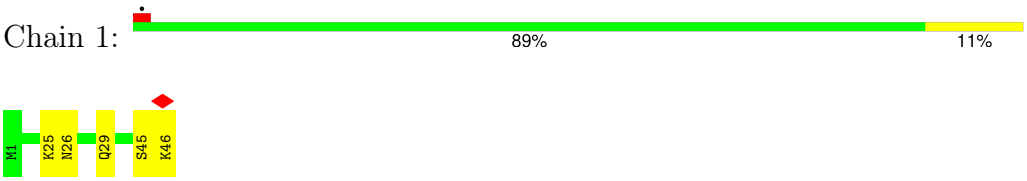
3 Residue-property plots (i)

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.

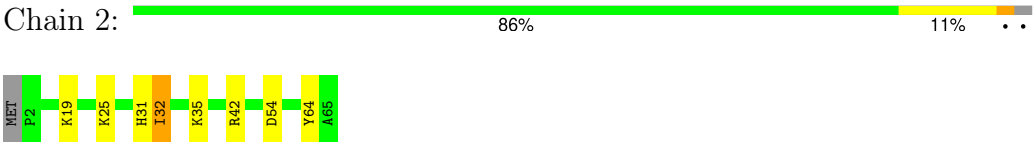
• Molecule 1: 50S ribosomal protein L33



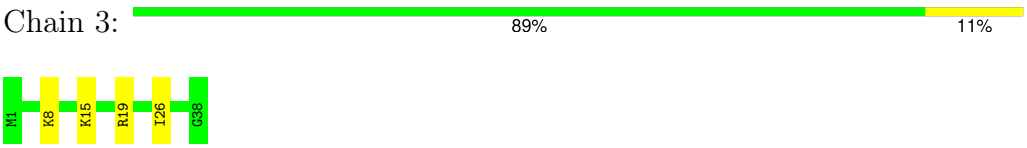
• Molecule 2: 50S ribosomal protein L34



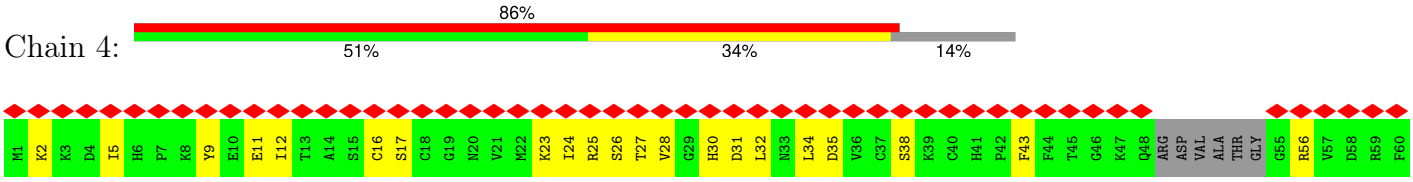
• Molecule 3: 50S ribosomal protein L35

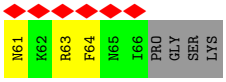


• Molecule 4: 50S ribosomal protein L36



• Molecule 5: 50S ribosomal protein L31

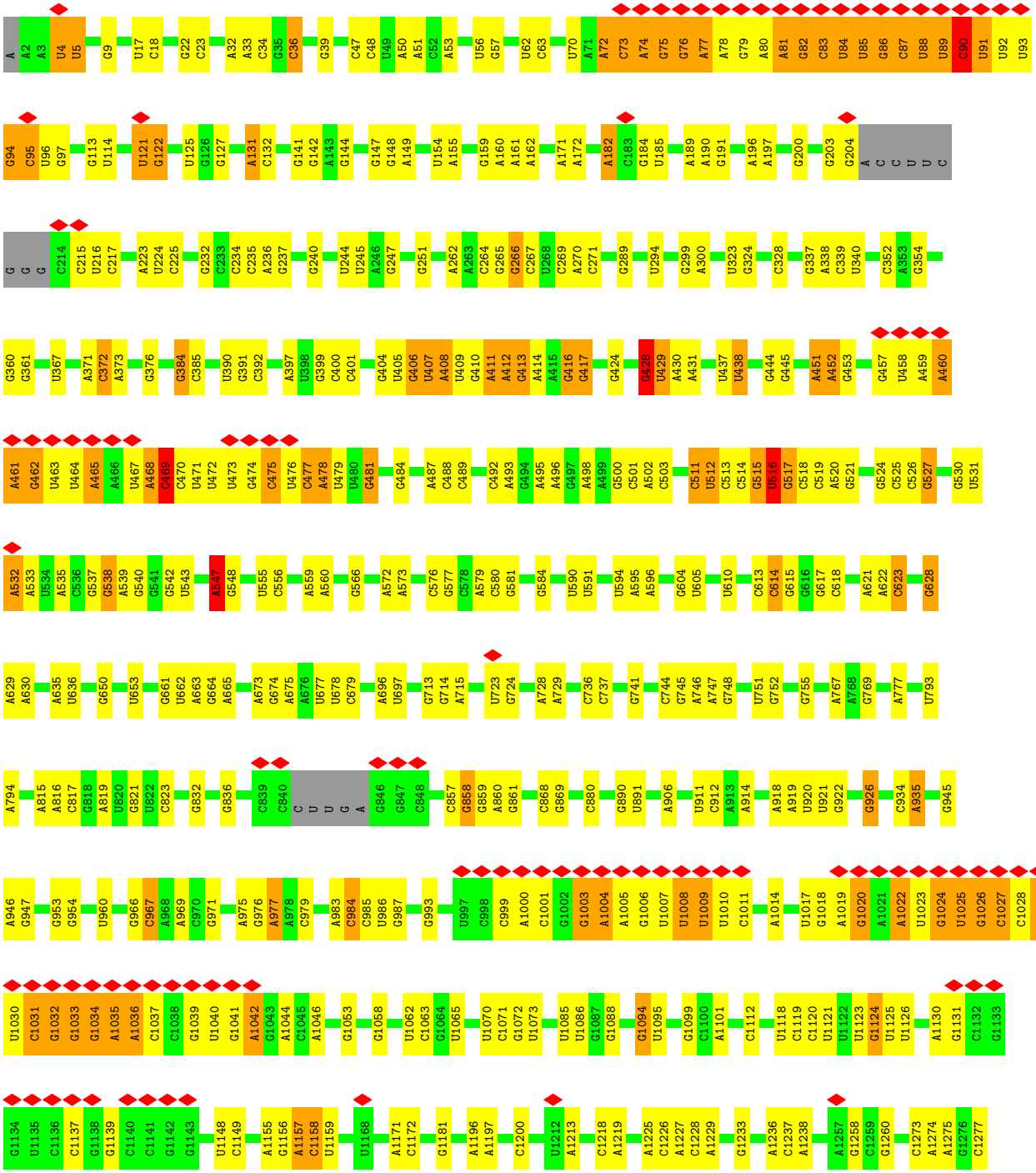


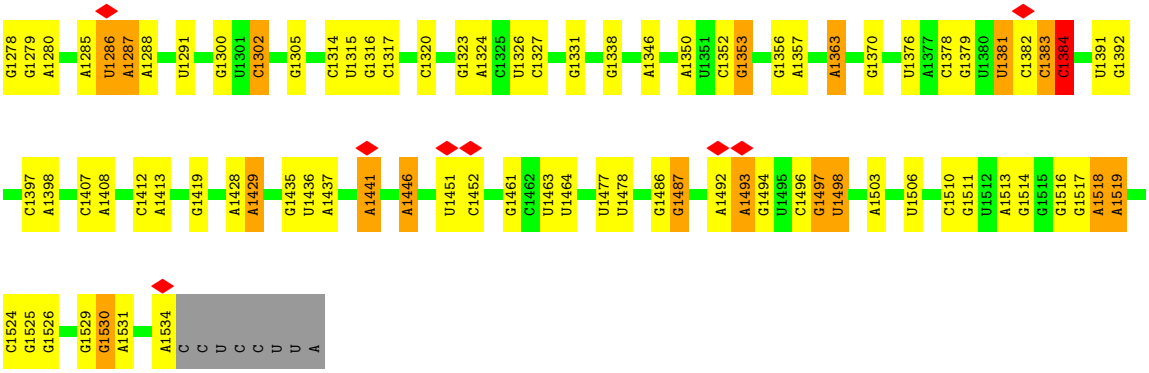


• Molecule 6: 16S rRNA

Chain A:



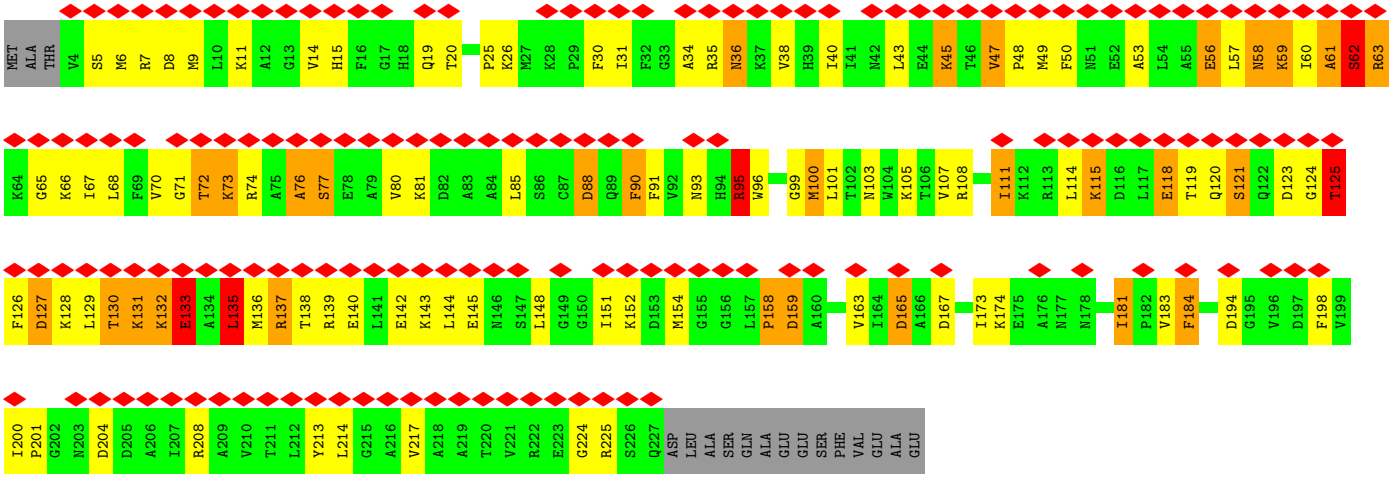




• Molecule 7: 30S ribosomal protein S2

Chain B:

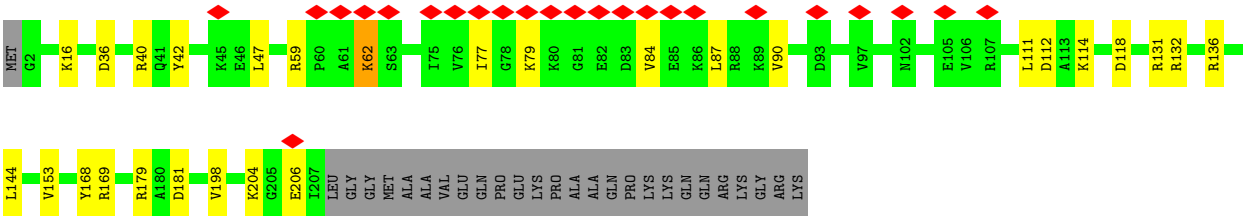




• Molecule 8: 30S ribosomal protein S3

Chain C:

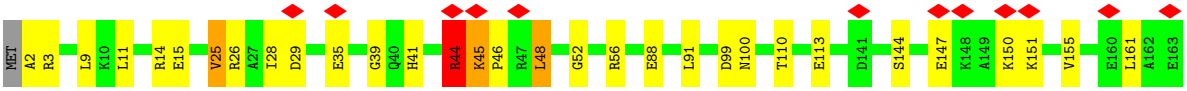


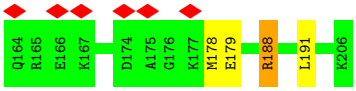


• Molecule 9: 30S ribosomal protein S4

Chain D:



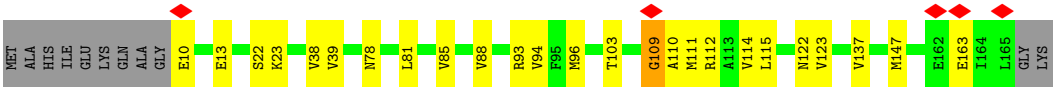




• Molecule 10: 30S ribosomal protein S5

Chain E:

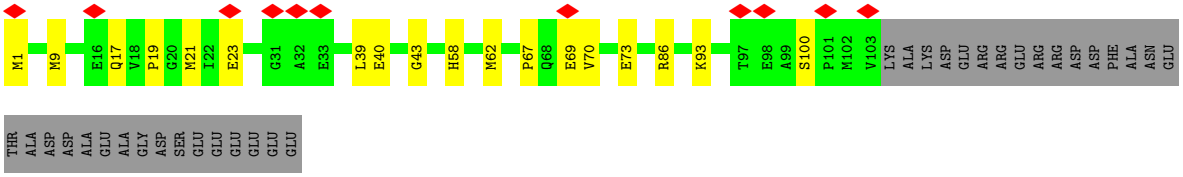




• Molecule 11: 30S ribosomal protein S6

Chain F:

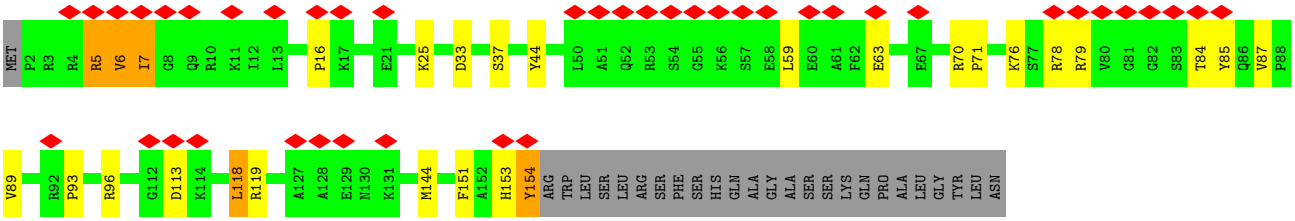




• Molecule 12: 30S ribosomal protein S7

Chain G:

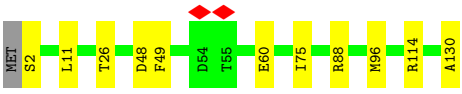




• Molecule 13: 30S ribosomal protein S8

Chain H:

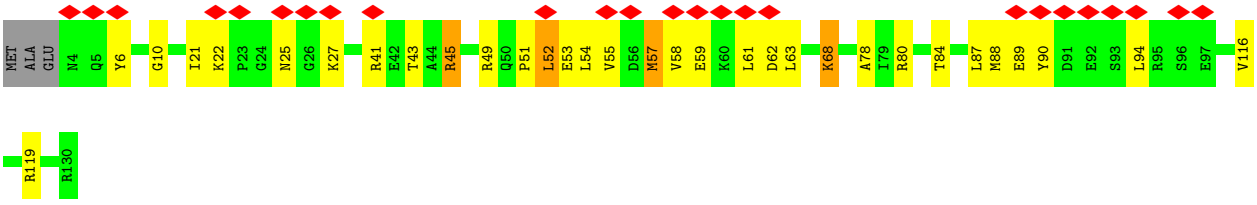




• Molecule 14: 30S ribosomal protein S9

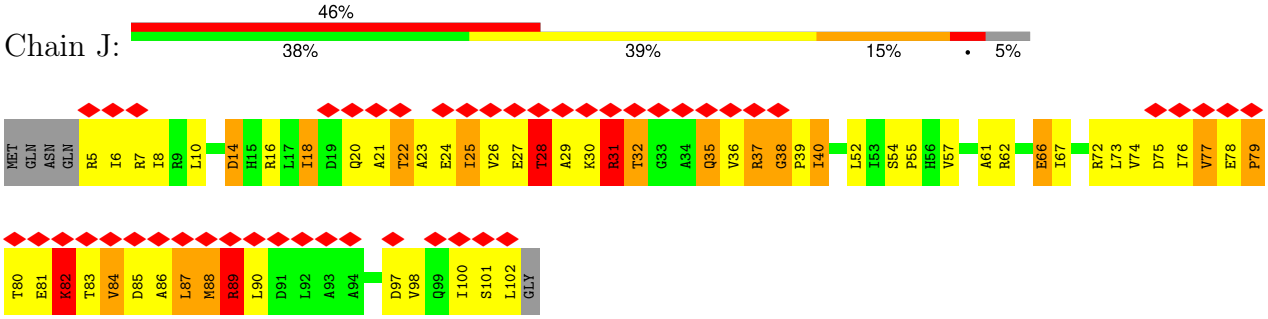
Chain I:





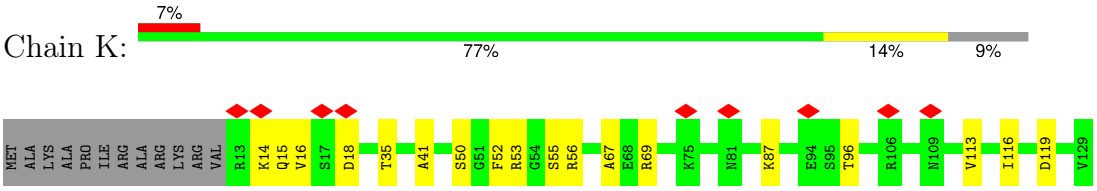
• Molecule 15: 30S ribosomal protein S10

Chain J:



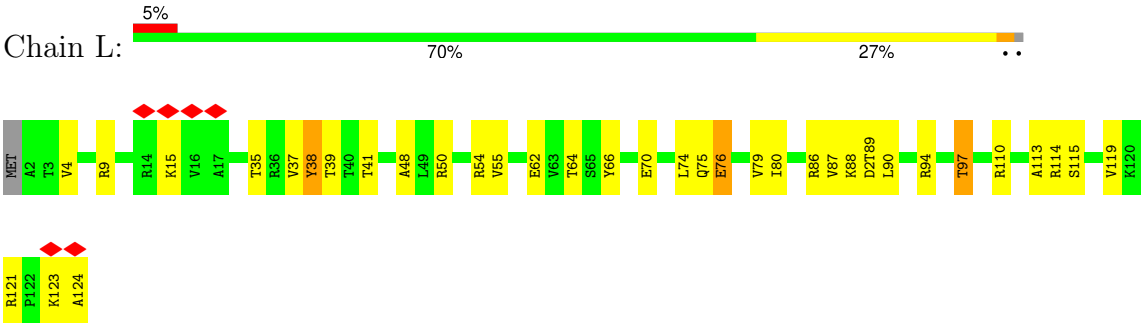
• Molecule 16: 30S ribosomal protein S11

Chain K:



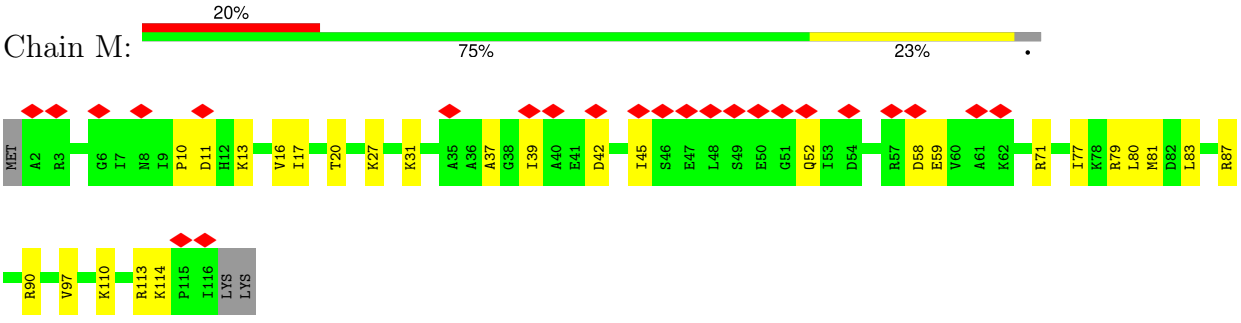
• Molecule 17: 30S ribosomal protein S12

Chain L:



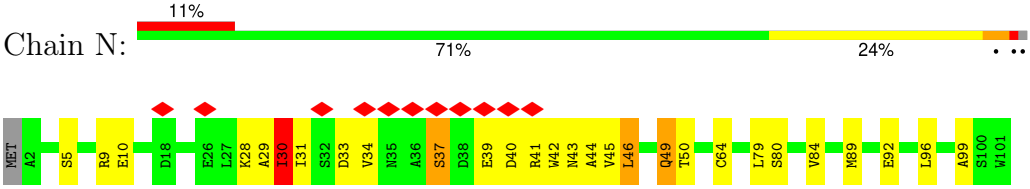
• Molecule 18: 30S ribosomal protein S13

Chain M:



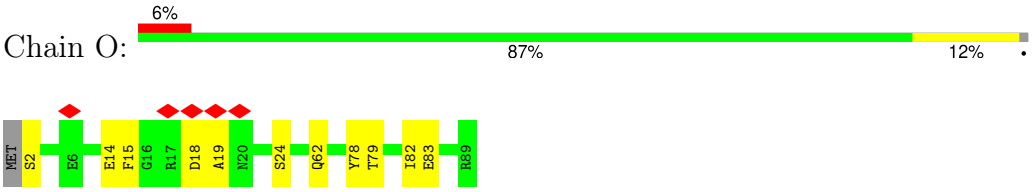
• Molecule 19: 30S ribosomal protein S14

Chain N:



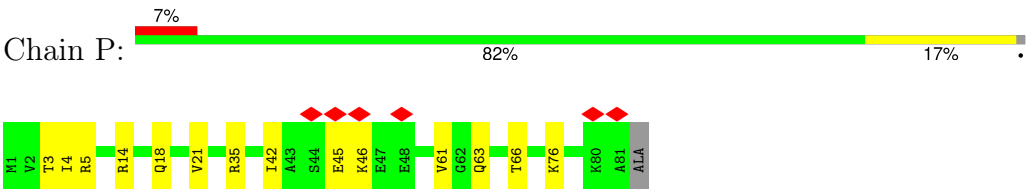
• Molecule 20: 30S ribosomal protein S15

Chain O:



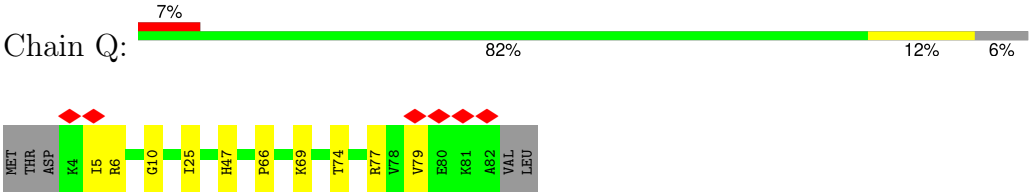
• Molecule 21: 30S ribosomal protein S16

Chain P:



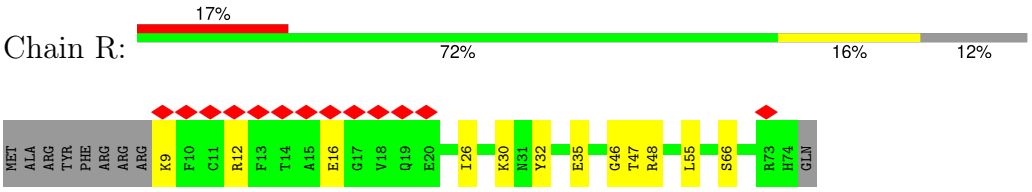
• Molecule 22: 30S ribosomal protein S17

Chain Q:



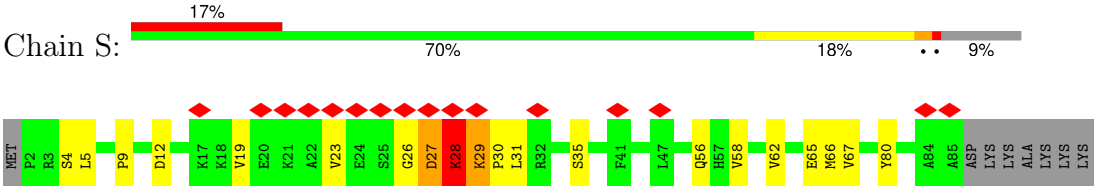
• Molecule 23: 30S ribosomal protein S18

Chain R:



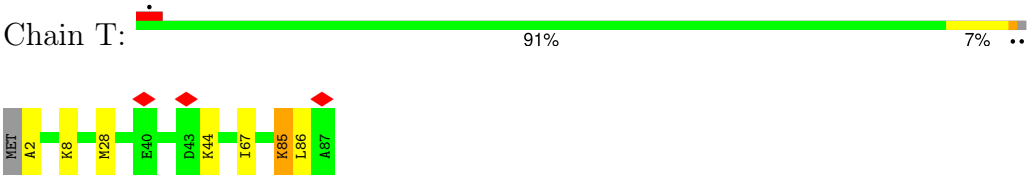
• Molecule 24: 30S ribosomal protein S19

Chain S:



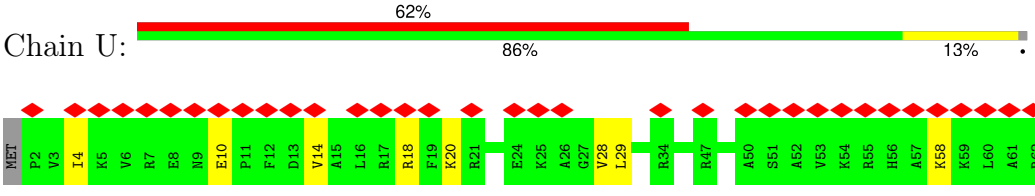
• Molecule 25: 30S ribosomal protein S20

Chain T:



• Molecule 26: 30S ribosomal protein S21

Chain U:



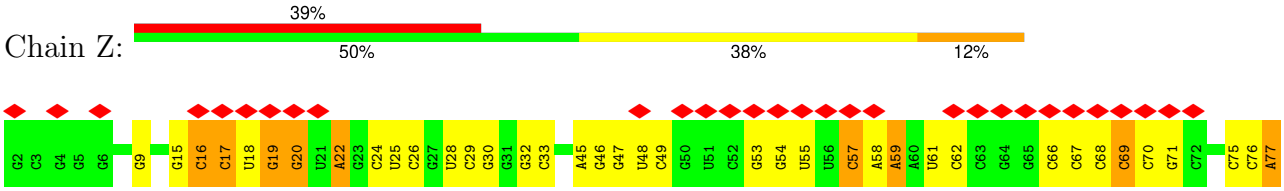
• Molecule 27: mRNA

Chain X:



• Molecule 28: P-site tRNA-fMet

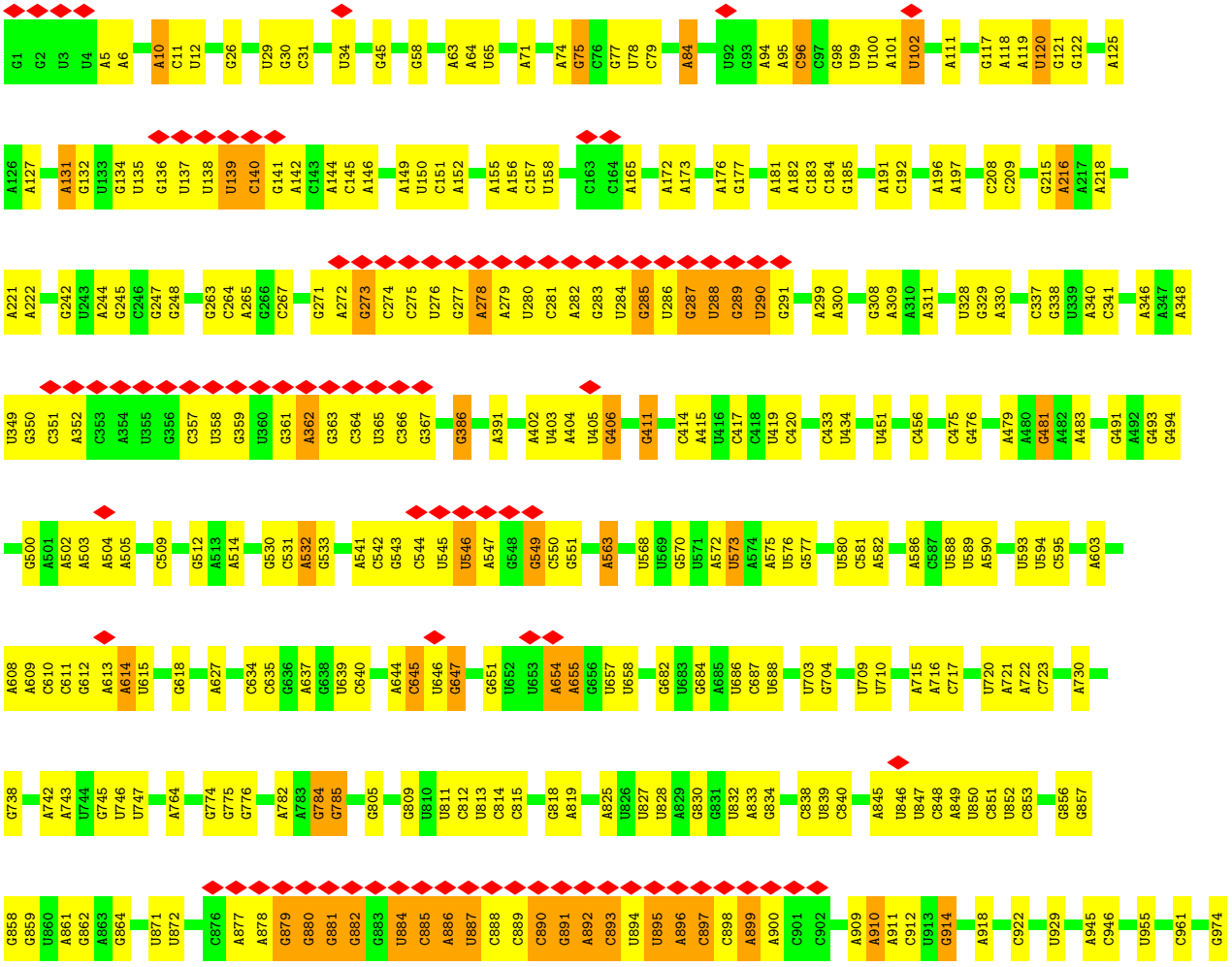
Chain Z:

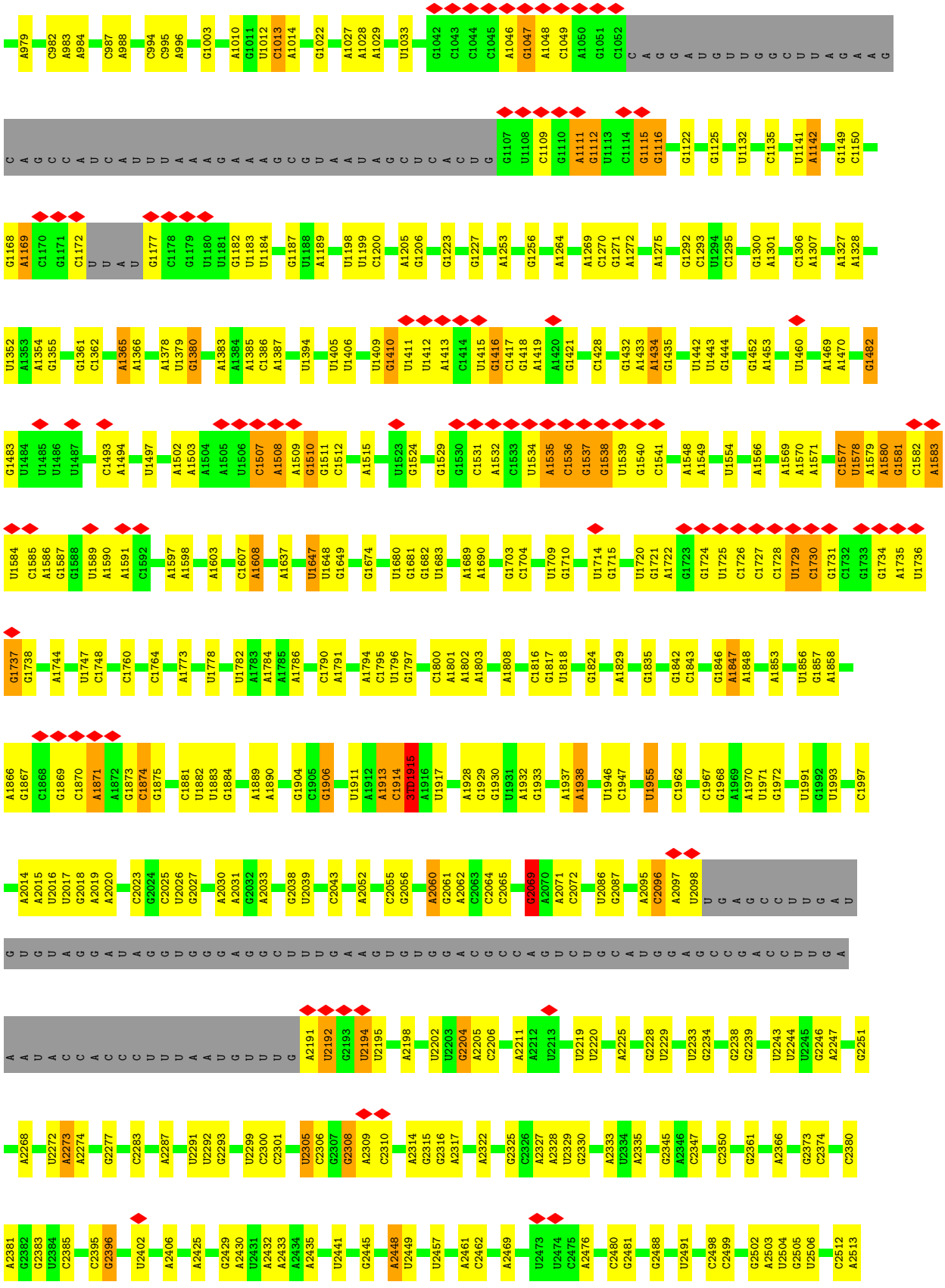


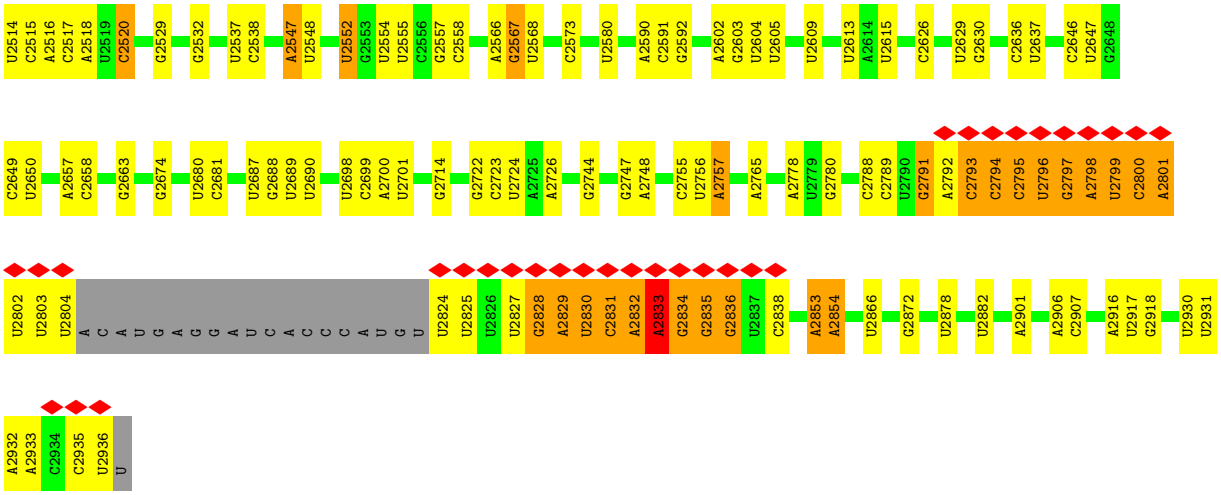
• Molecule 29: 23S rRNA

Chain a:





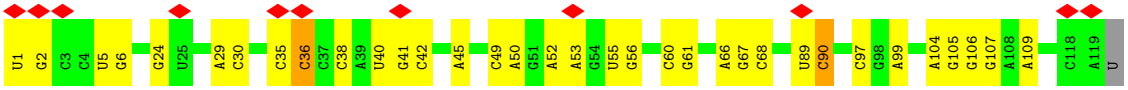




• Molecule 30: 5S rRNA

Chain b:

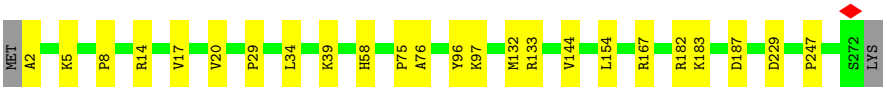




• Molecule 31: 50S ribosomal protein L2

Chain c:

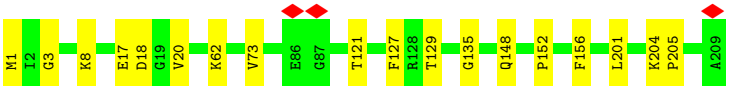




• Molecule 32: 50S ribosomal protein L3

Chain d:

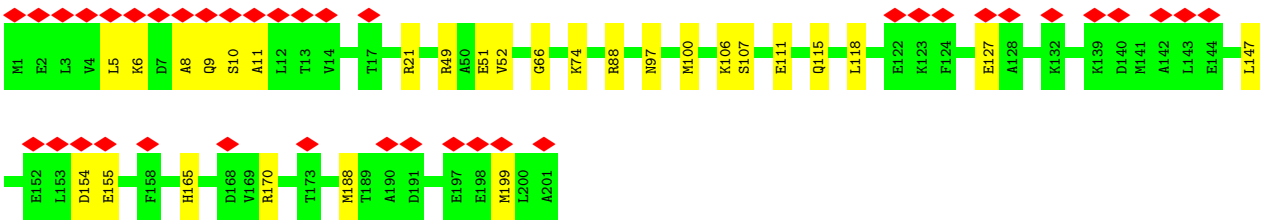




• Molecule 33: 50S ribosomal protein L4

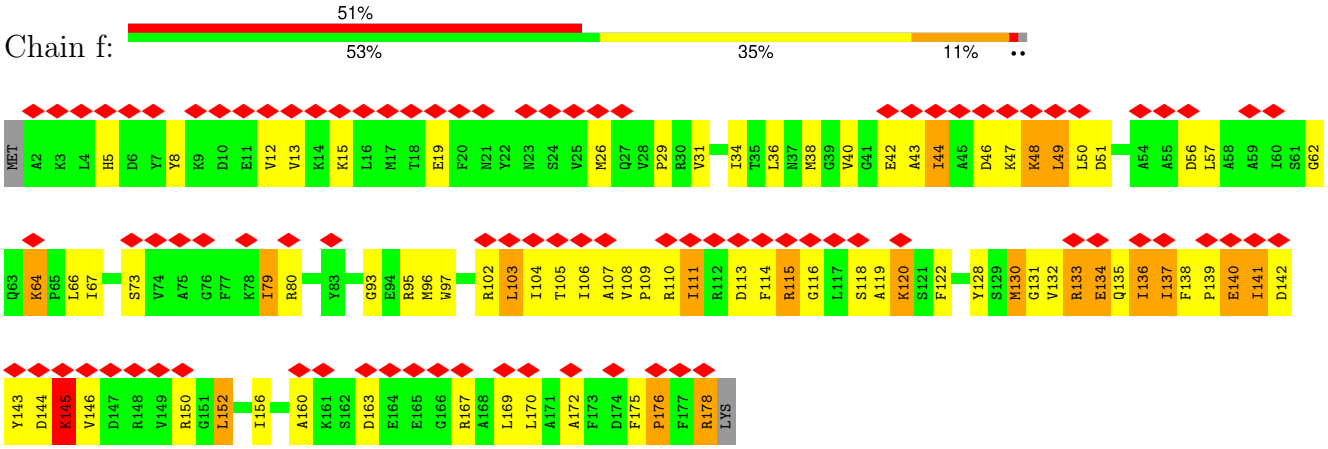
Chain e:





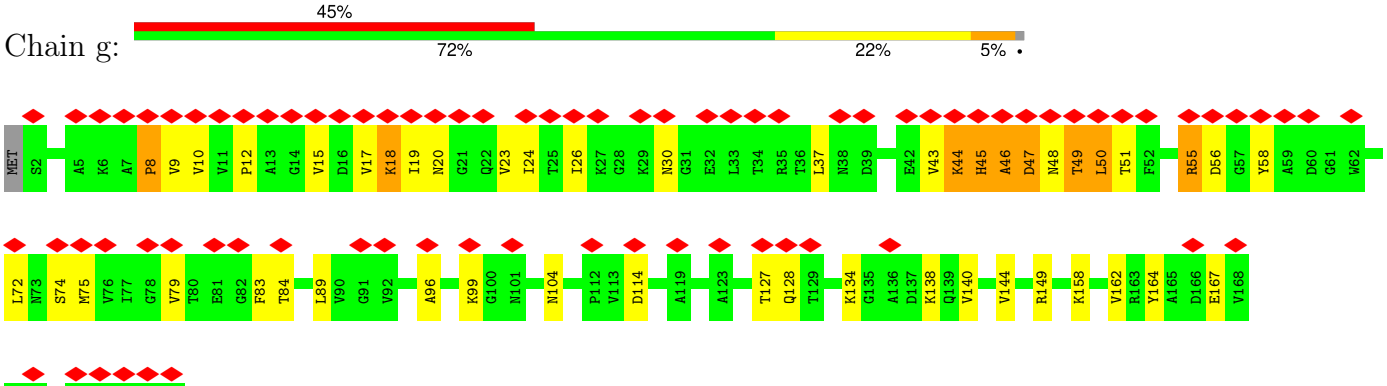
• Molecule 34: 50S ribosomal protein L5

Chain f:



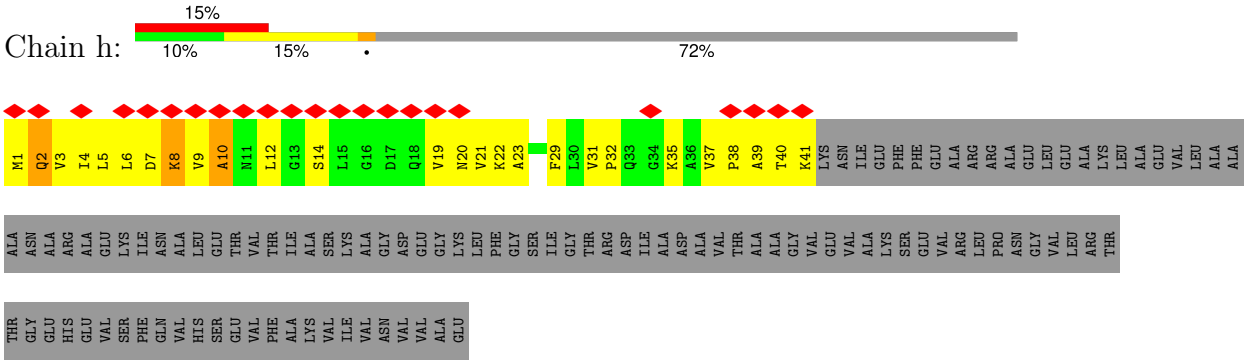
• Molecule 35: 50S ribosomal protein L6

Chain g:



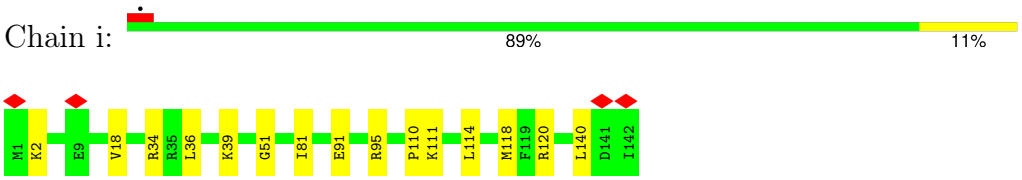
• Molecule 36: 50S ribosomal protein L9

Chain h:



• Molecule 37: 50S ribosomal protein L13

Chain i:



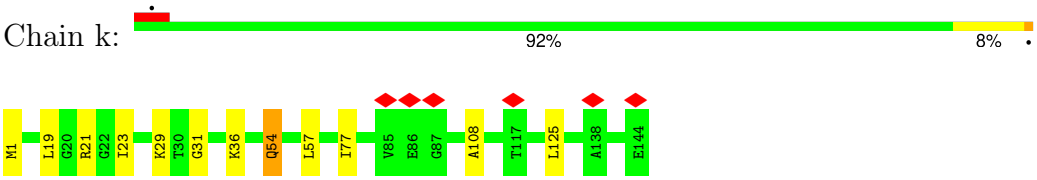
• Molecule 38: 50S ribosomal protein L14

Chain j:



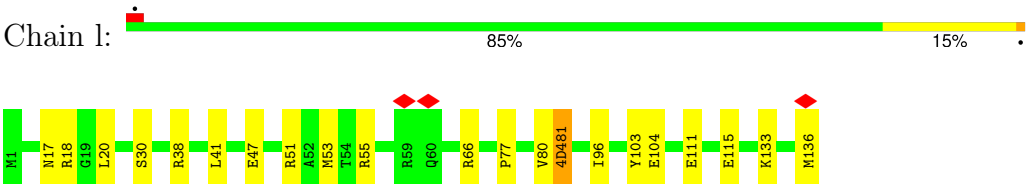
• Molecule 39: 50S ribosomal protein L15

Chain k:



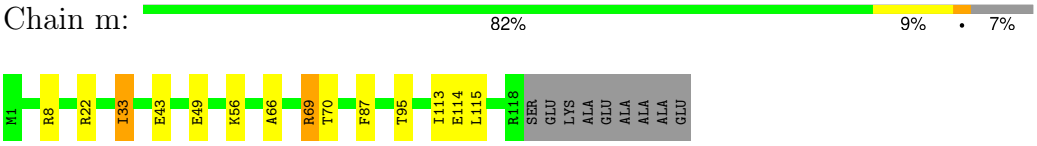
• Molecule 40: 50S ribosomal protein L16

Chain l:



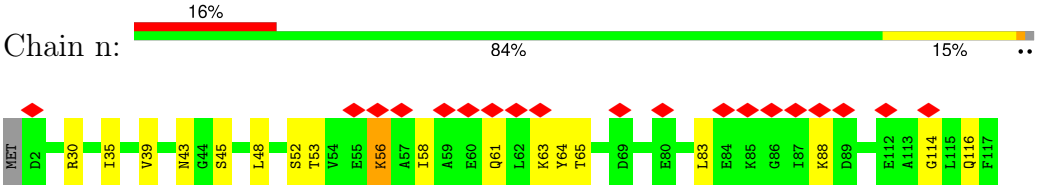
• Molecule 41: 50S ribosomal protein L17

Chain m:



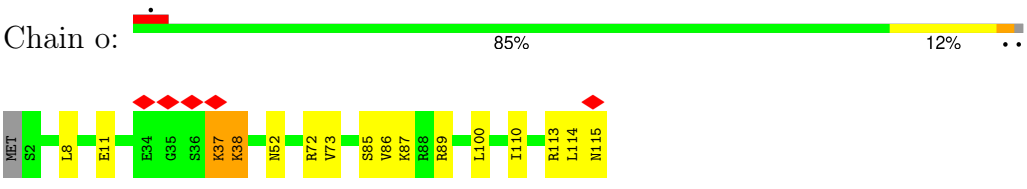
• Molecule 42: 50S ribosomal protein L18

Chain n:



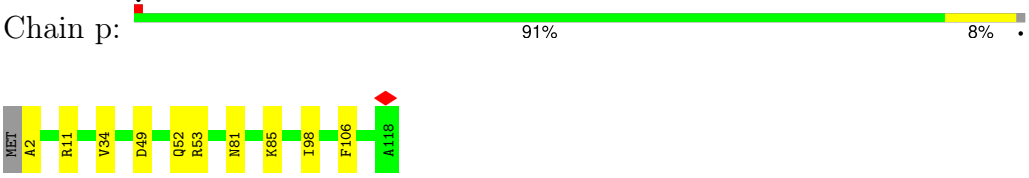
• Molecule 43: 50S ribosomal protein L19

Chain o:



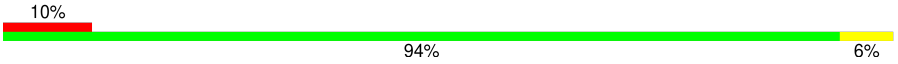
• Molecule 44: 50S ribosomal protein L20

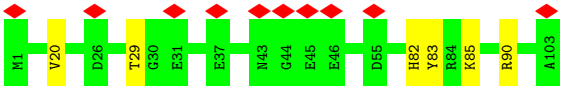
Chain p:



• Molecule 45: Ribosomal protein L21

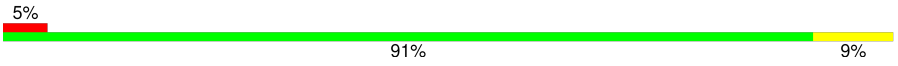
Chain q:

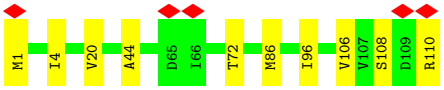




• Molecule 46: 50S ribosomal protein L22

Chain r:

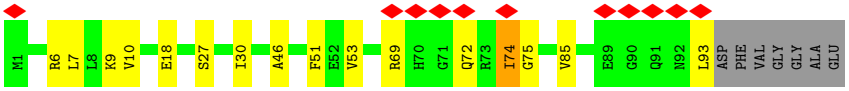




• Molecule 47: 50S ribosomal protein L23

Chain s:

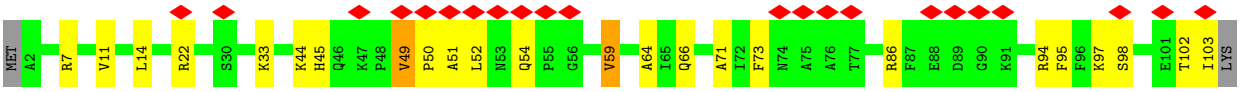




• Molecule 48: 50S ribosomal protein L24

Chain t:

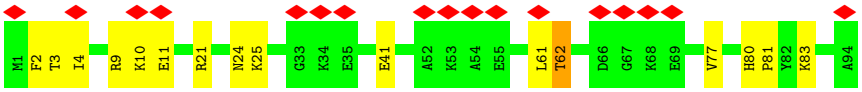




• Molecule 49: 50S ribosomal protein L25

Chain u:

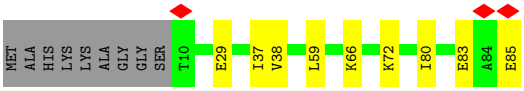




• Molecule 50: 50S ribosomal protein L27

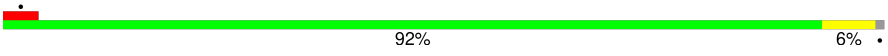
Chain v:

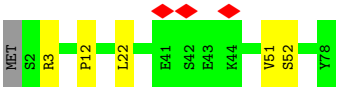




• Molecule 51: 50S ribosomal protein L28

Chain w:

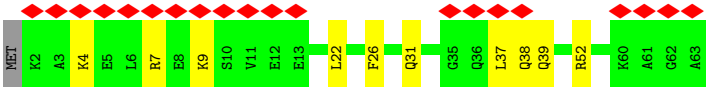




• Molecule 52: 50S ribosomal protein L29

Chain x:

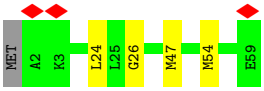




• Molecule 53: 50S ribosomal protein L30

Chain y:

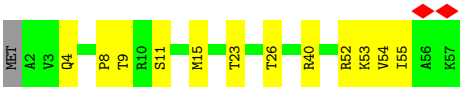




• Molecule 54: 50S ribosomal protein L32

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	601617	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.389	Depositor
Minimum map value	-3.990	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.269	Depositor
Recommended contour level	0.933	Depositor
Map size (Å)	369.5104, 369.5104, 369.5104	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8248, 0.8248, 0.8248	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: 6MZ, 2MA, MG, 5MC, UR3, 8AN, IAS, 5MU, OMU, FME, 4D4, 2MG, D2T, PSU, G7M, MEQ, 1MG, H2U, MA6, OMC, 3TD, MS6, 4OC, OMG

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	0	0.23	0/424	0.39	0/565
2	1	0.33	0/380	0.49	0/498
3	2	0.26	0/513	0.43	0/676
4	3	0.24	0/303	0.41	0/397
5	4	0.17	0/488	0.45	0/649
6	A	0.45	0/36236	0.45	10/56520 (0.0%)
7	B	0.92	1/1784 (0.1%)	1.37	11/2403 (0.5%)
8	C	0.30	0/1651	0.39	0/2225
9	D	0.35	0/1665	0.52	2/2227 (0.1%)
10	E	0.35	0/1165	0.48	1/1568 (0.1%)
11	F	0.28	0/858	0.37	0/1160
12	G	0.38	0/1219	0.60	0/1635
13	H	0.33	0/989	0.41	0/1326
14	I	0.69	0/1034	1.04	2/1375 (0.1%)
15	J	1.06	1/796 (0.1%)	1.42	7/1077 (0.6%)
16	K	0.27	0/884	0.39	0/1191
17	L	0.37	0/960	0.69	0/1286
18	M	0.28	0/900	0.37	0/1204
19	N	0.59	0/817	0.84	1/1088 (0.1%)
20	O	0.31	0/722	0.43	1/964 (0.1%)
21	P	0.35	0/653	0.54	0/877
22	Q	0.32	0/650	0.44	0/871
23	R	0.48	0/553	0.66	0/742
24	S	0.40	0/685	0.70	3/922 (0.3%)
25	T	0.36	0/676	0.56	0/895
26	U	0.20	0/597	0.30	0/792
27	X	0.45	0/210	0.81	0/324
28	Z	0.31	0/1787	0.47	0/2782
29	a	0.32	0/65975	0.47	3/102914 (0.0%)
30	b	0.23	0/2850	0.35	0/4444
31	c	0.25	0/2121	0.43	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	d	0.25	0/1576	0.44	0/2119
33	e	0.22	0/1571	0.40	0/2113
34	f	0.58	0/1434	0.88	1/1926 (0.1%)
35	g	0.47	0/1343	0.67	0/1816
36	h	0.87	0/306	1.15	1/413 (0.2%)
37	i	0.23	0/1152	0.39	0/1551
38	j	0.27	0/955	0.44	0/1279
39	k	0.25	0/1062	0.45	0/1413
40	l	0.23	0/1073	0.42	0/1433
41	m	0.49	1/958 (0.1%)	0.61	1/1281 (0.1%)
42	n	0.30	0/902	0.53	0/1209
43	o	0.35	0/929	0.51	0/1242
44	p	0.25	0/960	0.42	0/1278
45	q	0.26	0/829	0.44	1/1107 (0.1%)
46	r	0.24	0/864	0.40	0/1156
47	s	0.31	0/744	0.48	0/994
48	t	0.21	0/787	0.47	0/1051
49	u	0.23	0/766	0.44	0/1025
50	v	0.24	0/583	0.42	0/772
51	w	0.24	0/635	0.39	0/848
52	x	0.21	0/502	0.36	0/667
53	y	0.24	0/453	0.39	0/605
54	z	0.24	0/450	0.38	0/599
All	All	0.38	3/151379 (0.0%)	0.50	45/226346 (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
3	2	0	1
9	D	0	1
15	J	0	1
40	l	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	m	69	ARG	C-O	-6.66	1.15	1.23
15	J	55	PRO	C-O	-5.63	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	181	ILE	N-CA	5.11	1.50	1.46

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	547	A	C2'-C3'-O3'	9.22	123.34	109.50
6	A	5	U	C2'-C3'-O3'	-8.62	96.57	109.50
6	A	537	G	C4'-C3'-O3'	-8.51	100.23	113.00
7	B	121	SER	N-CA-C	-7.61	103.00	111.82
41	m	69	ARG	N-CA-C	-7.59	99.28	110.52

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	31	HIS	Peptide
9	D	188	ARG	Sidechain
15	J	38	GLY	Peptide
40	l	81	4D4	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	3	0
2	1	377	0	418	5	0
3	2	504	0	572	6	0
4	3	302	0	343	2	0
5	4	480	0	481	46	0
6	A	32612	0	16432	344	0
7	B	1753	0	1780	103	0
8	C	1624	0	1696	16	0
9	D	1643	0	1707	27	0
10	E	1152	0	1196	17	0
11	F	839	0	833	11	0
12	G	1203	0	1254	30	0
13	H	979	0	1031	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	1022	0	1070	28	0
15	J	786	0	828	56	0
16	K	877	0	884	10	0
17	L	957	0	1017	23	0
18	M	891	0	952	34	0
19	N	805	0	844	19	0
20	O	714	0	734	5	0
21	P	643	0	661	8	0
22	Q	641	0	682	10	0
23	R	544	0	565	6	0
24	S	668	0	692	27	0
25	T	670	0	719	4	0
26	U	589	0	629	5	0
27	X	189	0	96	12	0
28	Z	1623	0	827	28	0
29	a	59422	0	29916	528	0
30	b	2549	0	1291	21	0
31	c	2082	0	2154	15	0
32	d	1566	0	1618	11	0
33	e	1552	0	1619	18	0
34	f	1410	0	1444	99	0
35	g	1323	0	1371	34	0
36	h	303	0	327	18	0
37	i	1129	0	1162	10	0
38	j	946	0	1023	7	0
39	k	1053	0	1129	13	0
40	l	1075	0	1146	12	0
41	m	945	0	989	9	0
42	n	892	0	923	8	0
43	o	917	0	962	12	0
44	p	947	0	1019	7	0
45	q	816	0	839	4	0
46	r	857	0	922	5	0
47	s	738	0	807	11	0
48	t	779	0	831	17	0
49	u	753	0	780	10	0
50	v	576	0	588	5	0
51	w	625	0	652	4	0
52	x	501	0	531	10	0
53	y	449	0	488	4	0
54	z	444	0	458	8	0
55	A	81	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	a	195	0	0	0	0
55	b	5	0	0	0	0
55	c	1	0	0	0	0
55	d	1	0	0	0	0
55	z	1	0	0	0	0
56	a	10	0	10	3	0
57	0	7	0	0	0	0
57	1	24	0	0	0	0
57	2	19	0	0	1	0
57	3	2	0	0	0	0
57	A	1650	0	0	20	0
57	B	1	0	0	0	0
57	C	39	0	0	0	0
57	D	3	0	0	0	0
57	E	12	0	0	1	0
57	G	4	0	0	0	0
57	H	29	0	0	1	0
57	I	20	0	0	1	0
57	J	14	0	0	0	0
57	K	12	0	0	0	0
57	L	18	0	0	0	0
57	M	12	0	0	1	0
57	N	27	0	0	0	0
57	O	11	0	0	0	0
57	P	8	0	0	0	0
57	Q	4	0	0	0	0
57	R	2	0	0	0	0
57	S	10	0	0	2	0
57	T	2	0	0	0	0
57	U	4	0	0	0	0
57	X	6	0	0	1	0
57	Z	21	0	0	1	0
57	a	3559	0	0	18	0
57	b	93	0	0	3	0
57	c	90	0	0	1	0
57	d	40	0	0	0	0
57	e	44	0	0	0	0
57	f	9	0	0	1	0
57	h	3	0	0	0	0
57	i	16	0	0	1	0
57	j	14	0	0	0	0
57	k	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	l	27	0	0	0	0
57	m	26	0	0	0	0
57	n	23	0	0	0	0
57	o	12	0	0	0	0
57	p	28	0	0	0	0
57	q	20	0	0	0	0
57	r	21	0	0	0	0
57	s	12	0	0	1	0
57	t	2	0	0	0	0
57	u	4	0	0	0	0
57	v	15	0	0	0	0
57	w	18	0	0	0	0
57	x	2	0	0	1	0
57	y	5	0	0	0	0
57	z	28	0	0	0	0
All	All	146561	0	94393	1637	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 7.

The worst 5 of 1637 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)
5:4:56:ARG:NH1	18:M:79:ARG:NH2	1.71	1.36
5:4:56:ARG:NE	24:S:67:VAL:O	1.69	1.25
18:M:71:ARG:HH12	34:f:113:ASP:CG	1.51	1.19
5:4:56:ARG:NH1	24:S:65:GLU:O	1.76	1.16
6:A:533:A:OP1	57:A:1701:HOH:O	1.65	1.11

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	0	49/55 (89%)	49 (100%)	0	0	100 100
2	1	44/46 (96%)	44 (100%)	0	0	100 100
3	2	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	7 2
4	3	36/38 (95%)	36 (100%)	0	0	100 100
5	4	56/70 (80%)	53 (95%)	3 (5%)	0	100 100
7	B	222/241 (92%)	185 (83%)	21 (10%)	16 (7%)	1 0
8	C	204/233 (88%)	198 (97%)	6 (3%)	0	100 100
9	D	203/206 (98%)	199 (98%)	4 (2%)	0	100 100
10	E	154/167 (92%)	150 (97%)	4 (3%)	0	100 100
11	F	101/135 (75%)	99 (98%)	2 (2%)	0	100 100
12	G	151/179 (84%)	142 (94%)	9 (6%)	0	100 100
13	H	127/130 (98%)	122 (96%)	5 (4%)	0	100 100
14	I	125/130 (96%)	115 (92%)	10 (8%)	0	100 100
15	J	96/103 (93%)	80 (83%)	11 (12%)	5 (5%)	1 0
16	K	113/129 (88%)	109 (96%)	4 (4%)	0	100 100
17	L	120/124 (97%)	102 (85%)	16 (13%)	2 (2%)	7 1
18	M	113/118 (96%)	110 (97%)	3 (3%)	0	100 100
19	N	98/101 (97%)	95 (97%)	0	3 (3%)	3 0
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100 100
21	P	79/82 (96%)	76 (96%)	3 (4%)	0	100 100
22	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100 100
23	R	64/75 (85%)	60 (94%)	4 (6%)	0	100 100
24	S	82/92 (89%)	80 (98%)	1 (1%)	1 (1%)	10 2
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
26	U	68/71 (96%)	68 (100%)	0	0	100 100
31	c	269/273 (98%)	263 (98%)	6 (2%)	0	100 100
32	d	206/209 (99%)	202 (98%)	4 (2%)	0	100 100
33	e	199/201 (99%)	197 (99%)	2 (1%)	0	100 100
34	f	175/179 (98%)	159 (91%)	14 (8%)	2 (1%)	11 3
35	g	174/177 (98%)	160 (92%)	10 (6%)	4 (2%)	5 1
36	h	39/149 (26%)	33 (85%)	5 (13%)	1 (3%)	4 0
37	i	140/142 (99%)	140 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
39	k	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	18	8
40	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
41	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
42	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
43	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
44	p	115/118 (98%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
46	r	108/110 (98%)	108 (100%)	0	0	100	100
47	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
48	t	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
49	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
50	v	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
51	w	75/78 (96%)	75 (100%)	0	0	100	100
52	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
53	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
54	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5479/5913 (93%)	5237 (96%)	206 (4%)	36 (1%)	20	8

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	6	MET
7	B	62	SER
7	B	63	ARG
7	B	95	ARG
15	J	28	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	0	46/49 (94%)	45 (98%)	1 (2%)	45 32
2	1	38/38 (100%)	38 (100%)	0	100 100
3	2	51/52 (98%)	51 (100%)	0	100 100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37 22
5	4	55/62 (89%)	55 (100%)	0	100 100
7	B	186/199 (94%)	157 (84%)	29 (16%)	2 0
8	C	170/190 (90%)	167 (98%)	3 (2%)	51 40
9	D	172/173 (99%)	166 (96%)	6 (4%)	32 16
10	E	119/126 (94%)	119 (100%)	0	100 100
11	F	90/116 (78%)	89 (99%)	1 (1%)	65 57
12	G	126/147 (86%)	121 (96%)	5 (4%)	28 13
13	H	104/105 (99%)	104 (100%)	0	100 100
14	I	105/107 (98%)	98 (93%)	7 (7%)	15 4
15	J	86/90 (96%)	67 (78%)	19 (22%)	1 0
16	K	89/98 (91%)	89 (100%)	0	100 100
17	L	102/103 (99%)	93 (91%)	9 (9%)	9 1
18	M	93/96 (97%)	92 (99%)	1 (1%)	65 57
19	N	83/84 (99%)	77 (93%)	6 (7%)	13 3
20	O	76/77 (99%)	75 (99%)	1 (1%)	61 51
21	P	65/65 (100%)	65 (100%)	0	100 100
22	Q	73/78 (94%)	72 (99%)	1 (1%)	59 49
23	R	57/65 (88%)	56 (98%)	1 (2%)	51 40
24	S	72/79 (91%)	66 (92%)	6 (8%)	10 2
25	T	65/66 (98%)	62 (95%)	3 (5%)	24 9
26	U	60/61 (98%)	58 (97%)	2 (3%)	33 18
31	c	216/218 (99%)	216 (100%)	0	100 100
32	d	163/163 (100%)	161 (99%)	2 (1%)	63 55
33	e	165/165 (100%)	163 (99%)	2 (1%)	63 55
34	f	148/150 (99%)	125 (84%)	23 (16%)	2 0
35	g	137/138 (99%)	129 (94%)	8 (6%)	18 6
36	h	32/114 (28%)	26 (81%)	6 (19%)	1 0
37	i	116/116 (100%)	116 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	j	104/104 (100%)	104 (100%)	0	100 100
39	k	103/103 (100%)	102 (99%)	1 (1%)	68 60
40	l	107/107 (100%)	107 (100%)	0	100 100
41	m	98/103 (95%)	97 (99%)	1 (1%)	68 60
42	n	86/87 (99%)	81 (94%)	5 (6%)	18 6
43	o	99/100 (99%)	97 (98%)	2 (2%)	48 36
44	p	89/90 (99%)	89 (100%)	0	100 100
45	q	84/84 (100%)	83 (99%)	1 (1%)	63 55
46	r	93/93 (100%)	93 (100%)	0	100 100
47	s	80/84 (95%)	77 (96%)	3 (4%)	29 14
48	t	83/85 (98%)	81 (98%)	2 (2%)	43 28
49	u	78/78 (100%)	77 (99%)	1 (1%)	61 51
50	v	57/63 (90%)	56 (98%)	1 (2%)	51 40
51	w	67/68 (98%)	67 (100%)	0	100 100
52	x	54/55 (98%)	54 (100%)	0	100 100
53	y	48/49 (98%)	48 (100%)	0	100 100
54	z	47/48 (98%)	45 (96%)	2 (4%)	26 11
All	All	4571/4825 (95%)	4409 (96%)	162 (4%)	32 16

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	f	111	ILE
39	k	54	GLN
34	f	133	ARG
35	g	18	LYS
43	o	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
49	u	49	ASN
52	x	15	ASN
25	T	48	GLN
25	T	3	ASN

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Mol	Chain	Res	Type
52	x	25	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	8/27 (29%)	3 (37%)	0
28	Z	74/76 (97%)	19 (25%)	0
29	a	2762/2937 (94%)	339 (12%)	0
30	b	118/120 (98%)	12 (10%)	0
6	A	1516/1542 (98%)	222 (14%)	20 (1%)
All	All	4478/4702 (95%)	595 (13%)	20 (0%)

5 of 595 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	5	U
6	A	9	G
6	A	32	A
6	A	36	C

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	622	A
6	A	1035	A
6	A	1384	C
6	A	1124	G
6	A	360	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	PSU	a	1911	29	18,21,22	0.99	1 (5%)	21,30,33	0.73	0
29	H2U	a	2449	29	18,21,22	0.60	0	19,30,33	0.75	1 (5%)
29	5MU	a	1939	29	19,22,23	0.42	0	27,32,35	0.78	0
29	2MG	a	2445	29	23,26,27	1.49	5 (21%)	33,38,41	2.35	8 (24%)
29	PSU	a	2605	29	18,21,22	0.99	1 (5%)	21,30,33	0.84	0
29	PSU	a	955	29	18,21,22	1.03	1 (5%)	21,30,33	0.85	0
6	2MG	A	966	6	23,26,27	0.39	0	33,38,41	0.41	0
29	PSU	a	2457	29	18,21,22	1.05	1 (5%)	21,30,33	0.78	0
40	4D4	l	81	40	9,11,12	1.97	2 (22%)	7,13,15	1.10	1 (14%)
16	IAS	K	119	16	6,7,8	1.40	1 (16%)	3,8,10	0.92	0
29	OMC	a	2498	29,55	19,22,23	0.82	0	25,31,34	1.04	2 (8%)
6	PSU	A	516	55,6	18,21,22	0.97	1 (5%)	21,30,33	1.09	1 (4%)
28	8AN	Z	77	28	21,24,25	1.13	1 (4%)	26,35,38	0.65	1 (3%)
29	PSU	a	2504	29	18,21,22	1.49	4 (22%)	21,30,33	2.05	5 (23%)
40	MS6	l	82	40	5,7,8	0.20	0	2,7,9	0.19	0
29	5MU	a	747	29	19,22,23	0.35	0	27,32,35	0.54	0
29	OMG	a	2251	29,28	23,26,27	0.32	0	32,38,41	0.42	0
29	G7M	a	2069	29	23,26,27	1.49	3 (13%)	34,39,42	1.76	6 (17%)
6	UR3	A	1498	6	19,22,23	0.38	0	26,32,35	1.01	2 (7%)
29	6MZ	a	1618	29	22,25,26	0.29	0	29,36,39	0.62	0
6	2MG	A	1207	6	23,26,27	0.35	0	33,38,41	0.45	0
6	2MG	A	1516	6	23,26,27	0.38	0	33,38,41	0.52	0
29	3TD	a	1915	29	19,22,23	1.63	4 (21%)	23,32,35	2.22	4 (17%)
29	5MC	a	1962	29	19,22,23	0.74	1 (5%)	26,32,35	0.52	0
17	D2T	L	89	17	8,9,10	3.94	3 (37%)	6,11,13	1.63	2 (33%)
29	PSU	a	1917	29	18,21,22	1.01	1 (5%)	21,30,33	0.72	0
29	6MZ	a	2030	29	22,25,26	0.31	0	29,36,39	0.65	0
29	OMU	a	2552	29	19,22,23	1.36	3 (15%)	25,31,34	2.02	7 (28%)
29	PSU	a	2580	29	18,21,22	1.06	2 (11%)	21,30,33	0.89	1 (4%)
6	4OC	A	1402	6	20,23,24	0.41	0	25,32,35	0.50	0
6	5MC	A	967	6	19,22,23	0.83	1 (5%)	26,32,35	0.52	0
32	MEQ	d	150	32	8,9,10	0.46	0	5,10,12	0.33	0
29	PSU	a	2604	29	18,21,22	1.02	1 (5%)	21,30,33	0.82	0
29	PSU	a	746	29,55	18,21,22	1.41	3 (16%)	21,30,33	1.95	5 (23%)
29	2MG	a	1835	29	23,26,27	1.34	4 (17%)	33,38,41	2.50	9 (27%)
29	2MA	a	2503	29,55	22,25,26	1.52	4 (18%)	32,37,40	2.36	7 (21%)
6	5MC	A	1407	6	19,22,23	0.86	1 (5%)	26,32,35	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MA6	A	1518	6	23,26,27	1.42	5 (21%)	33,38,41	2.11	11 (33%)
29	1MG	a	745	29	23,26,27	1.25	4 (17%)	33,39,42	1.97	9 (27%)
6	MA6	A	1519	6	23,26,27	1.48	5 (21%)	33,38,41	2.24	10 (30%)
6	G7M	A	527	6	23,26,27	1.53	4 (17%)	34,39,42	1.74	5 (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
29	PSU	a	1911	29	-	0/7/25/26	0/2/2/2
29	H2U	a	2449	29	-	0/7/38/39	0/2/2/2
29	5MU	a	1939	29	-	1/7/25/26	0/2/2/2
29	2MG	a	2445	29	-	1/9/27/28	0/3/3/3
29	PSU	a	2605	29	-	0/7/25/26	0/2/2/2
29	PSU	a	955	29	-	0/7/25/26	0/2/2/2
6	2MG	A	966	6	-	0/9/27/28	0/3/3/3
29	PSU	a	2457	29	-	0/7/25/26	0/2/2/2
40	4D4	l	81	40	-	1/11/12/14	-
16	IAS	K	119	16	-	0/7/7/8	-
29	OMC	a	2498	29,55	-	1/9/27/28	0/2/2/2
6	PSU	A	516	55,6	-	0/7/25/26	0/2/2/2
28	8AN	Z	77	28	-	1/7/25/26	0/3/3/3
29	PSU	a	2504	29	-	1/7/25/26	0/2/2/2
40	MS6	l	82	40	-	1/4/6/8	-
29	5MU	a	747	29	-	1/7/25/26	0/2/2/2
29	OMG	a	2251	29,28	-	1/9/27/28	0/3/3/3
29	G7M	a	2069	29	-	2/7/25/26	0/3/3/3
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
29	6MZ	a	1618	29	-	0/9/27/28	0/3/3/3
6	2MG	A	1207	6	-	0/9/27/28	0/3/3/3
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
29	3TD	a	1915	29	-	2/7/25/26	0/2/2/2
29	5MC	a	1962	29	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	4/7/12/14	-
29	PSU	a	1917	29	-	0/7/25/26	0/2/2/2
29	6MZ	a	2030	29	-	2/9/27/28	0/3/3/3
29	OMU	a	2552	29	-	0/9/27/28	0/2/2/2
29	PSU	a	2580	29	-	0/7/25/26	0/2/2/2
6	4OC	A	1402	6	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
32	MEQ	d	150	32	-	2/8/9/11	-
29	PSU	a	2604	29	-	0/7/25/26	0/2/2/2
29	PSU	a	746	29,55	-	2/7/25/26	0/2/2/2
29	2MG	a	1835	29	-	0/9/27/28	0/3/3/3
29	2MA	a	2503	29,55	-	1/7/25/26	0/3/3/3
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
29	1MG	a	745	29	-	0/7/25/26	0/3/3/3
6	MA6	A	1519	6	-	2/11/29/30	0/3/3/3
6	G7M	A	527	6	-	1/7/25/26	0/3/3/3

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	89	D2T	CB-CA	9.42	1.57	1.54
6	A	527	G7M	C5-N7	-5.01	1.33	1.39
28	Z	77	8AN	C3'-N3'	-4.85	1.40	1.47
29	a	2069	G7M	C5-N7	-4.65	1.33	1.39
29	a	2503	2MA	C5-C4	4.38	1.46	1.39

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	1835	2MG	C2-N3-C4	8.59	122.75	112.00
29	a	1915	3TD	N1-C2-N3	8.54	122.34	116.13
29	a	2503	2MA	C5-C4-N3	-8.10	118.65	127.18
29	a	2445	2MG	C2-N3-C4	7.87	121.85	112.00
29	a	1835	2MG	C5-C4-N3	-6.95	117.33	128.39

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
17	L	89	D2T	SB-CB-CG-OD2
28	Z	77	8AN	C4'-C5'-O5'-P
29	a	2498	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	516	PSU	1	0
28	Z	77	8AN	5	0
29	a	2251	OMG	1	0
29	a	2069	G7M	1	0
6	A	1498	UR3	1	0
6	A	1516	2MG	1	0
29	a	1915	3TD	2	0
29	a	2030	6MZ	3	0
29	a	2552	OMU	1	0
6	A	967	5MC	1	0
6	A	1518	MA6	1	0
6	A	1519	MA6	3	0
6	A	527	G7M	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 285 ligands modelled in this entry, 284 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	FME	a	4196	-	8,9,10	0.78	0	8,9,11	1.10	1 (12%)

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
56	FME	a	4196	-	-	2/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	a	4196	FME	O-C-CA	-2.09	119.40	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	a	4196	FME	O1-CN-N-CA
56	a	4196	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	a	4196	FME	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	Z	1
29	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	5:G	O3'	6:G	P	3.17
1	a	1914:C	O3'	1915:3TD	P	2.35

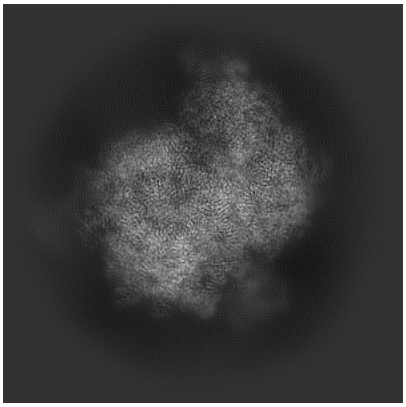
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29449. These allow visual inspection of the internal detail of the map and identification of artifacts.

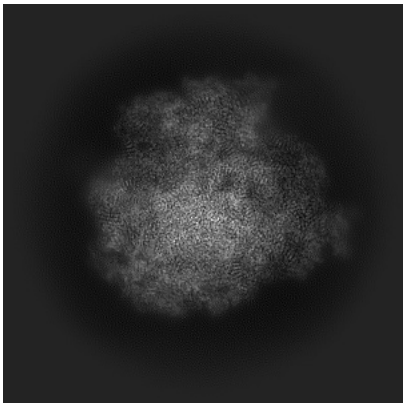
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

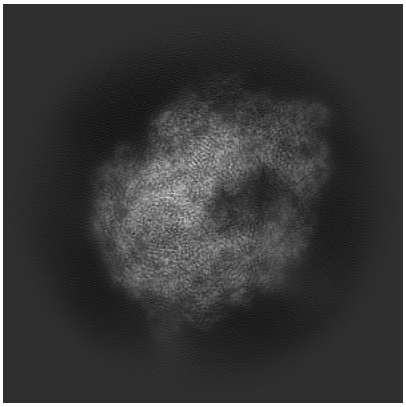
6.1.1 Primary map



X



Y

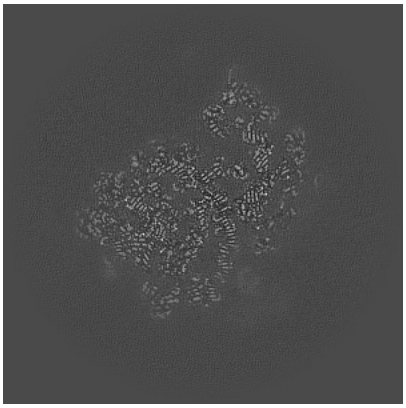


Z

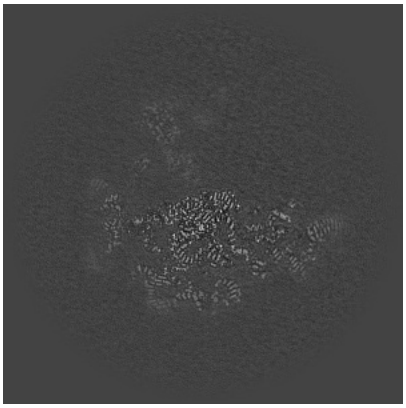
The images above show the map projected in three orthogonal directions.

6.2 Central slices

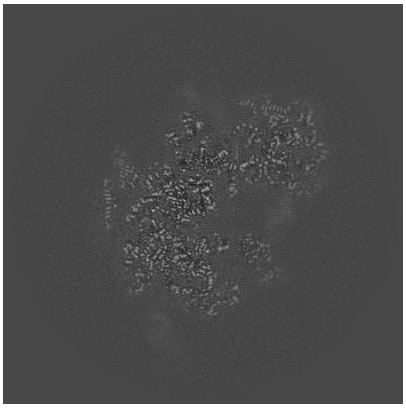
6.2.1 Primary map



X Index: 224



Y Index: 224

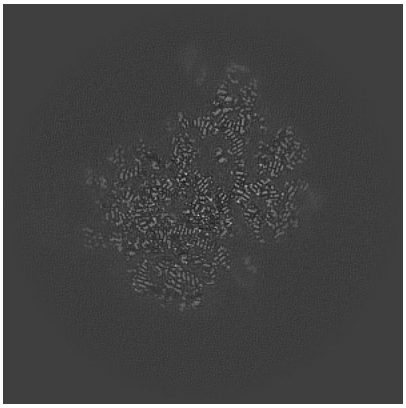


Z Index: 224

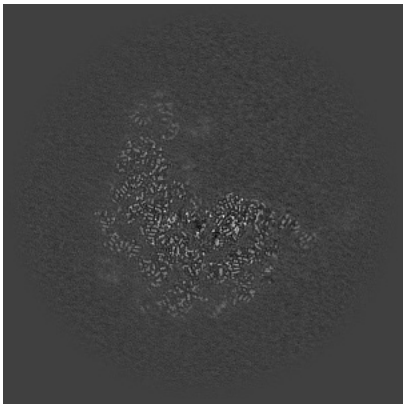
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

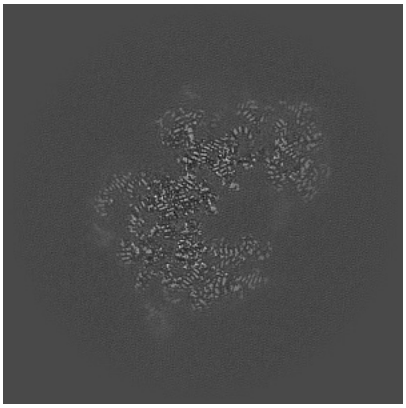
6.3.1 Primary map



X Index: 208



Y Index: 204

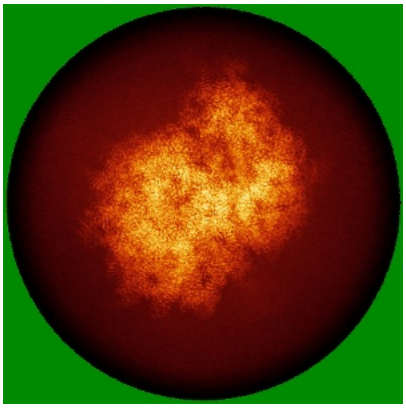


Z Index: 233

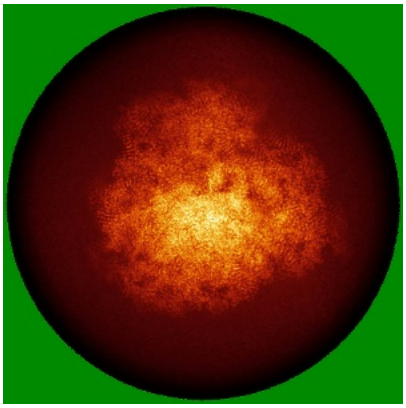
The images above show the largest variance slices of the map in three orthogonal directions.

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

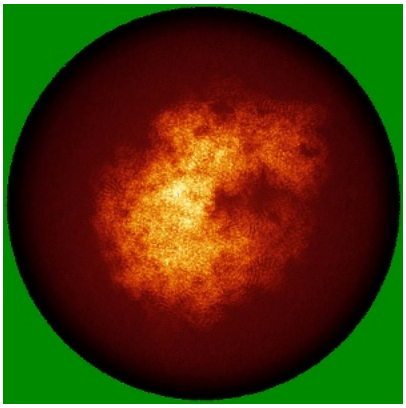
6.4.1 Primary map



X



Y

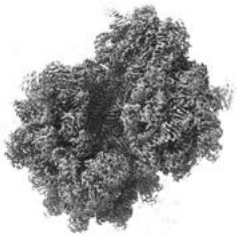


Z

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

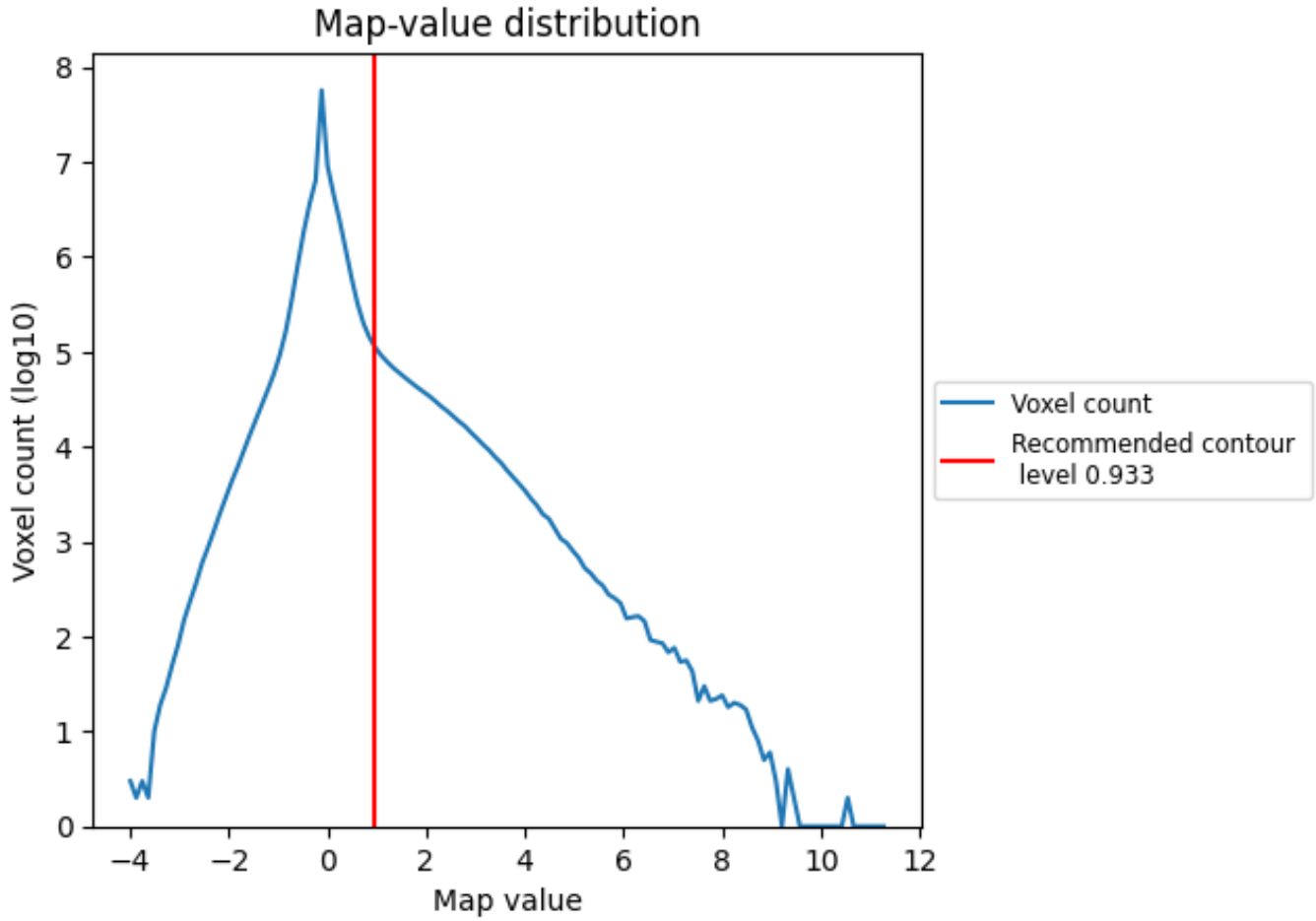
6.6 Mask visualisation (i)

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

7 Map analysis

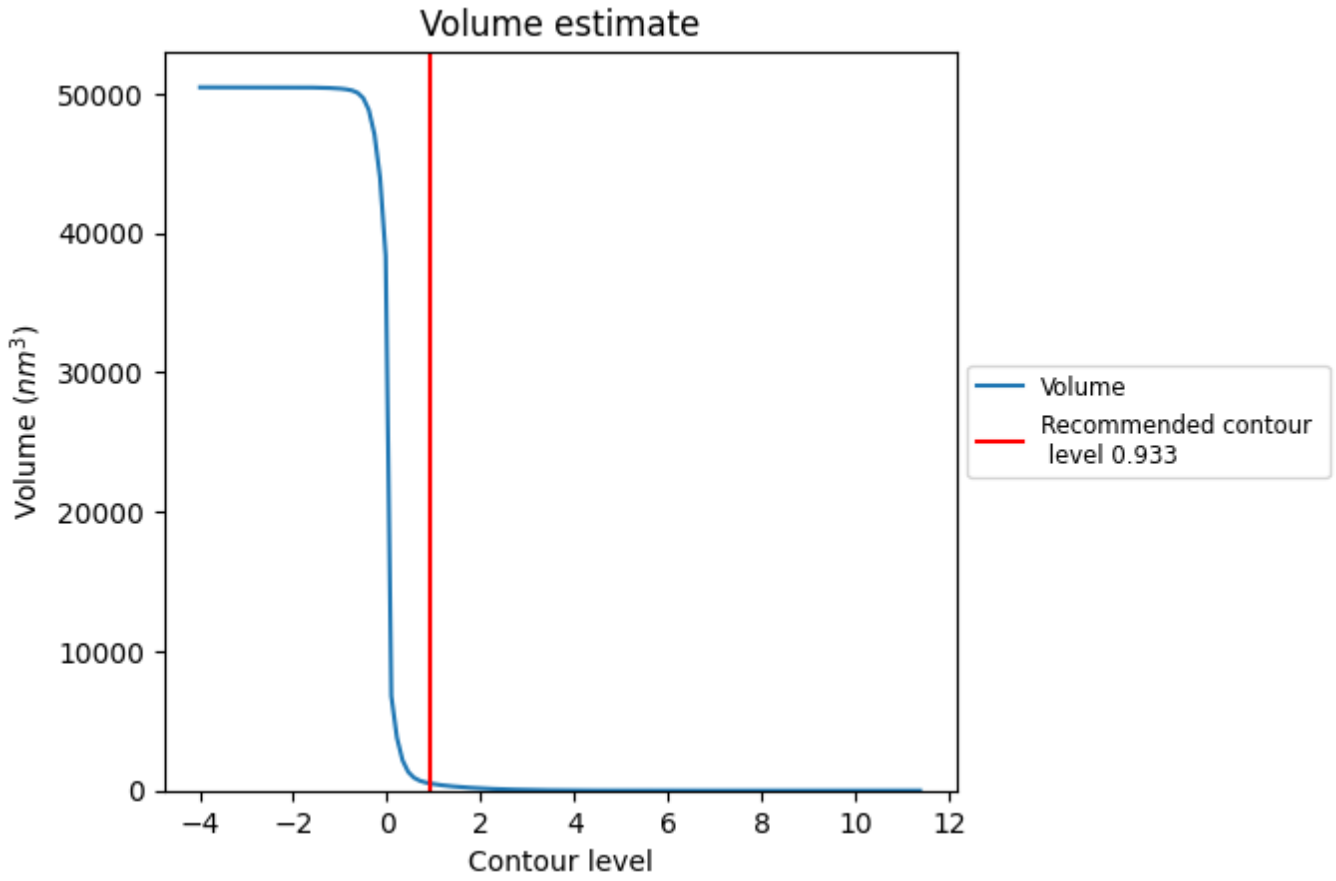
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

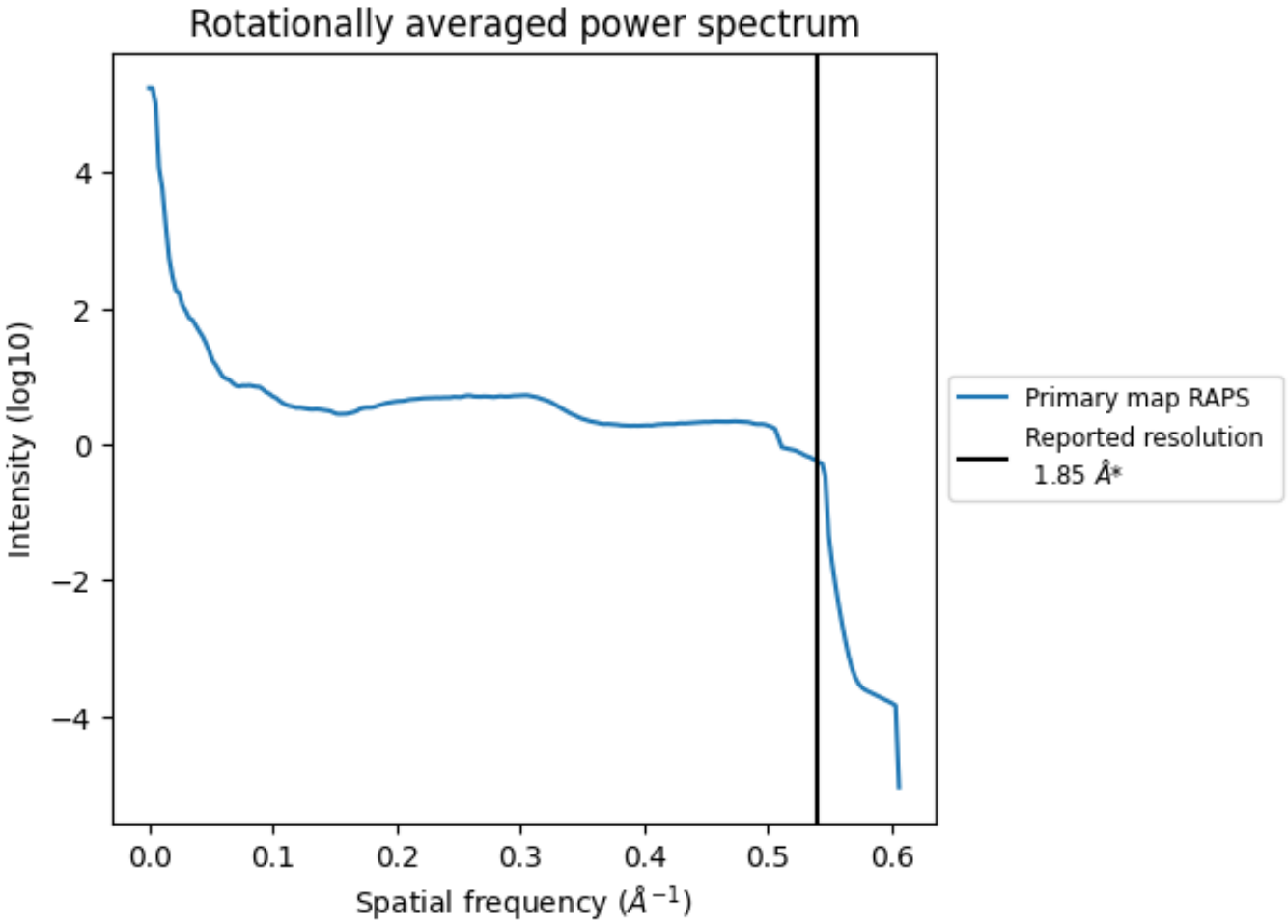
7.2 Volume estimate (i)



The volume at the recommended contour level is 505 nm^3; this corresponds to an approximate mass of 456 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 0.541 Å^{-1}

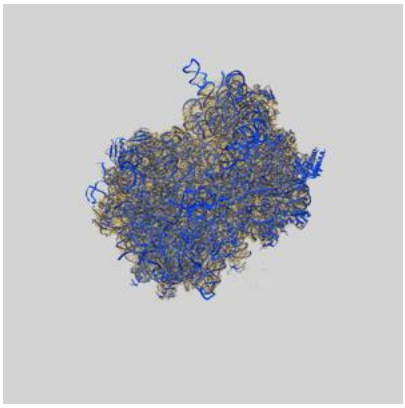
8 Fourier-Shell correlation (i)

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

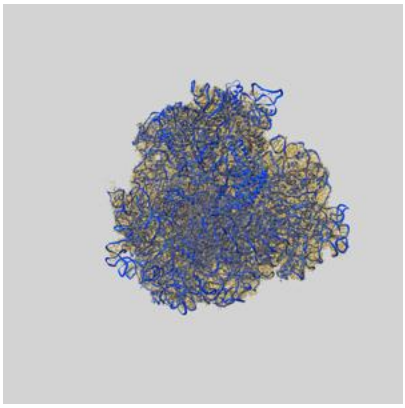
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29449 and PDB model 8FTO. Per-residue inclusion information can be found in section 3 on page 18.

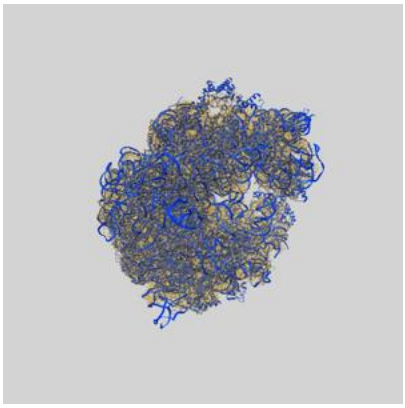
9.1 Map-model overlay



X



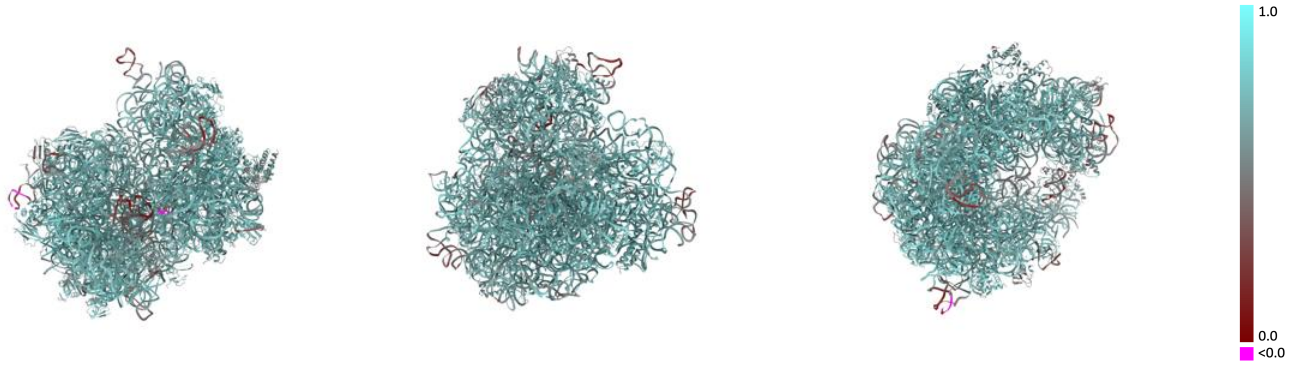
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.933 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.

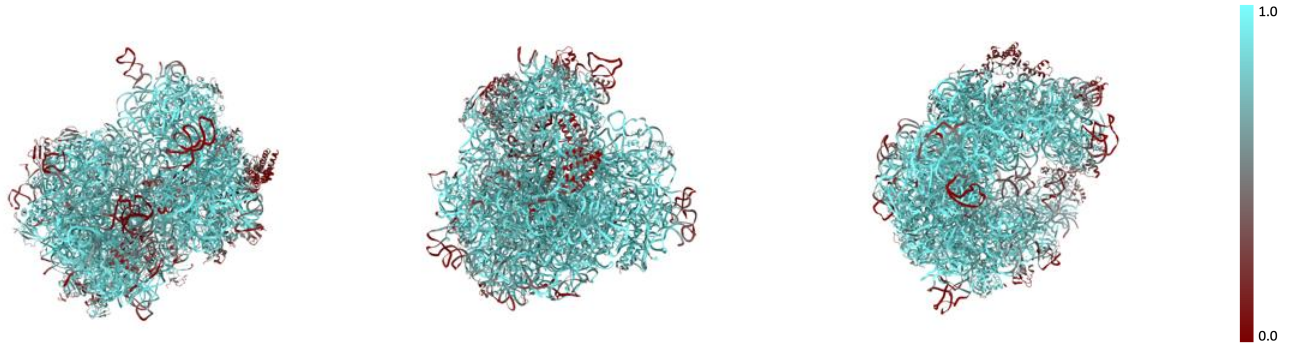
9.2 Q-score mapped to coordinate model (i)



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.

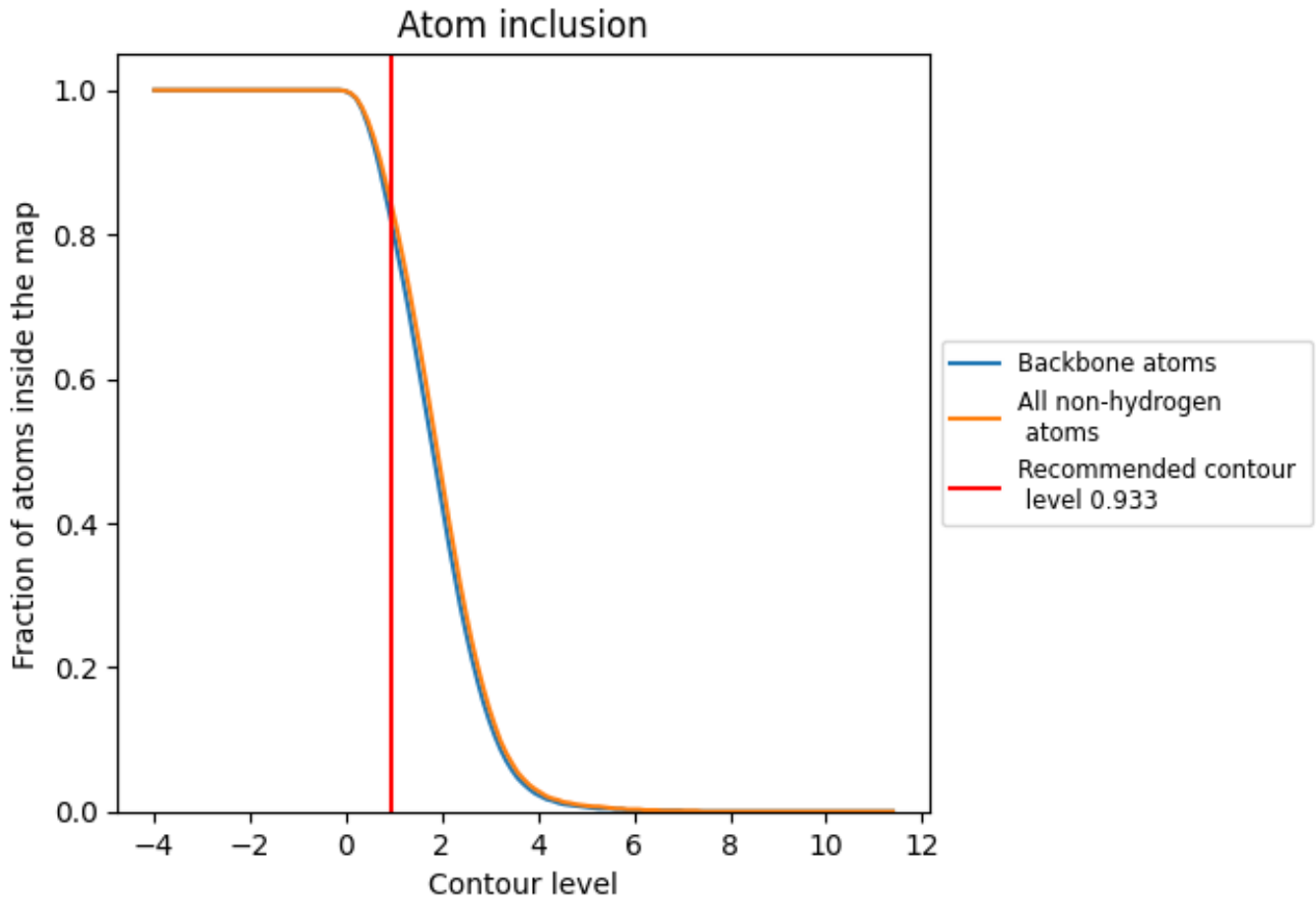
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.933).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.933) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.7220
0	0.8390	0.7580
1	0.9660	0.8080
2	0.9550	0.8060
3	0.9070	0.7630
4	0.0190	0.3530
A	0.8900	0.7120
B	0.2910	0.6140
C	0.7710	0.7130
D	0.8040	0.7240
E	0.8820	0.7480
F	0.7090	0.6820
G	0.6290	0.6690
H	0.8920	0.7460
I	0.6930	0.7000
J	0.5230	0.6490
K	0.8050	0.7110
L	0.8890	0.7340
M	0.6720	0.6880
N	0.8240	0.7230
O	0.8590	0.7340
P	0.8730	0.7320
Q	0.8060	0.6960
R	0.7000	0.6570
S	0.6860	0.6810
T	0.8850	0.7340
U	0.3830	0.5970
X	0.4550	0.5630
Z	0.5420	0.5700
a	0.8970	0.7360
b	0.7800	0.6930
c	0.9610	0.7940
d	0.9270	0.7840
e	0.7320	0.7320
f	0.3950	0.5940



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Chain	Atom inclusion	Q-score
g	0.4510	0.5970
h	0.4530	0.6330
i	0.9090	0.7760
j	0.9330	0.7840
k	0.8740	0.7730
l	0.8910	0.7770
m	0.9840	0.8020
n	0.7090	0.7110
o	0.8990	0.7660
p	0.9470	0.7960
q	0.7990	0.7480
r	0.8980	0.7810
s	0.7840	0.7240
t	0.6390	0.6800
u	0.7030	0.7110
v	0.9040	0.7870
w	0.8780	0.7680
x	0.5810	0.6670
y	0.8720	0.7620
z	0.8880	0.7700