wwPDB EM Validation Summary Report (i)

Sep 29, 2024 – 10:03 AM EDT

PDB ID	:	3JCJ
EMDB ID	:	EMD-6559
Title	:	Structures of ribosome-bound initiation factor 2 reveal the mechanism of subunit association
Authors	:	Sprink, T.; Ramrath, D.J.F.; Yamamoto, H.; Yamamoto, K.; Loerke, J.; Ismer, J.; Hildebrand, P.W.; Scheerer, P.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on	:	2015-12-18
Resolution	:	3.70 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:

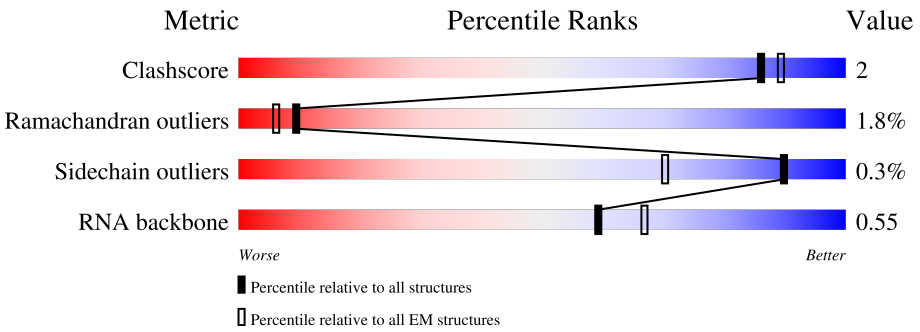
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	118	• 91% 9%
2	1	75	27% 69% • 27%
3	2	71	49% 69% • 28%
4	3	87	20% 93% 5% •
5	4	52	6% 6% 88%
6	A	2904	6% 86% 12% •
7	B	273	11% 94% 5% •

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Mol	Chain	Length	Quality of chain
8	C	209	10% 91% 9%
9	D	201	30% 97%
10	E	179	63% 97%
11	F	177	20% 97%
12	G	149	25% 32% 66%
13	H	142	99% 97%
14	I	142	13% 95% 5%
15	J	123	17% 89% 11%
16	K	144	20% 96%
17	L	136	12% 96%
18	M	127	5% 94% 6%
19	N	117	20% 94% 5%
20	O	115	20% 95%
21	P	118	10% 97%
22	Q	103	20% 97%
23	R	110	10% 96%
24	S	100	22% 87% 6% 7%
25	T	104	25% 93% 5%
26	U	94	10% 100%
27	V	85	31% 82% 9% 7%
28	W	78	17% 96%
29	X	63	17% 98%
30	Y	59	8% 98%
31	Z	57	11% 95%
32	a	55	31% 89% 9%

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Mol	Chain	Length	Quality of chain
33	b	46	7% 100%
34	c	65	6% 97%
35	d	38	11% 95% 5%
36	e	165	69% 68% 29%
37	f	890	19% 57% 43%
38	g	1542	5% 88% 12%
39	h	233	30% 87% 12%
40	j	241	58% 88% 10%
41	k	167	15% 86% 10%
42	l	206	26% 98%
43	m	179	72% 84% 16%
44	n	135	43% 72% 26%
45	o	130	47% 95%
46	p	130	15% 98%
47	q	129	40% 90% 9%
48	r	102	53% 94%
49	s	118	62% 96%
50	t	124	20% 97%
51	u	89	22% 99%
52	v	77	27% 73% 19% 8%
53	w	101	35% 93% 5%
54	x	84	20% 94% 5%
55	y	82	15% 98%
56	z	92	54% 86% 14%

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 148348 atoms, of which 1 is hydrogen and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	0	118	2529	1126	464	821	118	0	0

- Molecule 2 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	55	455	288	86	81	0	0

- Molecule 3 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	51	425	265	86	73	1	0	0

- Molecule 4 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	85	665	411	137	114	3	0	0

- Molecule 5 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	4	6	129	58	24	41	6	0	0

- Molecule 6 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	A	2854	61274	27334	11279	19807	2854	0	0

- Molecule 7 is a protein called 50S ribosomal protein L2.

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

- Molecule 8 is a protein called 50S ribosomal protein L3.

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

- Molecule 9 is a protein called 50S ribosomal protein L4.

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

- Molecule 10 is a protein called 50S ribosomal protein L5.

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

- Molecule 11 is a protein called 50S ribosomal protein L6.

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

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	50	384	247	68	68	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L11.

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

- Molecule 14 is a protein called 50S ribosomal protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

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

- Molecule 16 is a protein called 50S ribosomal protein L15.

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

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L17.

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

- Molecule 19 is a protein called 50S ribosomal protein L18.

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

- Molecule 20 is a protein called 50S ribosomal protein L19.

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

- Molecule 21 is a protein called 50S ribosomal protein L20.

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

- Molecule 22 is a protein called 50S ribosomal protein L21.

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

- Molecule 23 is a protein called 50S ribosomal protein L22.

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

- Molecule 24 is a protein called 50S ribosomal protein L23.

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

- Molecule 25 is a protein called 50S ribosomal protein L24.

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

- Molecule 26 is a protein called 50S ribosomal protein L25.

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

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	V	79	596	367	120	108	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	e	117	884	559	157	163	5	0	0

- Molecule 37 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	f	509	3847	2409	675	748	15	0	0

- Molecule 38 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	g	1539	33015	14725	6052	10699	1539	0	0

- Molecule 39 is a protein called 30S ribosomal protein S3.

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

- Molecule 40 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	218	1704	1081	305	311	7	0	0

- Molecule 41 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k	150	1105	687	211	201	6	0	0

- Molecule 42 is a protein called 30S ribosomal protein S4.

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

- Molecule 43 is a protein called 30S ribosomal protein S7.

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

- Molecule 44 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n	100	817	515	148	148	6	0	0

- Molecule 45 is a protein called 30S ribosomal protein S9.

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

- Molecule 46 is a protein called 30S ribosomal protein S8.

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

- Molecule 47 is a protein called 30S ribosomal protein S11.

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

- Molecule 48 is a protein called 30S ribosomal protein S10.

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

- Molecule 49 is a protein called 30S ribosomal protein S13.

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

- Molecule 50 is a protein called 30S ribosomal protein S12.

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

- Molecule 51 is a protein called 30S ribosomal protein S15.

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

- Molecule 52 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
52	v	77	1643	733	297	535	77	1	0	0

- Molecule 53 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	w	96	774	483	160	128	3	0	0

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S16.

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

- Molecule 56 is a protein called 30S ribosomal protein S19.

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

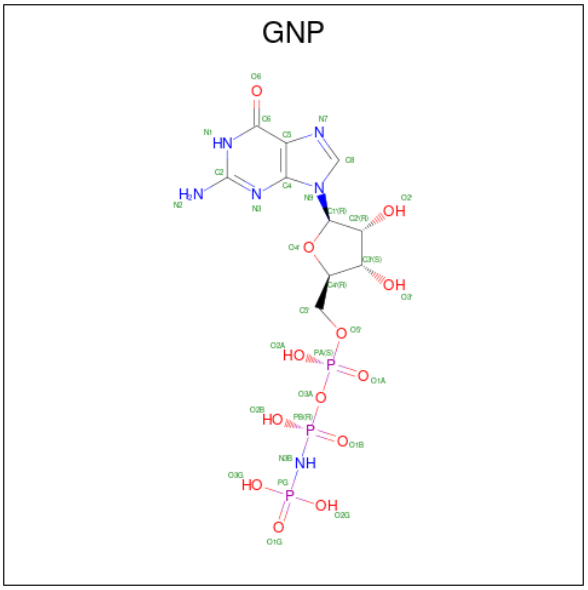
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	3	1	1	1	0
57	A	137	137	137	0
57	B	1	1	1	0
57	d	1	1	1	0
57	g	54	54	54	0
57	w	1	1	1	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

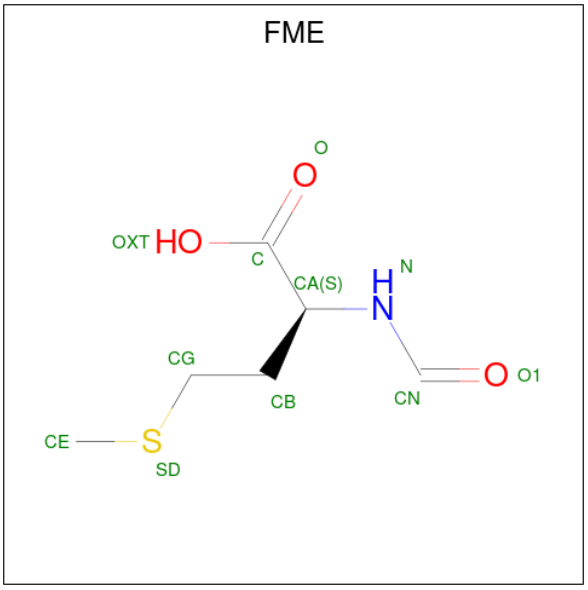
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
58	d	1	1	1	0

- Molecule 59 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	f	1	32	10	6	13	3	0

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



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
60	v	1	10	6	1	1	1	1	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
61	3	4	4	4	0
61	A	599	599	599	0
61	B	7	7	7	0
61	C	2	2	2	0
61	D	2	2	2	0
61	I	1	1	1	0
61	K	8	8	8	0
61	M	5	5	5	0

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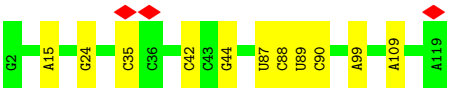
Mol	Chain	Residues	Atoms	AltConf
61	P	3	Total O 3 3	0
61	Q	3	Total O 3 3	0
61	R	3	Total O 3 3	0
61	S	2	Total O 2 2	0
61	b	1	Total O 1 1	0
61	d	3	Total O 3 3	0
61	g	189	Total O 189 189	0
61	q	1	Total O 1 1	0
61	t	2	Total O 2 2	0
61	w	2	Total O 2 2	0

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.

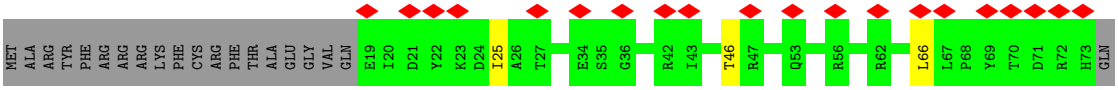
- Molecule 1: 5S ribosomal RNA

Chain 0:



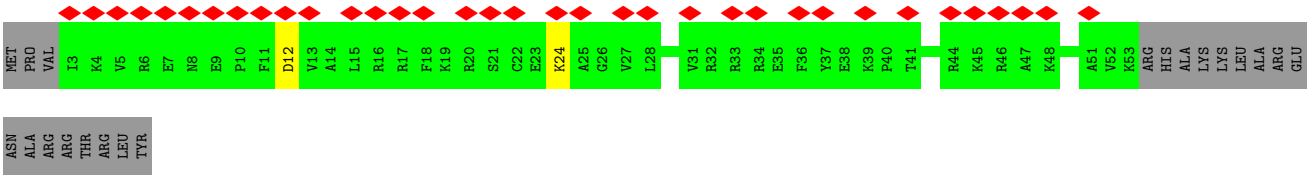
- Molecule 2: 30S ribosomal protein S18

Chain 1:



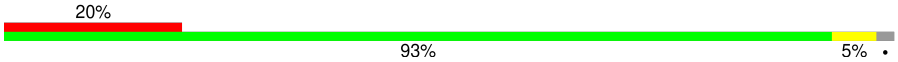
- Molecule 3: 30S ribosomal protein S21

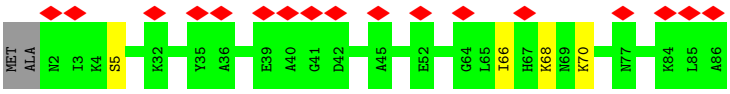
Chain 2:



- Molecule 4: 30S ribosomal protein S20

Chain 3:



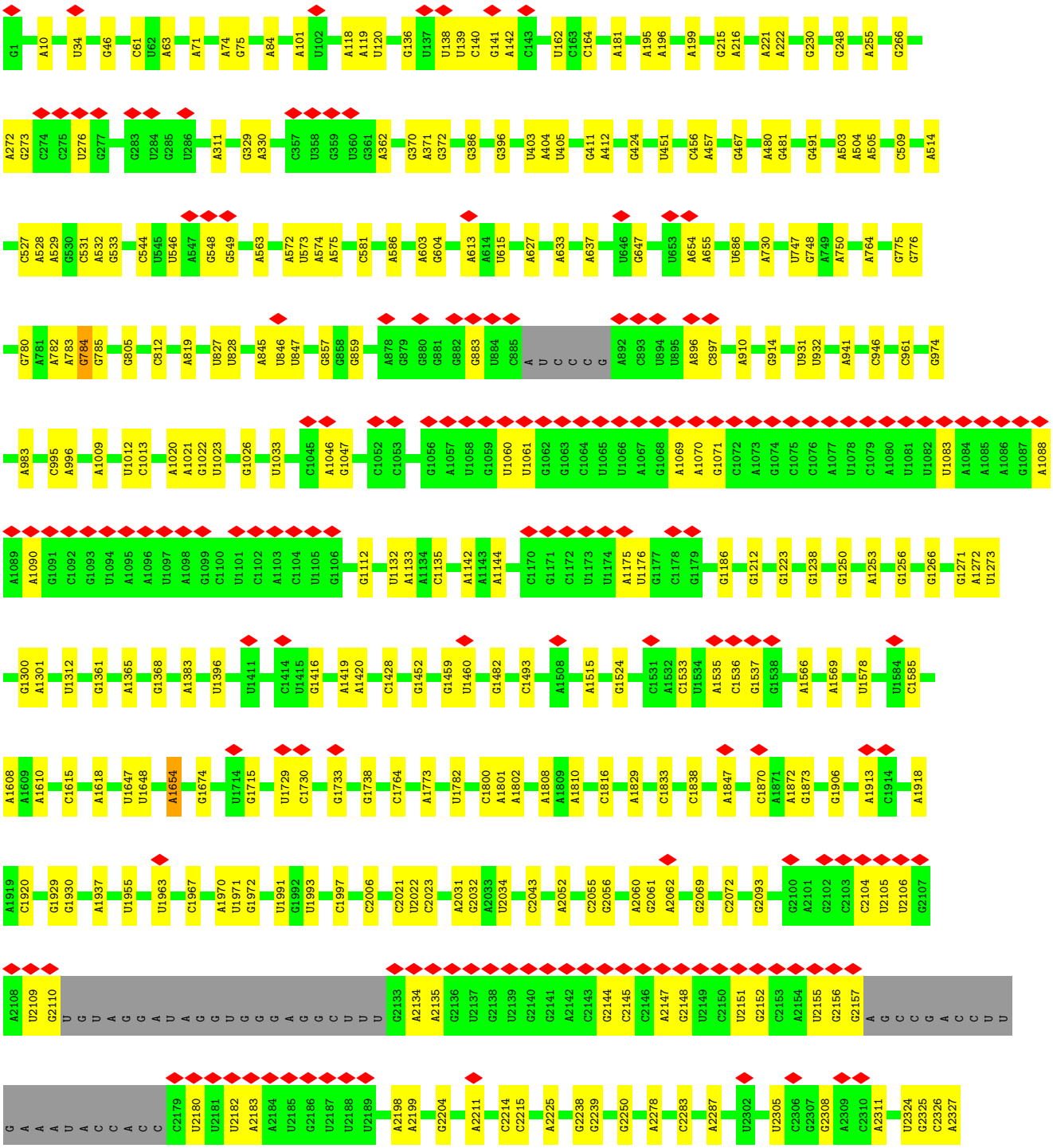


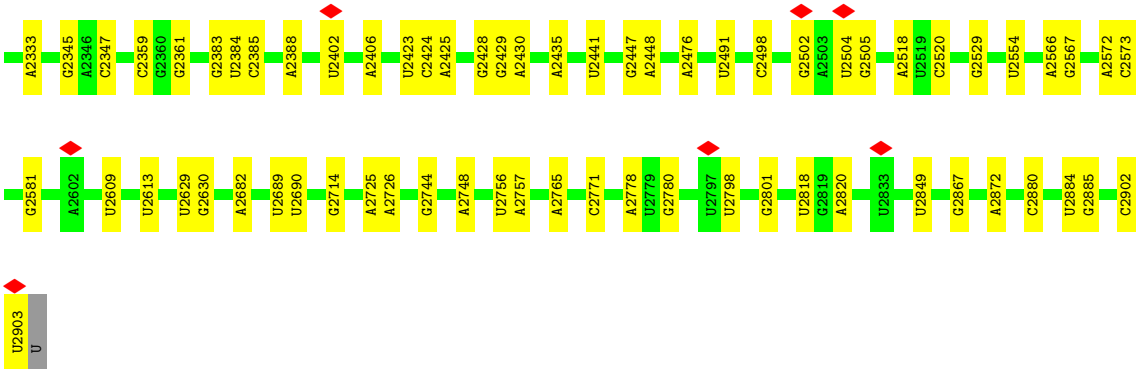
- Molecule 5: messenger RNA

Chain 4:

• Molecule 6: 23S ribosomal RNA

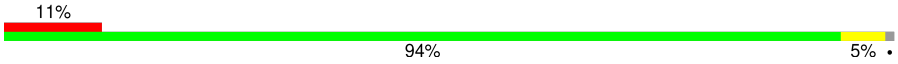
Chain A:

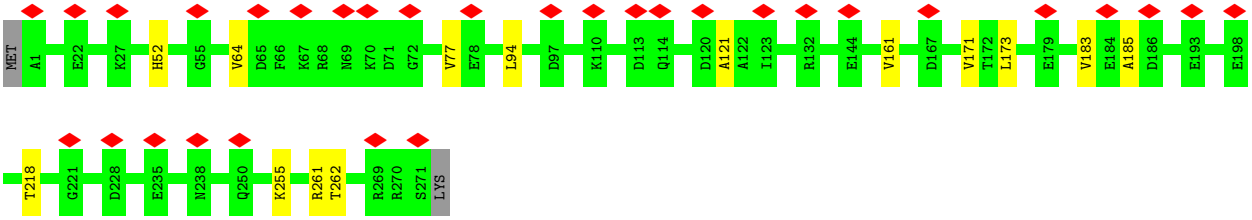




- Molecule 7: 50S ribosomal protein L2

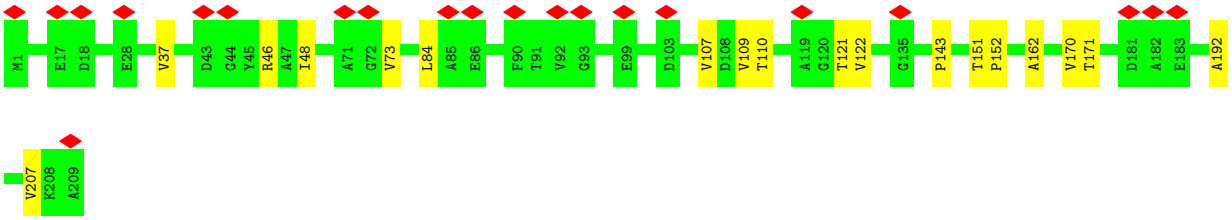
Chain B:





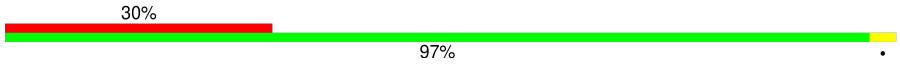
- Molecule 8: 50S ribosomal protein L3

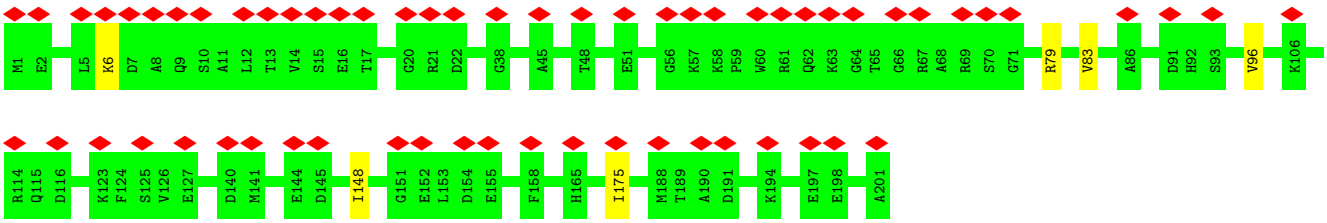
Chain C:



- Molecule 9: 50S ribosomal protein L4

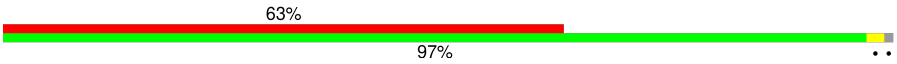
Chain D:

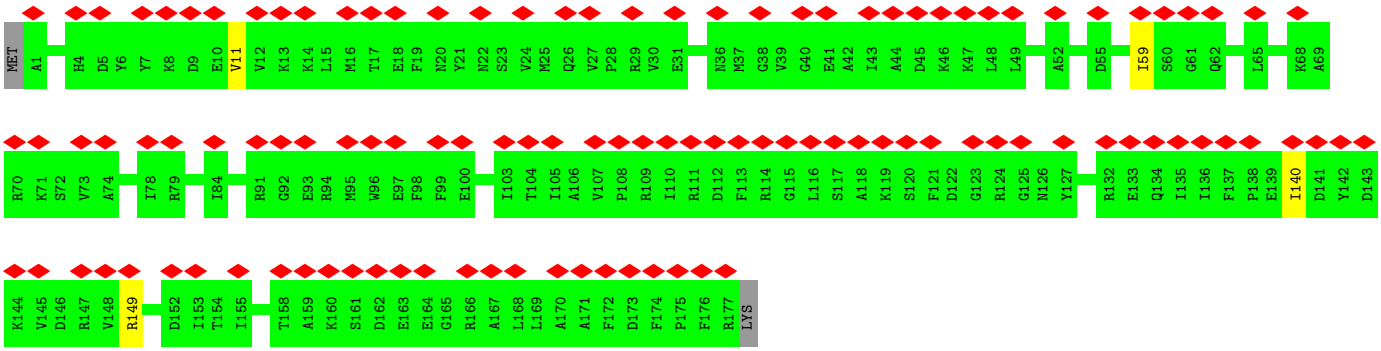




- Molecule 10: 50S ribosomal protein L5

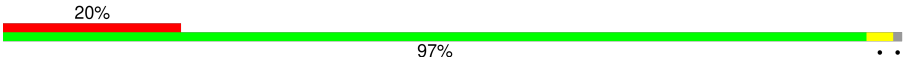
Chain E:

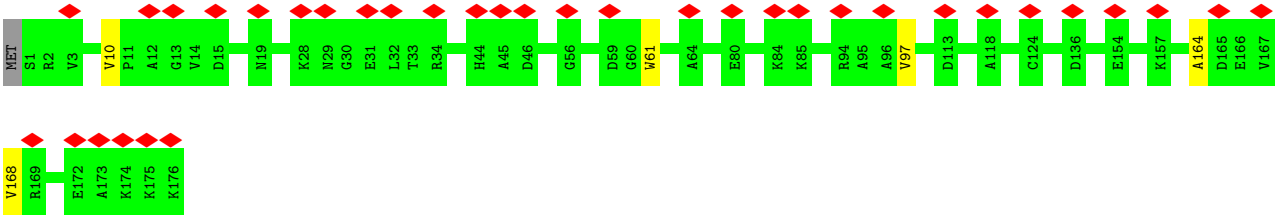




- Molecule 11: 50S ribosomal protein L6

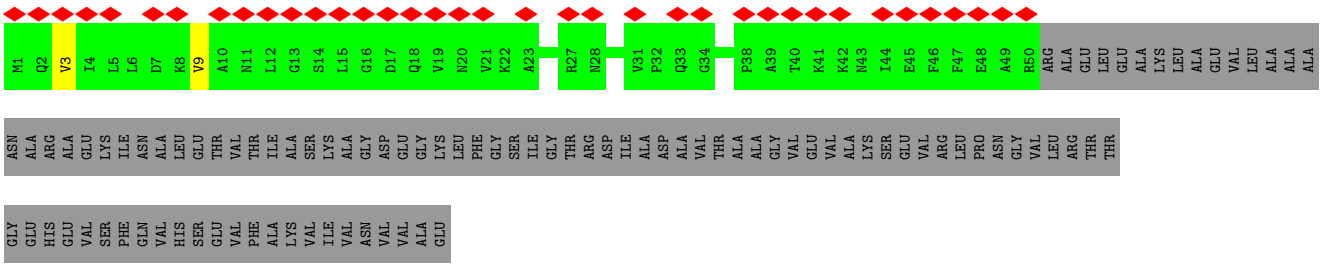
Chain F:





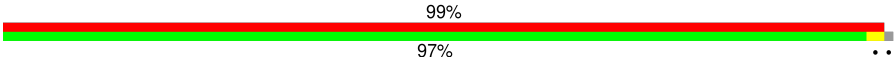
- Molecule 12: 50S ribosomal protein L9

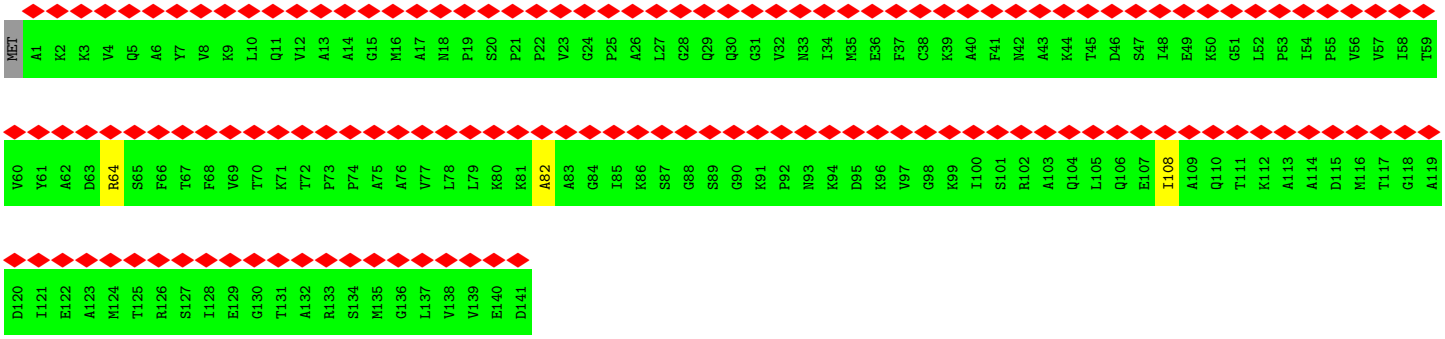
Chain G:



- Molecule 13: 50S ribosomal protein L11

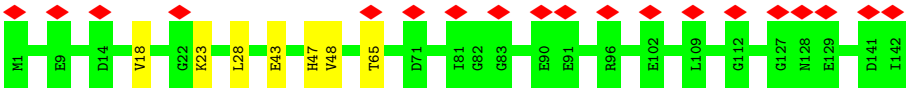
Chain H:





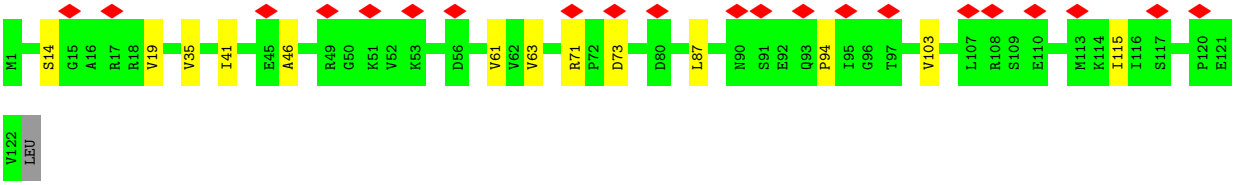
- Molecule 14: 50S ribosomal protein L13

Chain I: 13% 95% 5%



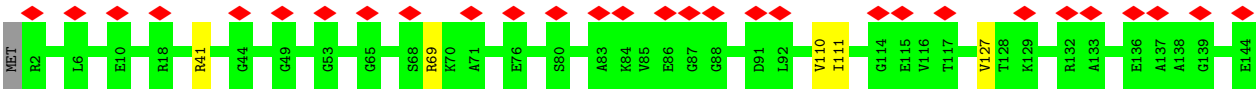
• Molecule 15: 50S ribosomal protein L14

Chain J: 17% 89% 11%



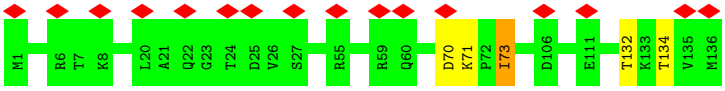
• Molecule 16: 50S ribosomal protein L15

Chain K: 20% 96%



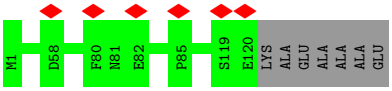
• Molecule 17: 50S ribosomal protein L16

Chain L: 12% 96%



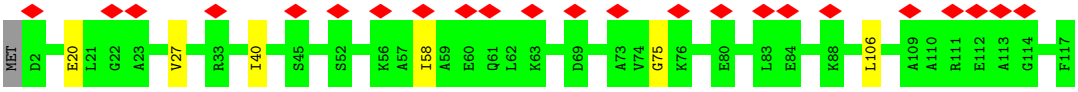
• Molecule 18: 50S ribosomal protein L17

Chain M: 5% 94% 6%



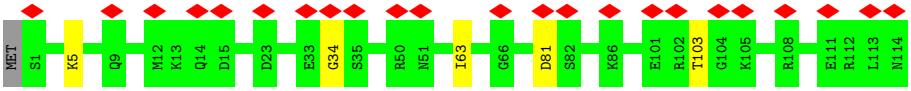
• Molecule 19: 50S ribosomal protein L18

Chain N: 20% 94% 5%



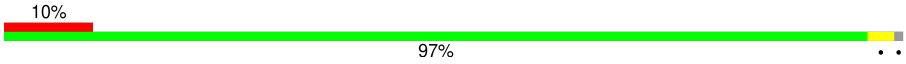
• Molecule 20: 50S ribosomal protein L19

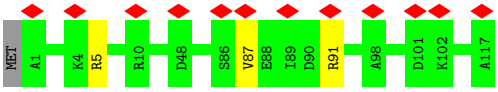
Chain O: 20% 95%



• Molecule 21: 50S ribosomal protein L20

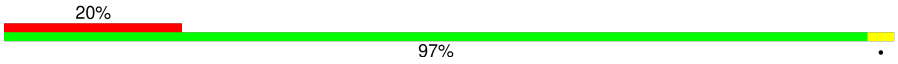
Chain P:

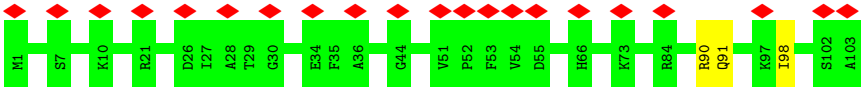




• Molecule 22: 50S ribosomal protein L21

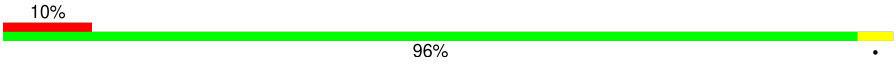
Chain Q:

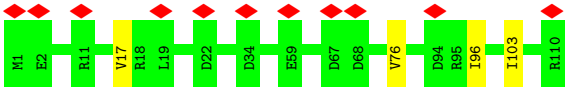




• Molecule 23: 50S ribosomal protein L22

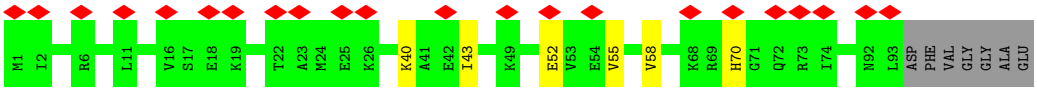
Chain R:





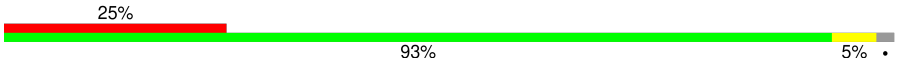
• Molecule 24: 50S ribosomal protein L23

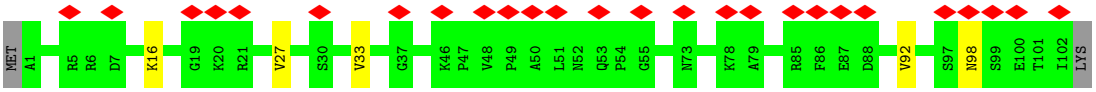
Chain S:



• Molecule 25: 50S ribosomal protein L24

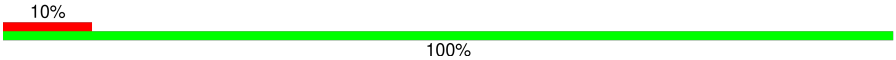
Chain T:

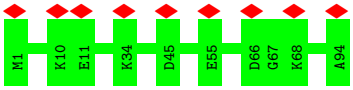




• Molecule 26: 50S ribosomal protein L25

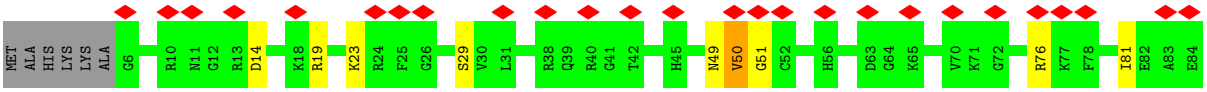
Chain U:



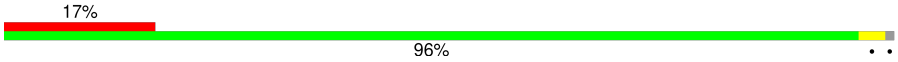


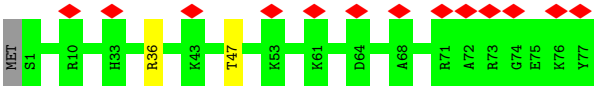
• Molecule 27: 50S ribosomal protein L27

Chain V:

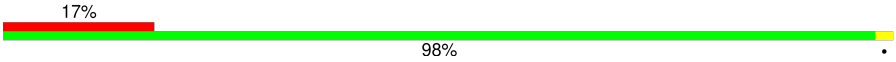


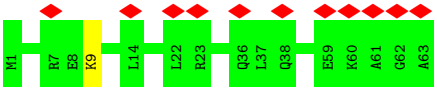
- Molecule 28: 50S ribosomal protein L28

Chain W: 

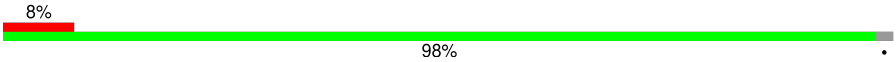


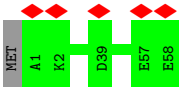
- Molecule 29: 50S ribosomal protein L29

Chain X: 

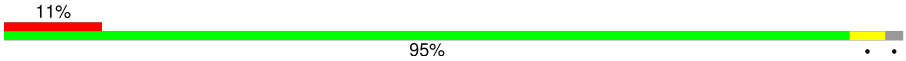


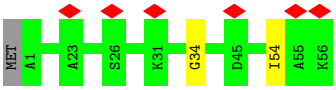
- Molecule 30: 50S ribosomal protein L30

Chain Y: 



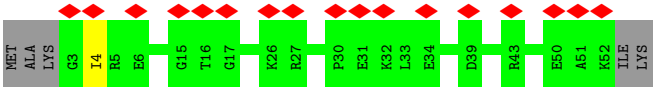
- Molecule 31: 50S ribosomal protein L32

Chain Z: 



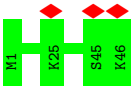
- Molecule 32: 50S ribosomal protein L33

Chain a:



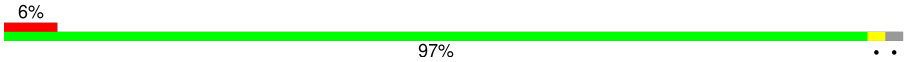
- Molecule 33: 50S ribosomal protein L34

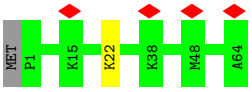
Chain b:



- Molecule 34: 50S ribosomal protein L35

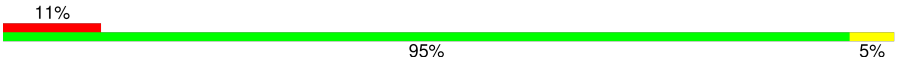
Chain c:

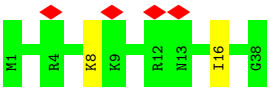




- Molecule 35: 50S ribosomal protein L36

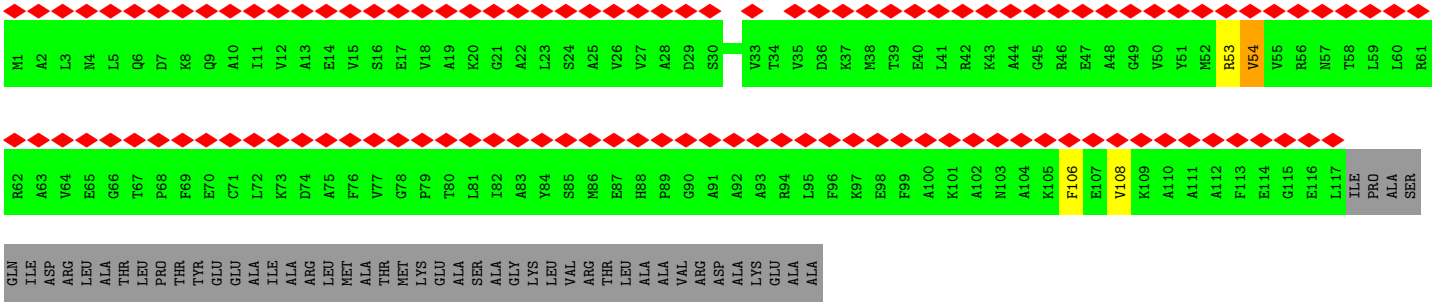
Chain d:





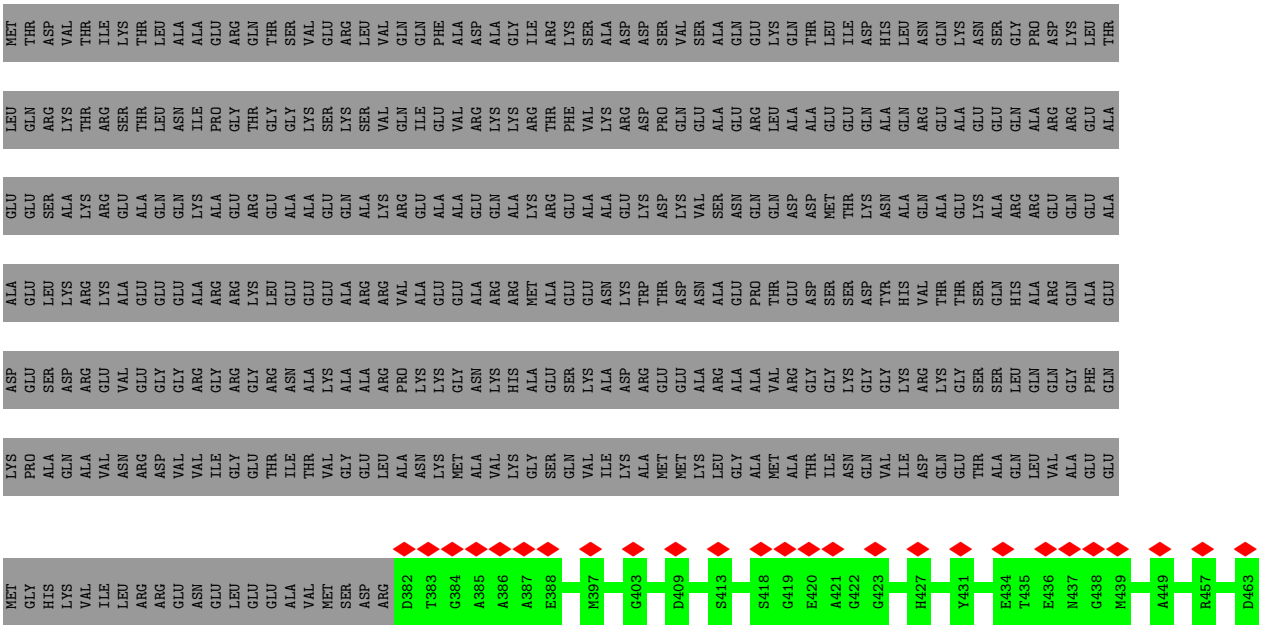
- Molecule 36: 50S ribosomal protein L10

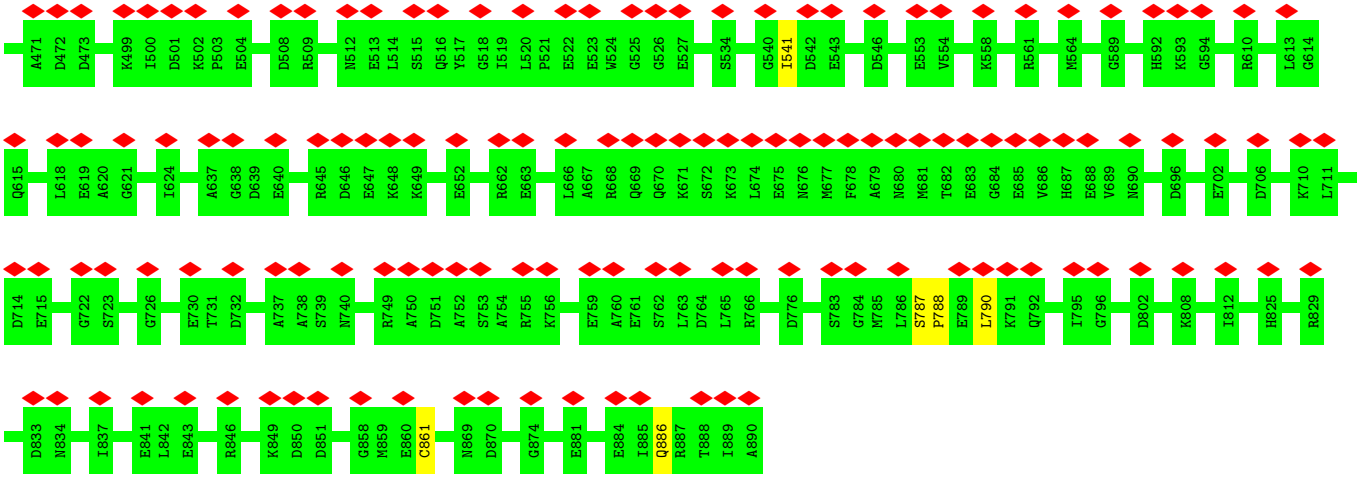
Chain e:



- Molecule 37: Translation initiation factor IF-2

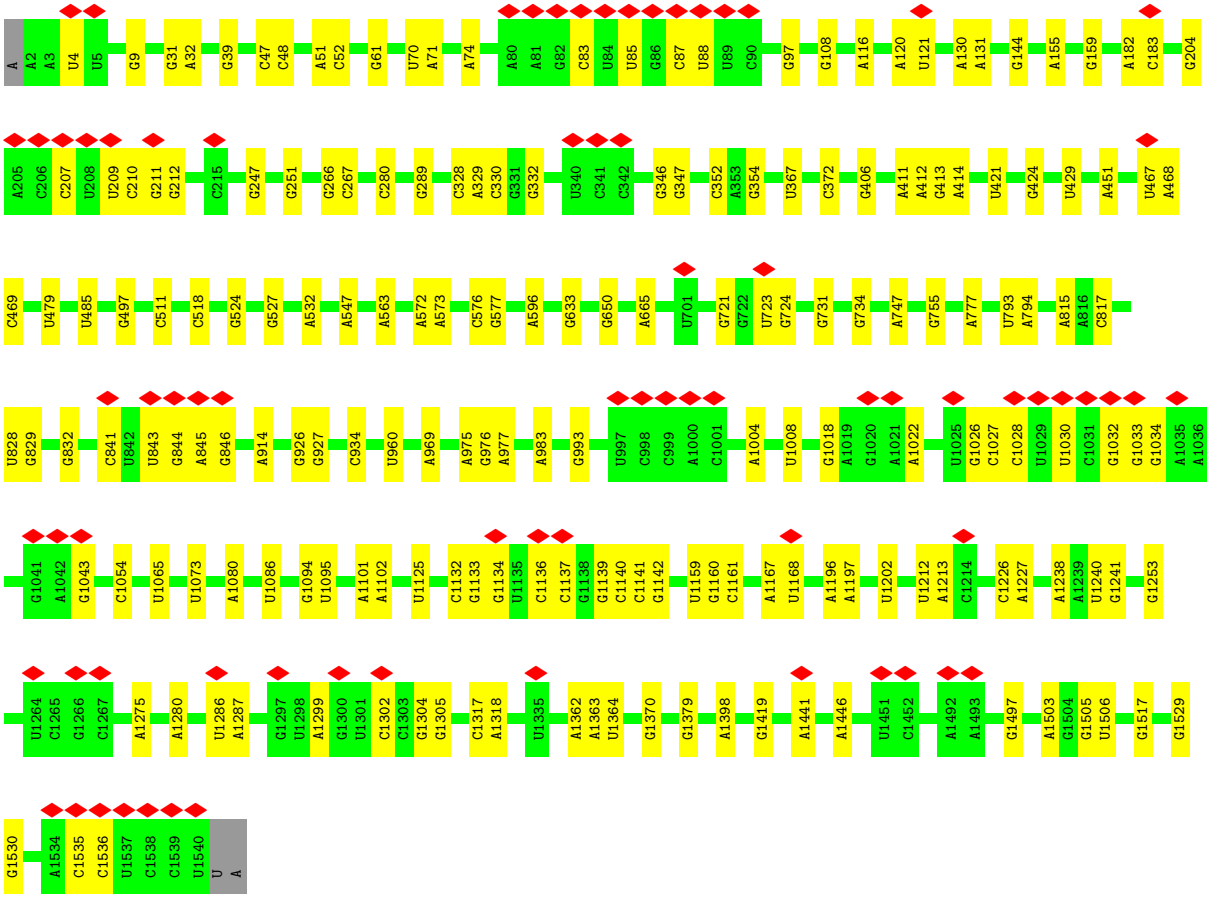
Chain f:





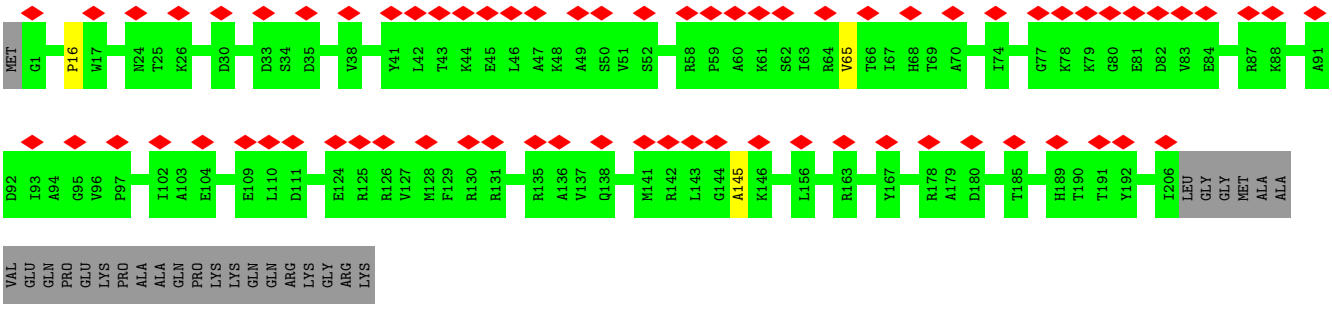
- Molecule 38: 16S ribosomal RNA

Chain g:



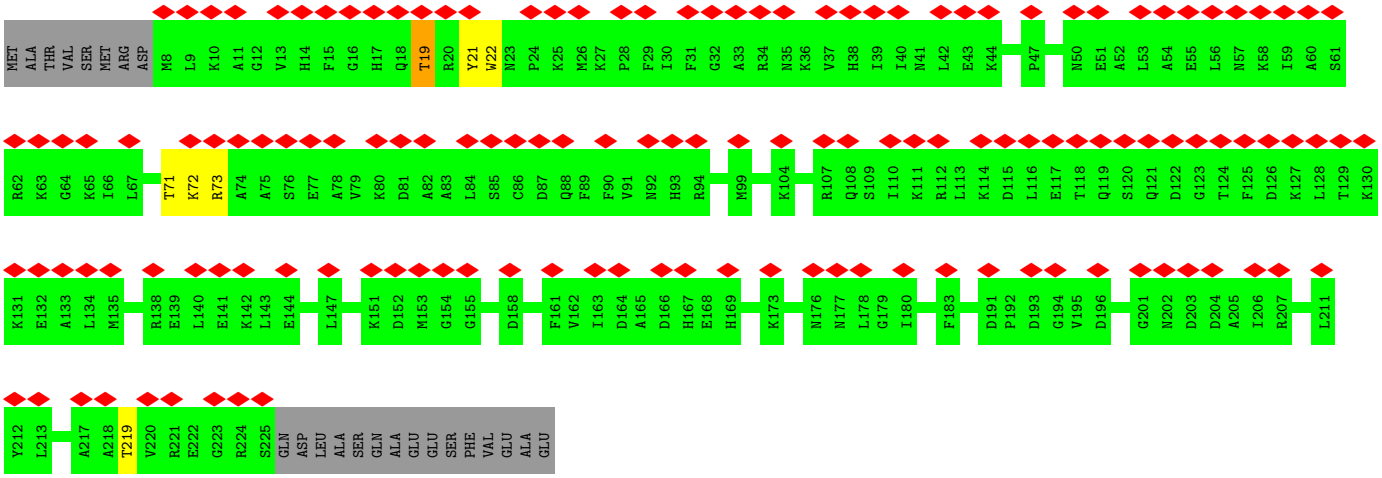
- Molecule 39: 30S ribosomal protein S3

Chain h:



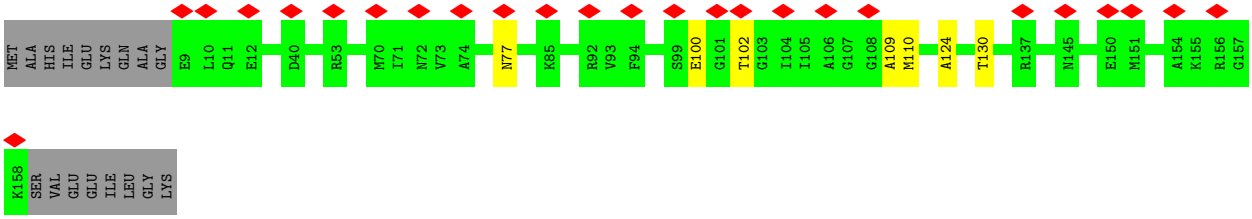
- Molecule 40: 30S ribosomal protein S2

Chain j:



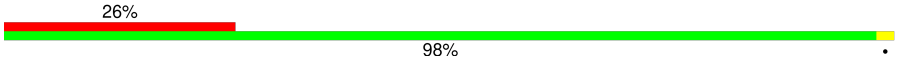
- Molecule 41: 30S ribosomal protein S5

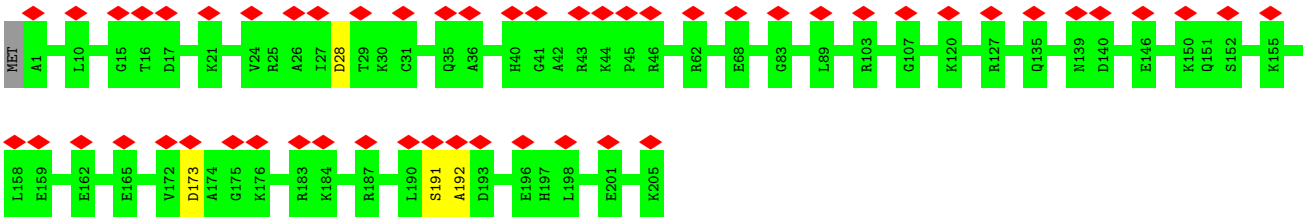
Chain k:



- Molecule 42: 30S ribosomal protein S4

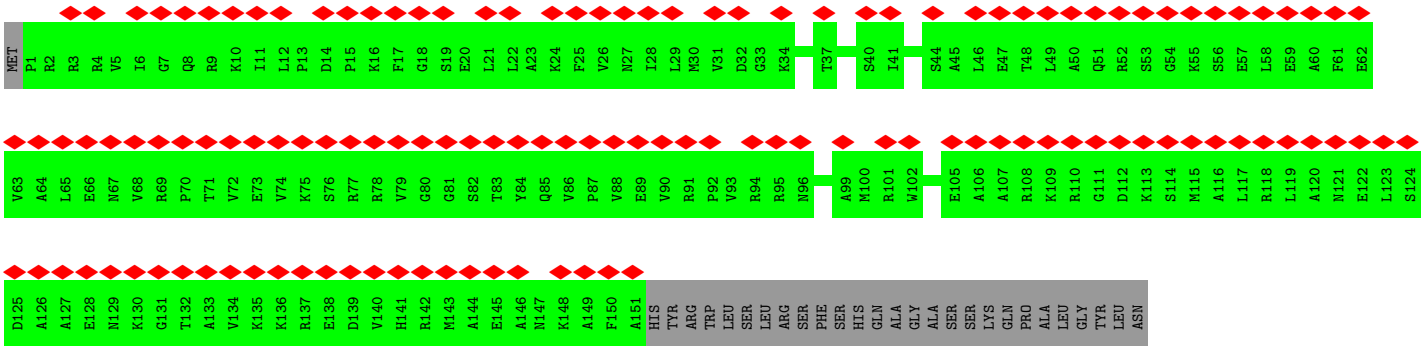
Chain l:





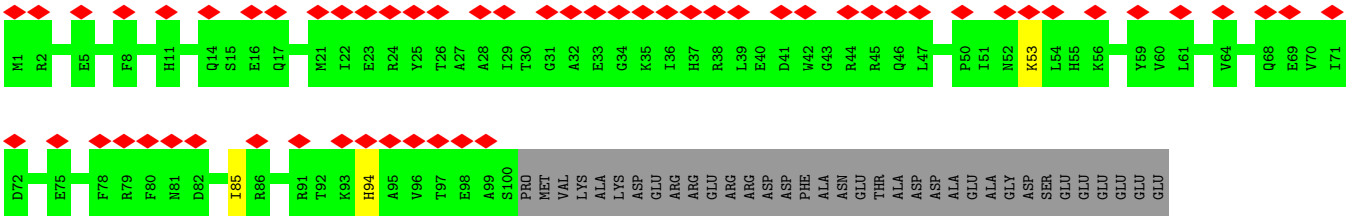
- Molecule 43: 30S ribosomal protein S7

Chain m:



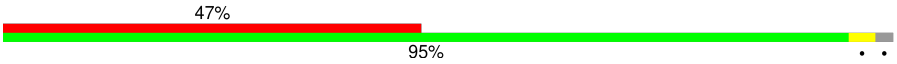
- Molecule 44: 30S ribosomal protein S6

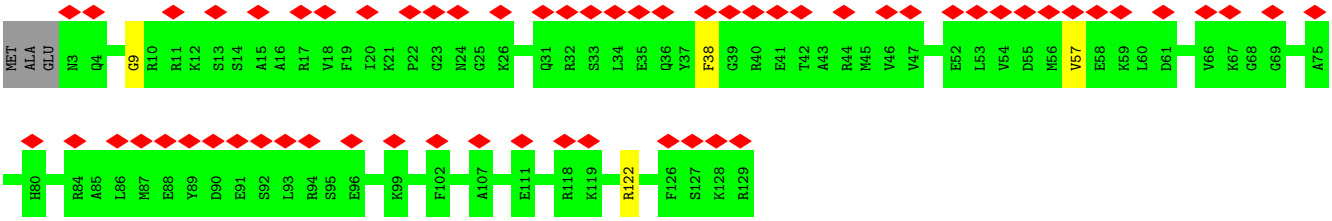
Chain n:



- Molecule 45: 30S ribosomal protein S9

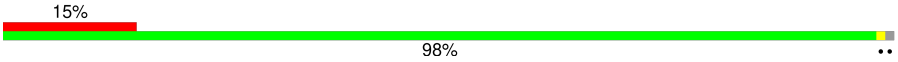
Chain o:

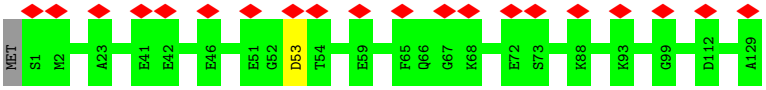




- Molecule 46: 30S ribosomal protein S8

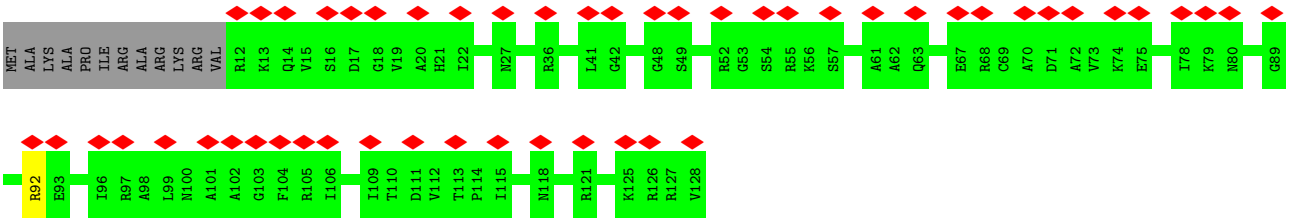
Chain p:





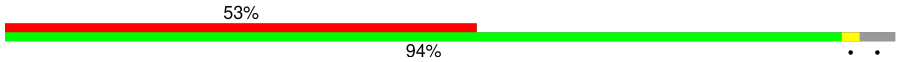
- Molecule 47: 30S ribosomal protein S11

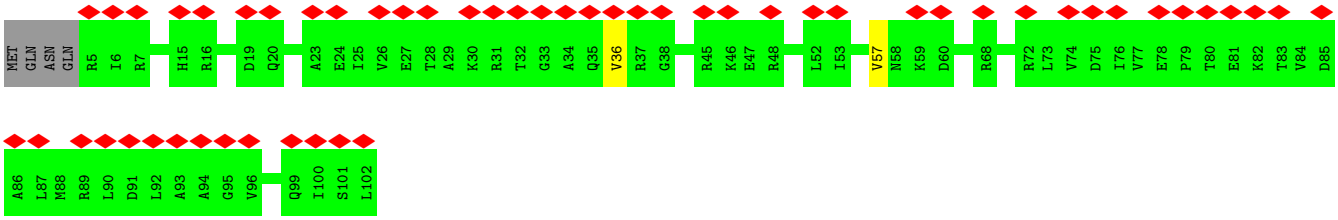
Chain q:



- Molecule 48: 30S ribosomal protein S10

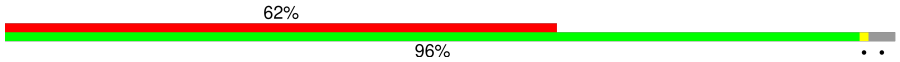
Chain r:

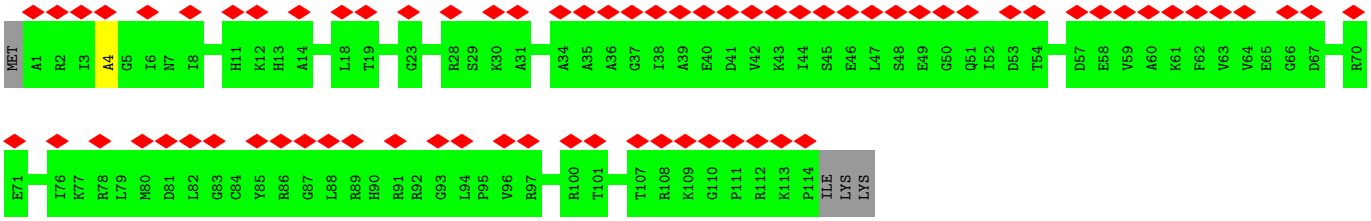




- Molecule 49: 30S ribosomal protein S13

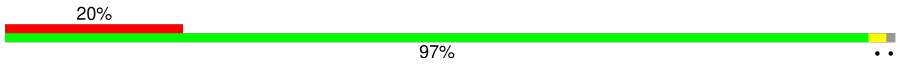
Chain s:

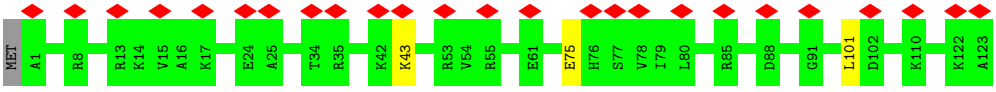




- Molecule 50: 30S ribosomal protein S12

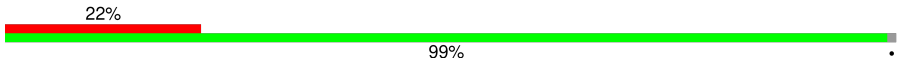
Chain t:

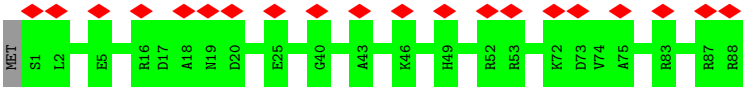




- Molecule 51: 30S ribosomal protein S15

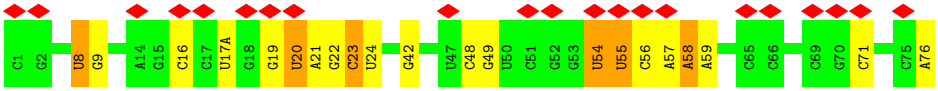
Chain u:





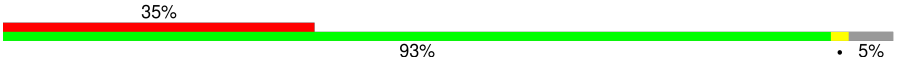
- Molecule 52: tRNA

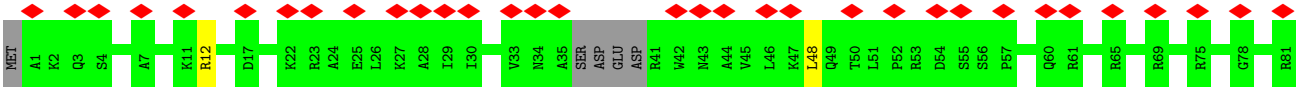
Chain v:

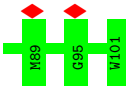


- Molecule 53: 30S ribosomal protein S14

Chain w:

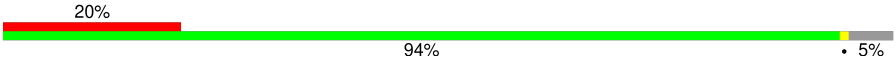


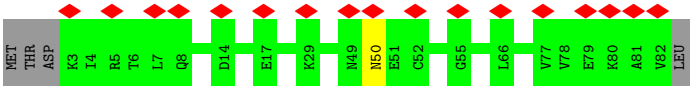




- Molecule 54: 30S ribosomal protein S17

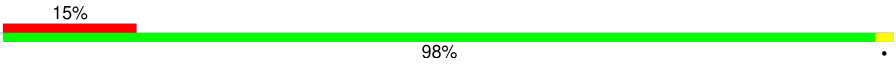
Chain x:

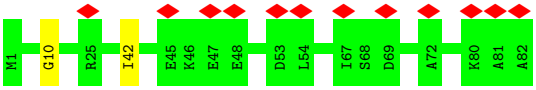




- Molecule 55: 30S ribosomal protein S16

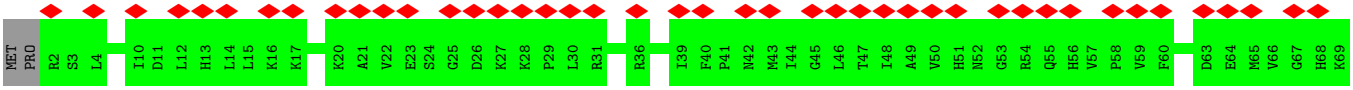
Chain y:

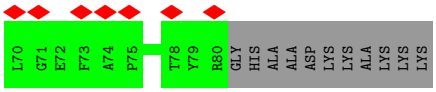




- Molecule 56: 30S ribosomal protein S19

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND4	Depositor
Microscope	FEI POLARA 300, FEI POLARA 300	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	640, 190	Depositor
Maximum defocus (nm)	7180, 7570	Depositor
Magnification	39000, 39000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	13.350	Depositor
Minimum map value	-6.028	Depositor
Average map value	0.091	Depositor
Map value standard deviation	0.658	Depositor
Recommended contour level	2.2	Depositor
Map size (Å)	369.0, 369.0, 369.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.025, 1.025, 1.025	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: PSU, GNP, ZN, FME, MG, 5MU, 4SU, H2U

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	0.21	0/2828	0.66	0/4410
2	1	0.51	0/462	0.71	0/621
3	2	0.54	0/430	0.80	0/570
4	3	0.46	0/671	0.63	0/888
5	4	0.39	0/144	1.37	4/222 (1.8%)
6	A	0.21	0/68626	0.65	1/107056 (0.0%)
7	B	0.46	0/2121	0.72	0/2852
8	C	0.47	0/1586	0.65	0/2134
9	D	0.46	0/1571	0.63	0/2113
10	E	0.49	0/1434	0.65	0/1926
11	F	0.46	0/1343	0.61	0/1816
12	G	0.50	0/389	0.61	0/523
13	H	0.48	0/1046	0.57	0/1410
14	I	0.48	0/1152	0.65	0/1551
15	J	0.47	0/947	0.73	0/1268
16	K	0.48	0/1054	0.72	0/1403
17	L	0.45	0/1093	0.64	0/1460
18	M	0.49	0/973	0.69	0/1301
19	N	0.46	0/902	0.64	0/1209
20	O	0.49	0/929	0.72	0/1242
21	P	0.48	0/960	0.71	0/1278
22	Q	0.44	0/829	0.62	0/1107
23	R	0.44	0/864	0.68	0/1156
24	S	0.48	0/744	0.70	0/994
25	T	0.47	0/787	0.66	0/1051
26	U	0.45	0/766	0.60	0/1025
27	V	0.49	0/603	0.72	0/797
28	W	0.46	0/635	0.69	0/848
29	X	0.47	0/510	0.67	0/677
30	Y	0.48	0/453	0.69	0/605
31	Z	0.44	0/450	0.67	0/599
32	a	0.46	0/416	0.63	0/554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.46	0/380	0.77	0/498
34	c	0.44	0/513	0.69	0/676
35	d	0.45	0/303	0.72	0/397
36	e	0.52	0/895	0.69	0/1203
37	f	0.25	0/3895	0.46	1/5264 (0.0%)
38	g	0.21	0/36966	0.66	0/57666
39	h	0.47	0/1651	0.63	0/2225
40	j	0.50	0/1735	0.66	0/2338
41	k	0.48	0/1118	0.68	0/1504
42	l	0.48	0/1665	0.69	0/2227
43	m	0.47	0/1195	0.66	0/1602
44	n	0.50	0/835	0.69	0/1128
45	o	0.50	0/1034	0.78	0/1375
46	p	0.45	0/989	0.60	0/1326
47	q	0.47	0/893	0.63	0/1205
48	r	0.47	0/797	0.70	0/1077
49	s	0.47	0/892	0.72	0/1193
50	t	0.46	0/969	0.72	0/1300
51	u	0.47	0/722	0.65	0/964
52	v	0.21	0/1746	0.77	3/2721 (0.1%)
53	w	0.50	0/785	0.78	1/1043 (0.1%)
54	x	0.49	0/657	0.69	0/881
55	y	0.47	0/659	0.69	0/884
56	z	0.48	0/652	0.66	0/877
All	All	0.31	0/159664	0.66	10/238240 (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
36	e	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	f	787	SER	C-N-CD	5.40	139.74	128.40
5	4	17	U	N1-C1'-C2'	-5.37	106.09	112.00
5	4	15	U	C4'-C3'-O3'	5.33	123.67	113.00
5	4	16	A	N9-C1'-C2'	-5.33	106.14	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	v	23	C	C2'-C3'-O3'	-5.32	97.80	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	e	53	ARG	Peptide

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	2529	0	1281	0	0
2	1	455	0	478	1	0
3	2	425	0	449	0	0
4	3	665	0	714	1	0
5	4	129	0	65	31	0
6	A	61274	0	30819	12	0
7	B	2082	0	2157	5	0
8	C	1565	0	1616	8	0
9	D	1552	0	1619	0	0
10	E	1410	0	1447	1	0
11	F	1323	0	1374	0	0
12	G	384	0	405	0	0
13	H	1032	0	1088	1	0
14	I	1129	0	1162	3	0
15	J	938	0	1012	5	0
16	K	1045	0	1117	1	0
17	L	1074	0	1157	1	0
18	M	960	0	1000	0	0
19	N	892	0	923	3	0
20	O	917	0	965	0	0
21	P	947	0	1022	1	0
22	Q	816	0	839	1	0
23	R	857	0	922	2	0
24	S	738	0	807	1	0
25	T	779	0	834	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	U	753	0	780	0	0
27	V	596	0	610	4	0
28	W	625	0	655	1	0
29	X	509	0	543	0	0
30	Y	449	0	491	0	0
31	Z	444	0	461	0	0
32	a	409	0	440	0	0
33	b	377	0	418	0	0
34	c	504	0	574	0	0
35	d	302	0	342	0	0
36	e	884	0	913	0	0
37	f	3847	0	3909	0	0
38	g	33015	0	16616	0	0
39	h	1624	0	1699	0	0
40	j	1704	0	1732	0	0
41	k	1105	0	1148	0	0
42	l	1643	0	1710	0	0
43	m	1181	0	1240	0	0
44	n	817	0	808	0	0
45	o	1022	0	1070	0	0
46	p	979	0	1034	0	0
47	q	877	0	887	0	0
48	r	787	0	828	0	0
49	s	883	0	944	0	0
50	t	955	0	1019	0	0
51	u	714	0	737	0	0
52	v	1643	0	836	0	0
53	w	774	0	827	0	0
54	x	648	0	691	0	0
55	y	649	0	666	0	0
56	z	637	0	665	0	0
57	3	1	0	0	0	0
57	A	137	0	0	0	0
57	B	1	0	0	0	0
57	d	1	0	0	0	0
57	g	54	0	0	0	0
57	w	1	0	0	0	0
58	d	1	0	0	0	0
59	f	32	0	13	0	0
60	v	9	1	10	0	0
61	3	4	0	0	0	0
61	A	599	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B	7	0	0	0	0
61	C	2	0	0	0	0
61	D	2	0	0	0	0
61	I	1	0	0	0	0
61	K	8	0	0	0	0
61	M	5	0	0	0	0
61	P	3	0	0	0	0
61	Q	3	0	0	0	0
61	R	3	0	0	0	0
61	S	2	0	0	0	0
61	b	1	0	0	0	0
61	d	3	0	0	0	0
61	g	189	0	0	0	0
61	q	1	0	0	0	0
61	t	2	0	0	0	0
61	w	2	0	0	0	0
All	All	148347	1	100588	79	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 2.

The worst 5 of 79 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)
5:4:16:A:C2	5:4:17:U:C4	2.49	1.00
5:4:13:A:O2'	5:4:14:A:O4'	1.85	0.94
5:4:13:A:H2'	5:4:14:A:C8	2.04	0.91
5:4:16:A:C2	5:4:17:U:N3	2.47	0.82
5:4:14:A:O2'	5:4:15:U:H5"	1.86	0.76

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	6	35
3	2	49/71 (69%)	37 (76%)	10 (20%)	2 (4%)	2	22
4	3	83/87 (95%)	80 (96%)	1 (1%)	2 (2%)	5	30
7	B	269/273 (98%)	239 (89%)	25 (9%)	5 (2%)	6	35
8	C	207/209 (99%)	179 (86%)	22 (11%)	6 (3%)	3	28
9	D	199/201 (99%)	169 (85%)	24 (12%)	6 (3%)	3	27
10	E	175/179 (98%)	154 (88%)	19 (11%)	2 (1%)	12	43
11	F	174/177 (98%)	153 (88%)	17 (10%)	4 (2%)	5	31
12	G	48/149 (32%)	42 (88%)	4 (8%)	2 (4%)	2	21
13	H	139/142 (98%)	121 (87%)	17 (12%)	1 (1%)	19	51
14	I	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	19	51
15	J	120/123 (98%)	101 (84%)	15 (12%)	4 (3%)	3	26
16	K	141/144 (98%)	124 (88%)	14 (10%)	3 (2%)	5	33
17	L	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	5	32
18	M	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
19	N	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	14	47
20	O	112/115 (97%)	99 (88%)	8 (7%)	5 (4%)	2	19
21	P	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	14	47
22	Q	101/103 (98%)	90 (89%)	9 (9%)	2 (2%)	6	34
23	R	108/110 (98%)	104 (96%)	3 (3%)	1 (1%)	14	47
24	S	91/100 (91%)	68 (75%)	19 (21%)	4 (4%)	2	20
25	T	100/104 (96%)	82 (82%)	15 (15%)	3 (3%)	3	27
26	U	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
27	V	77/85 (91%)	51 (66%)	22 (29%)	4 (5%)	1	18
28	W	75/78 (96%)	68 (91%)	7 (9%)	0	100	100
29	X	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	8	37
30	Y	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
31	Z	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	2	24
32	a	48/55 (87%)	46 (96%)	1 (2%)	1 (2%)	5	33
33	b	44/46 (96%)	39 (89%)	5 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	c	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	8	37
35	d	36/38 (95%)	28 (78%)	6 (17%)	2 (6%)	1	16
36	e	115/165 (70%)	99 (86%)	13 (11%)	3 (3%)	4	29
37	f	507/890 (57%)	488 (96%)	17 (3%)	2 (0%)	30	62
39	h	204/233 (88%)	185 (91%)	16 (8%)	3 (2%)	8	38
40	j	216/241 (90%)	187 (87%)	24 (11%)	5 (2%)	5	31
41	k	148/167 (89%)	128 (86%)	15 (10%)	5 (3%)	3	26
42	l	203/206 (98%)	184 (91%)	15 (7%)	4 (2%)	6	34
43	m	149/179 (83%)	140 (94%)	9 (6%)	0	100	100
44	n	98/135 (73%)	84 (86%)	11 (11%)	3 (3%)	3	27
45	o	125/130 (96%)	106 (85%)	15 (12%)	4 (3%)	3	27
46	p	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
47	q	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	14	47
48	r	96/102 (94%)	80 (83%)	14 (15%)	2 (2%)	5	33
49	s	112/118 (95%)	105 (94%)	6 (5%)	1 (1%)	14	47
50	t	121/124 (98%)	108 (89%)	10 (8%)	3 (2%)	4	30
51	u	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
53	w	92/101 (91%)	76 (83%)	16 (17%)	0	100	100
54	x	78/84 (93%)	65 (83%)	12 (15%)	1 (1%)	10	40
55	y	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4	30
56	z	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
All	All	6144/7039 (87%)	5468 (89%)	567 (9%)	109 (2%)	9	35

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	121	ALA
12	G	3	VAL
27	V	14	ASP
39	h	16	PRO
42	l	28	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	48/65 (74%)	48 (100%)	0	100	100
3	2	44/61 (72%)	44 (100%)	0	100	100
4	3	65/66 (98%)	65 (100%)	0	100	100
7	B	216/218 (99%)	216 (100%)	0	100	100
8	C	164/164 (100%)	164 (100%)	0	100	100
9	D	165/165 (100%)	165 (100%)	0	100	100
10	E	148/150 (99%)	148 (100%)	0	100	100
11	F	137/138 (99%)	136 (99%)	1 (1%)	81	88
12	G	40/114 (35%)	40 (100%)	0	100	100
13	H	109/110 (99%)	109 (100%)	0	100	100
14	I	116/116 (100%)	115 (99%)	1 (1%)	75	84
15	J	103/104 (99%)	102 (99%)	1 (1%)	73	82
16	K	102/103 (99%)	102 (100%)	0	100	100
17	L	109/109 (100%)	108 (99%)	1 (1%)	75	84
18	M	100/103 (97%)	100 (100%)	0	100	100
19	N	86/87 (99%)	86 (100%)	0	100	100
20	O	99/100 (99%)	99 (100%)	0	100	100
21	P	89/90 (99%)	88 (99%)	1 (1%)	70	80
22	Q	84/84 (100%)	84 (100%)	0	100	100
23	R	93/93 (100%)	93 (100%)	0	100	100
24	S	80/84 (95%)	80 (100%)	0	100	100
25	T	83/85 (98%)	83 (100%)	0	100	100
26	U	78/78 (100%)	78 (100%)	0	100	100
27	V	59/63 (94%)	58 (98%)	1 (2%)	56	73
28	W	67/68 (98%)	67 (100%)	0	100	100
29	X	55/55 (100%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Y	48/49 (98%)	48 (100%)	0	100	100
31	Z	47/48 (98%)	47 (100%)	0	100	100
32	a	45/49 (92%)	45 (100%)	0	100	100
33	b	38/38 (100%)	38 (100%)	0	100	100
34	c	51/52 (98%)	51 (100%)	0	100	100
35	d	34/34 (100%)	34 (100%)	0	100	100
36	e	88/123 (72%)	87 (99%)	1 (1%)	70	80
37	f	409/713 (57%)	406 (99%)	3 (1%)	81	88
39	h	170/190 (90%)	170 (100%)	0	100	100
40	j	180/199 (90%)	177 (98%)	3 (2%)	56	73
41	k	113/126 (90%)	111 (98%)	2 (2%)	54	71
42	l	172/173 (99%)	172 (100%)	0	100	100
43	m	124/147 (84%)	124 (100%)	0	100	100
44	n	87/116 (75%)	87 (100%)	0	100	100
45	o	105/107 (98%)	105 (100%)	0	100	100
46	p	104/105 (99%)	103 (99%)	1 (1%)	73	82
47	q	90/99 (91%)	90 (100%)	0	100	100
48	r	86/90 (96%)	86 (100%)	0	100	100
49	s	92/96 (96%)	92 (100%)	0	100	100
50	t	103/104 (99%)	103 (100%)	0	100	100
51	u	76/77 (99%)	76 (100%)	0	100	100
53	w	79/84 (94%)	78 (99%)	1 (1%)	65	77
54	x	74/78 (95%)	74 (100%)	0	100	100
55	y	65/65 (100%)	65 (100%)	0	100	100
56	z	70/79 (89%)	70 (100%)	0	100	100
All	All	5089/5714 (89%)	5072 (100%)	17 (0%)	90	94

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

Mol	Chain	Res	Type
41	k	130	THR
53	w	48	LEU
37	f	541	ILE

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Mol	Chain	Res	Type
37	f	790	LEU
37	f	861	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
37	f	426	GLN
49	s	51	GLN
37	f	484	GLN
51	u	34	GLN
44	n	46	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	117/118 (99%)	11 (9%)	0
38	g	1538/1542 (99%)	187 (12%)	0
5	4	6/52 (11%)	5 (83%)	4 (66%)
52	v	76/77 (98%)	21 (27%)	0
6	A	2850/2904 (98%)	332 (11%)	14 (0%)
All	All	4587/4693 (97%)	556 (12%)	18 (0%)

5 of 556 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	A
1	0	24	G
1	0	35	C
1	0	42	C
1	0	44	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	2423	U
6	A	2902	C
6	A	2756	U
6	A	784	G
6	A	2384	U

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

4 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	$\#\|Z\| > 2$
52	5MU	v	54	52	19,22,23	1.43	6 (31%)	27,32,35	2.18	7 (25%)
52	H2U	v	20	52	18,21,22	0.82	0	19,30,33	1.02	1 (5%)
52	PSU	v	55	52	18,21,22	1.34	2 (11%)	21,30,33	2.21	5 (23%)
52	4SU	v	8	52	18,21,22	1.97	5 (27%)	25,30,33	2.61	11 (44%)

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
52	5MU	v	54	52	-	2/7/25/26	0/2/2/2
52	H2U	v	20	52	-	2/7/38/39	0/2/2/2
52	PSU	v	55	52	-	1/7/25/26	0/2/2/2
52	4SU	v	8	52	-	3/7/25/26	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	8	4SU	C4-S4	-4.91	1.60	1.68
52	v	8	4SU	C4-N3	-3.99	1.33	1.37
52	v	55	PSU	C6-C5	3.44	1.39	1.35
52	v	54	5MU	C6-C5	2.82	1.39	1.34
52	v	55	PSU	C4-N3	-2.61	1.34	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	v	8	4SU	C4-N3-C2	-6.64	120.95	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	v	55	PSU	N1-C2-N3	6.38	121.90	115.17
52	v	8	4SU	C5-C4-N3	5.60	119.96	114.75
52	v	54	5MU	C4-N3-C2	-5.08	120.68	127.34
52	v	54	5MU	N3-C2-N1	4.95	121.33	114.89

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	v	8	4SU	O4'-C1'-N1-C2
52	v	8	4SU	O4'-C1'-N1-C6
52	v	20	H2U	O4'-C1'-N1-C6
52	v	54	5MU	O4'-C1'-N1-C6
52	v	20	H2U	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 198 ligands modelled in this entry, 196 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
59	GNP	f	901	-	29,34,34	3.22	7 (24%)	33,54,54	1.88	6 (18%)
60	FME	v	101	52	8,8,10	0.43	0	7,8,11	0.98	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GNP	f	901	-	-	3/14/38/38	0/3/3/3
60	FME	v	101	52	-	1/7/7/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	f	901	GNP	PG-O1G	10.09	1.61	1.46
59	f	901	GNP	PB-O1B	10.08	1.61	1.46
59	f	901	GNP	PG-N3B	4.61	1.75	1.63
59	f	901	GNP	PB-N3B	4.59	1.75	1.63
59	f	901	GNP	C5-C6	4.19	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	f	901	GNP	C2-N3-C4	5.15	121.04	115.48
59	f	901	GNP	C2-N1-C6	4.58	122.33	115.96
59	f	901	GNP	C5-C6-N1	-4.04	118.01	123.42
59	f	901	GNP	N3-C2-N1	-3.45	122.82	127.21
59	f	901	GNP	C4-C5-N7	-2.64	106.55	109.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	f	901	GNP	PB-N3B-PG-O1G
59	f	901	GNP	PG-N3B-PB-O1B
59	f	901	GNP	PG-N3B-PB-O3A
60	v	101	FME	C-CA-N-CN

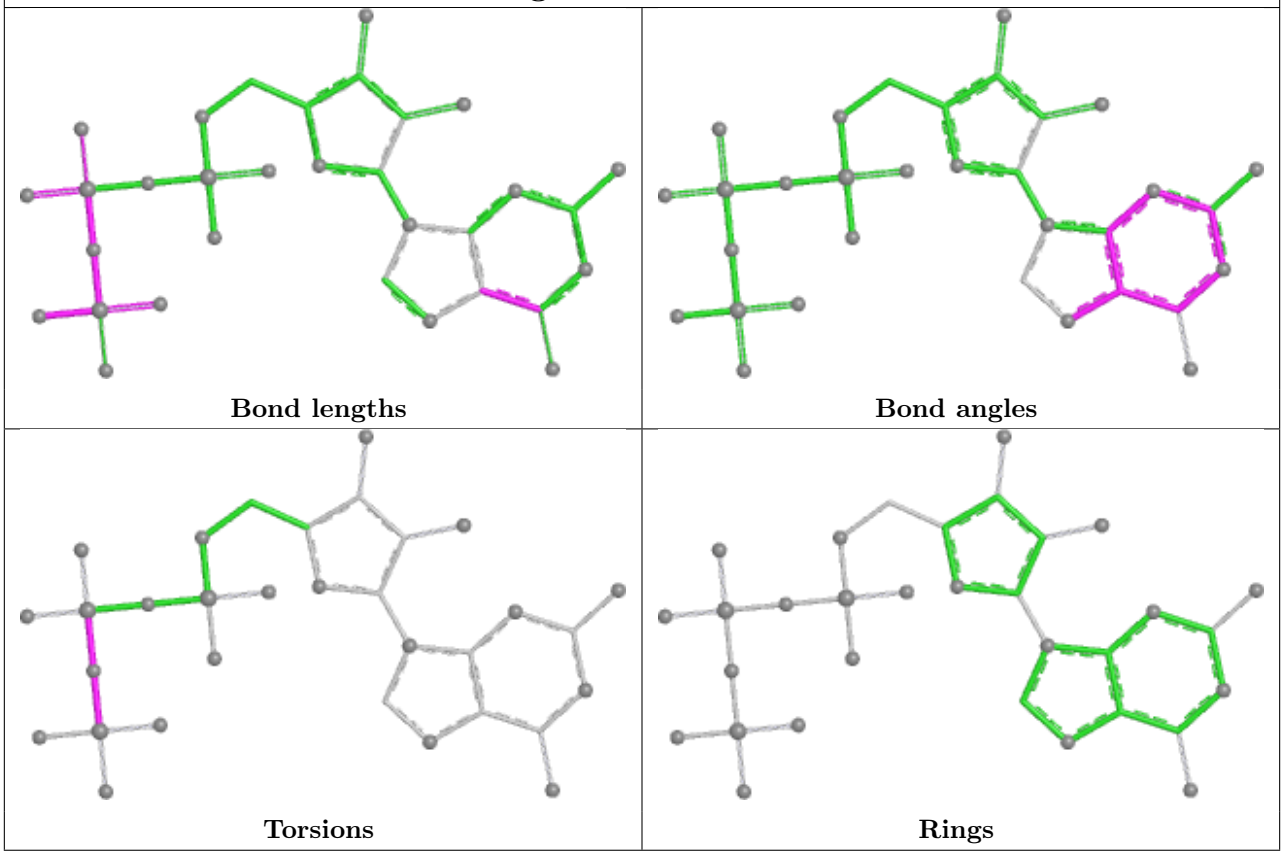
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP f 901



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.

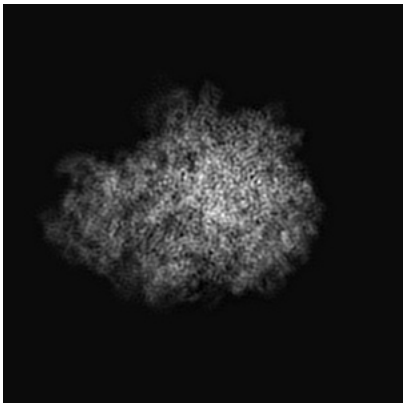
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6559. These allow visual inspection of the internal detail of the map and identification of artifacts.

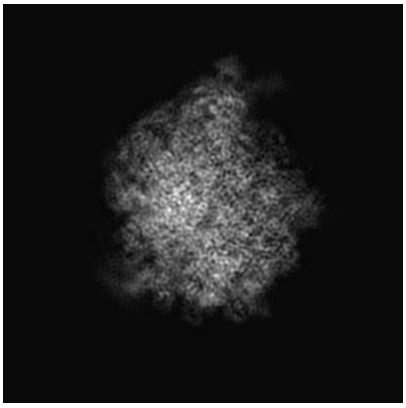
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

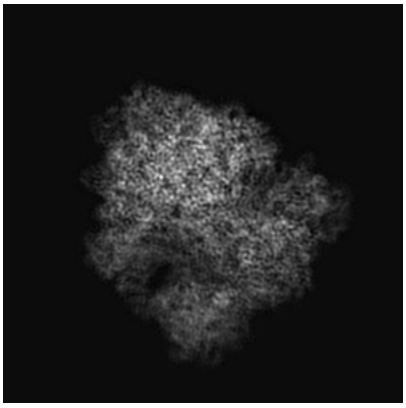
6.1.1 Primary map



X



Y

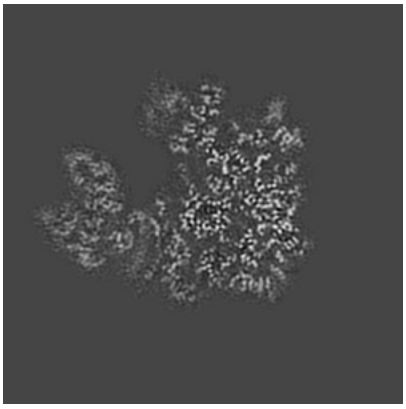


Z

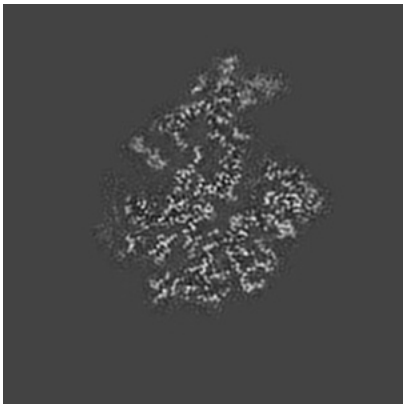
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

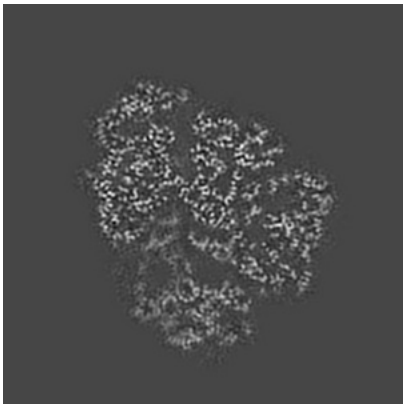
6.2.1 Primary map



X Index: 180



Y Index: 180

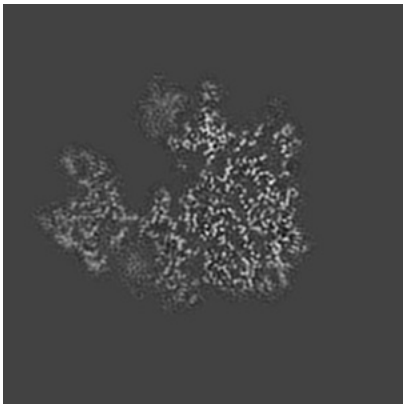


Z Index: 180

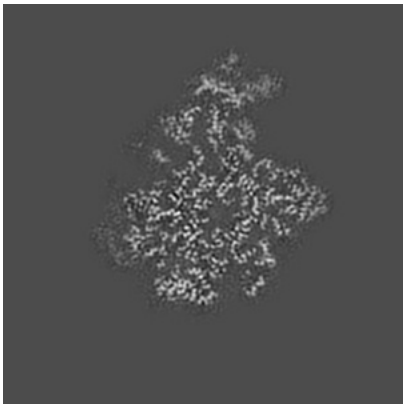
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

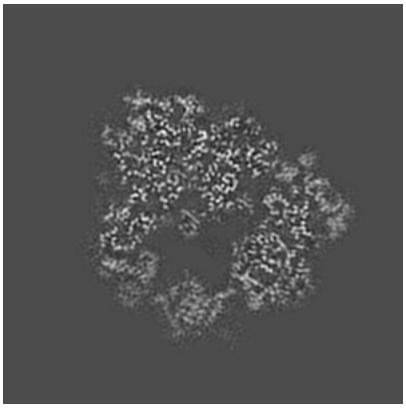
6.3.1 Primary map



X Index: 185



Y Index: 184

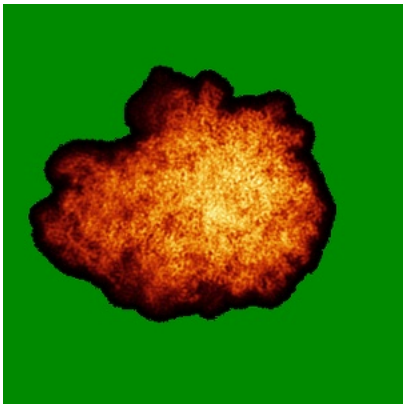


Z Index: 196

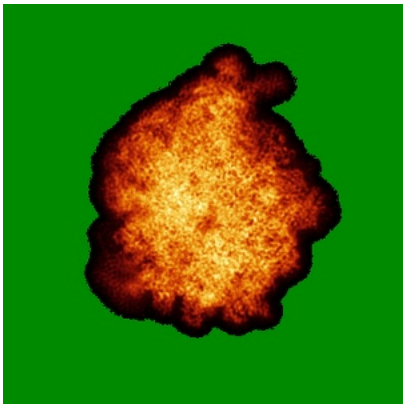
The images above show the largest variance slices of the map in three orthogonal directions.

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

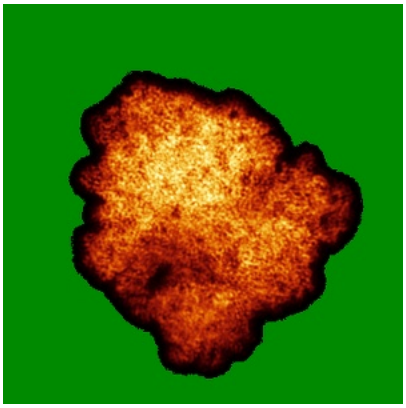
6.4.1 Primary map



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

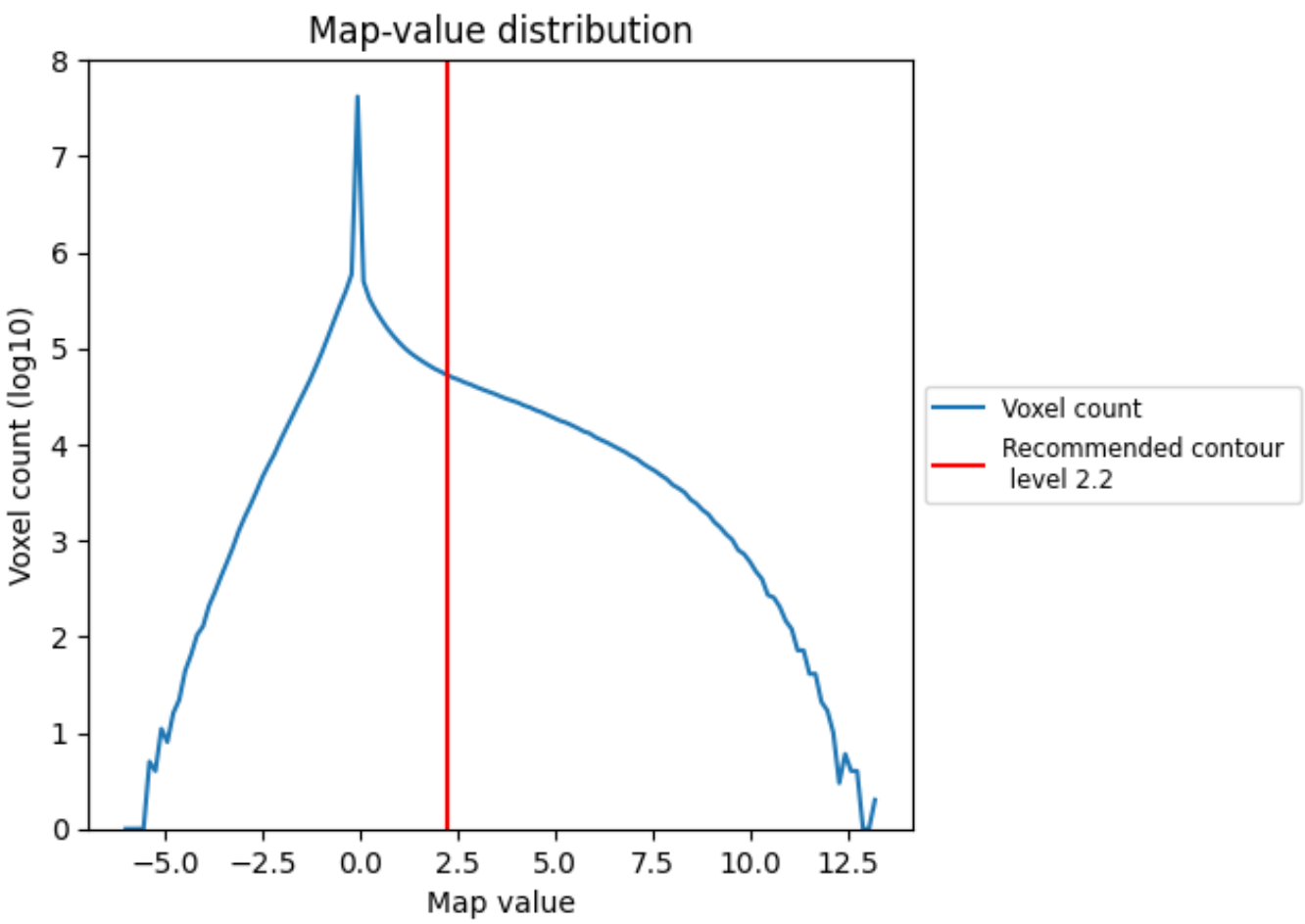
6.6 Mask visualisation (i)

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

7 Map analysis (i)

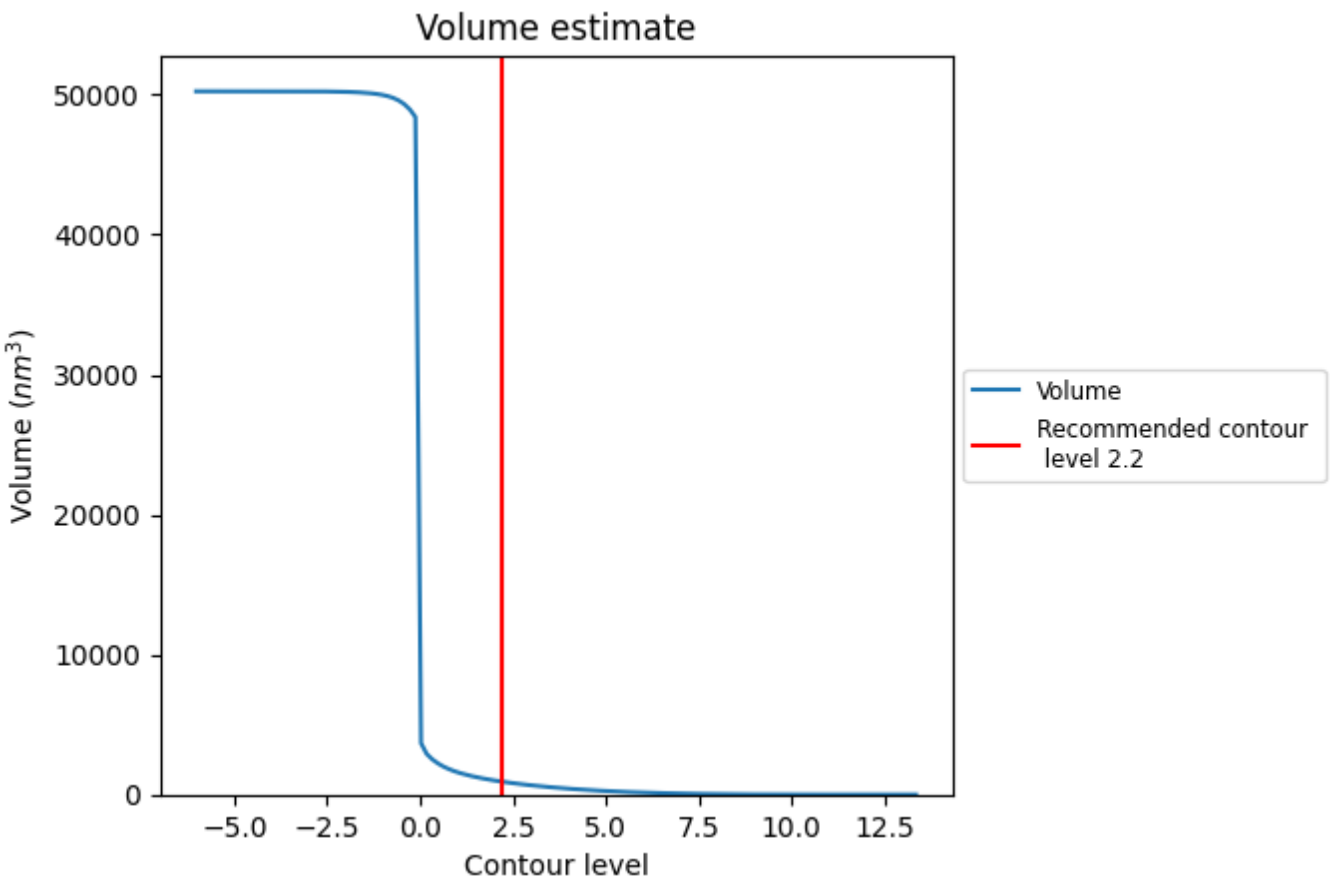
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

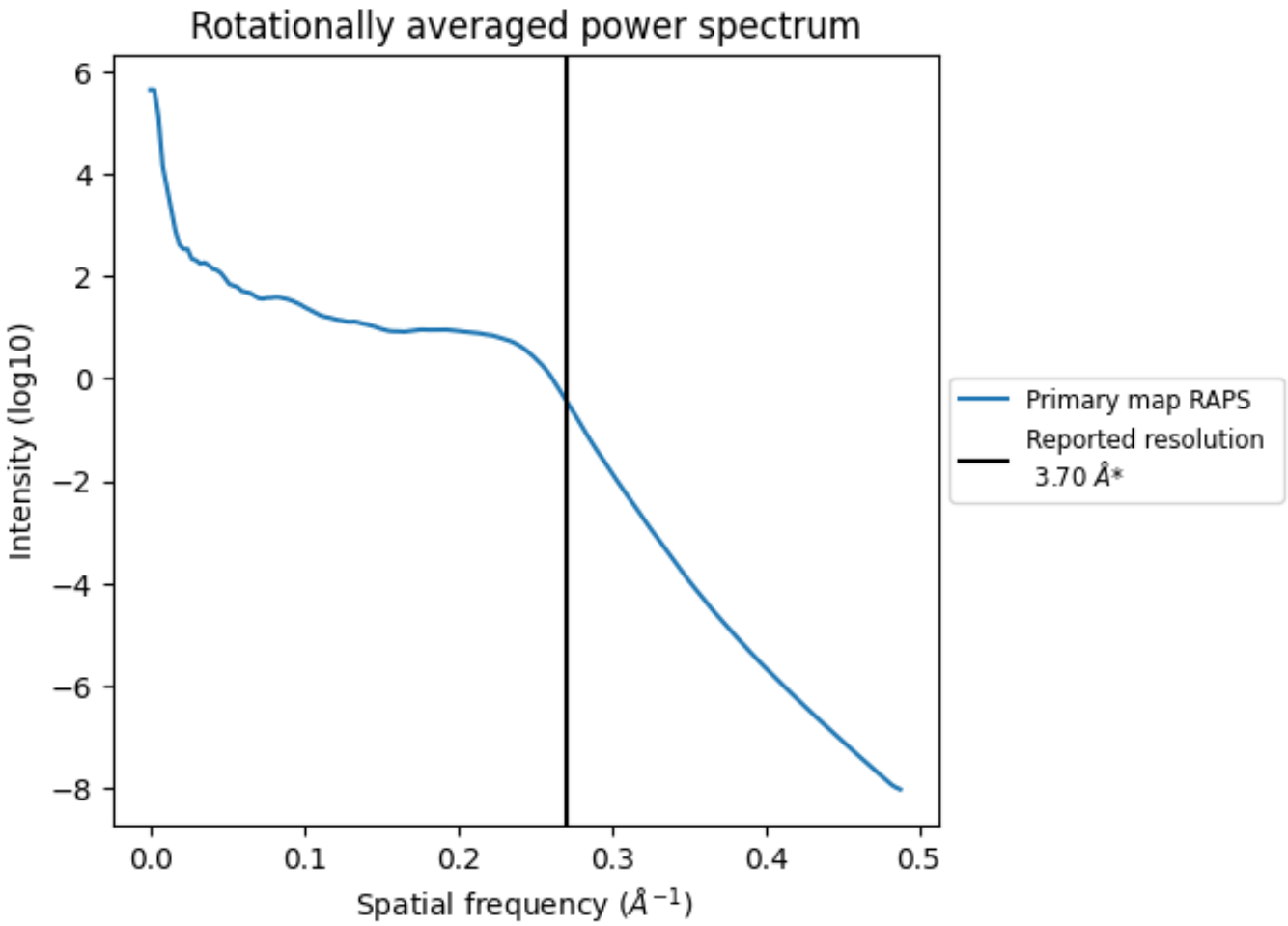
7.2 Volume estimate (i)



The volume at the recommended contour level is 925 nm^3; this corresponds to an approximate mass of 836 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 0.270 Å^{-1}

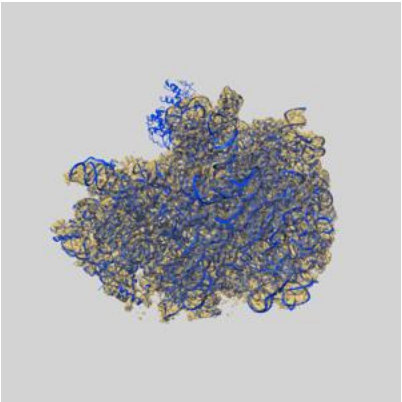
8 Fourier-Shell correlation (i)

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

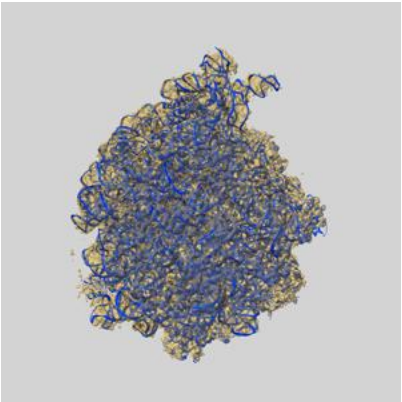
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6559 and PDB model 3JCJ. Per-residue inclusion information can be found in section 3 on page 16.

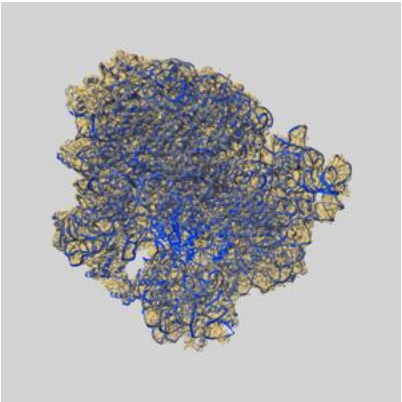
9.1 Map-model overlay (i)



X



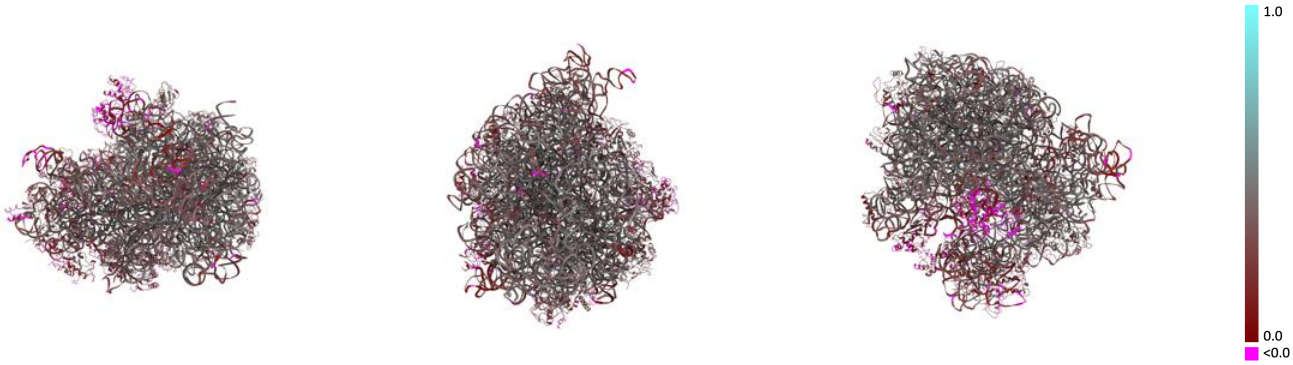
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.2 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.

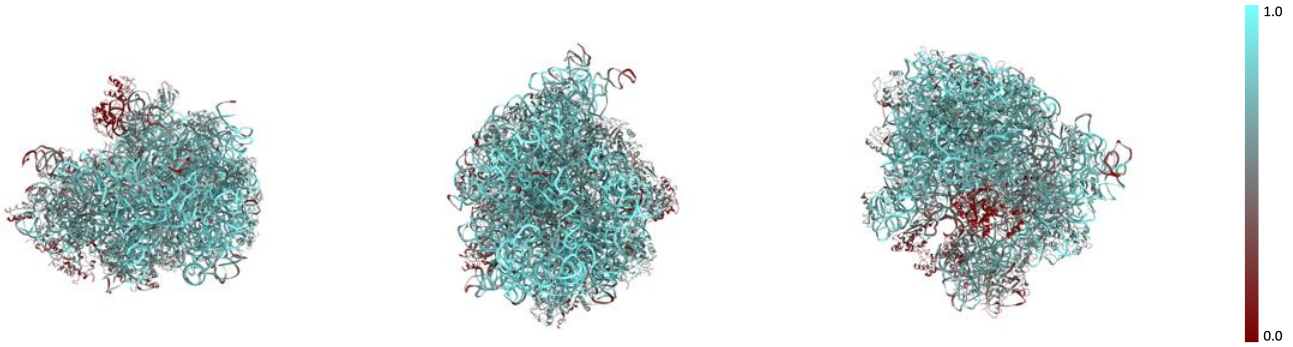
9.2 Q-score mapped to coordinate model (i)



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.

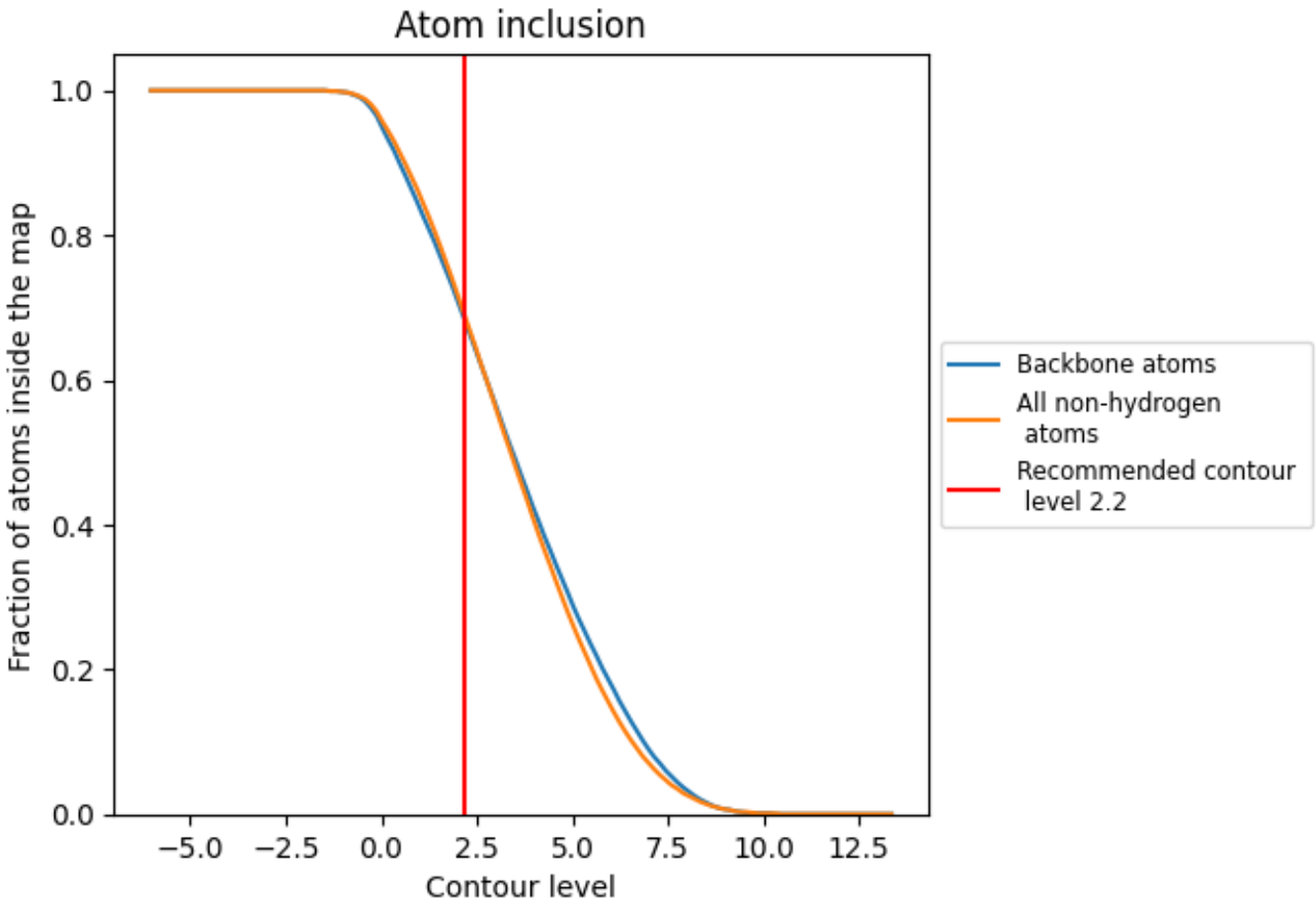
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.2).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.3500
0	0.8090	0.3700
1	0.4790	0.2780
2	0.2590	0.1050
3	0.5700	0.2790
4	0.6200	0.3990
A	0.7990	0.3970
B	0.6270	0.3710
C	0.6360	0.3580
D	0.5370	0.3050
E	0.3150	0.1120
F	0.5610	0.3060
G	0.2220	0.1410
H	0.0040	-0.0020
I	0.6160	0.3500
J	0.5840	0.3530
K	0.5860	0.3380
L	0.6130	0.3700
M	0.6630	0.3800
N	0.5900	0.3040
O	0.5810	0.3250
P	0.6640	0.3780
Q	0.6050	0.3480
R	0.6330	0.3860
S	0.5500	0.2840
T	0.5550	0.3160
U	0.6130	0.3750
V	0.5100	0.2390
W	0.6060	0.3390
X	0.5630	0.2810
Y	0.6360	0.3780
Z	0.6470	0.3900
a	0.4940	0.3080
b	0.6450	0.3760
c	0.6580	0.3830

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Chain	Atom inclusion	Q-score
d	0.6120	0.3390
e	0.0200	0.0150
f	0.4980	0.3440
g	0.7600	0.3580
h	0.5010	0.2720
j	0.3040	0.1930
k	0.5920	0.3310
l	0.5370	0.3010
m	0.1860	0.1460
n	0.3520	0.1580
o	0.4200	0.2080
p	0.5680	0.3490
q	0.4440	0.2490
r	0.3750	0.2150
s	0.3300	0.1560
t	0.5640	0.3450
u	0.5450	0.2860
v	0.5130	0.2710
w	0.4780	0.2640
x	0.5520	0.2800
y	0.6250	0.3510
z	0.3210	0.1830