wwPDB EM Validation Summary Report (i)

Feb 22, 2024 – 10:36 PM EST

PDB ID	:	4V65
EMDB ID	:	EMD-1055
Title	:	Structure of the E. coli ribosome in the Pre-accommodation state
Authors	:	Devkota, B.; Caulfield, T.R.; Tan, R.-Z.; Harvey, S.C.
Deposited on	:	2008-08-03
Resolution	:	9.00 Å(reported)
Based on initial models	:	1EHZ, 2I2P

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

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

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

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

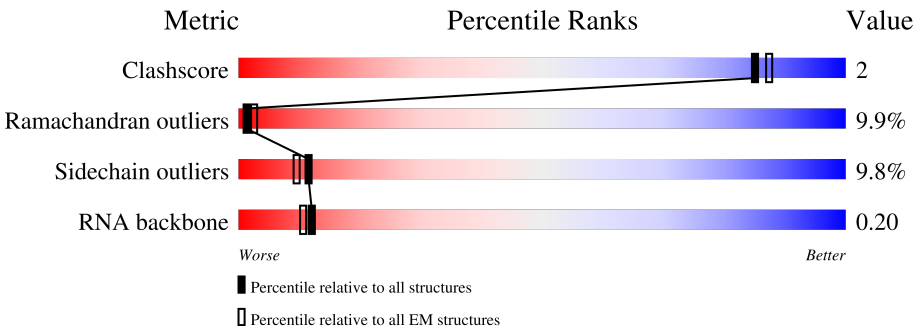
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	76	57%; 11%, 51%, 37%, •
1	AE	76	58%; 30%, 49%, 21%
1	AP	76	50%; 18%, 46%, 34%, •
2	AM	20	25%; 15%, 50%, 35%
3	A1	1530	65%; 17%, 45%, 39%
4	AB	241	71%; 69%, 17%, •, 10%
5	AC	129	47%; 66%, 22%, • •, 9%

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Mol	Chain	Length	Quality of chain
6	AD	124	76% 59% 30% 9%
7	AF	118	55% 68% 23% 6%
8	AG	101	88% 67% 22% 5% 5%
9	AH	89	84% 69% 25%
10	AI	82	100% 65% 27% 7%
11	AJ	84	73% 68% 21% 6% 5%
12	AK	75	29% 53% 19% 27%
13	AL	92	82% 54% 23% 9% 14%
14	AN	87	56% 77% 17%
15	AO	233	31% 65% 20% 12%
16	AQ	71	39% 45% 18% 7% 28%
17	AR	206	62% 69% 25%
18	AS	159	38% 68% 21% 6%
19	AT	135	55% 54% 16% 26%
20	AU	179	35% 59% 20% 5% 16%
21	AV	130	48% 84% 13%
22	AW	130	81% 75% 18% 5%
23	AX	103	73% 58% 32% 5% 5%
24	BA	117	71% 25% 49% 26%
25	BB	2903	52% 17% 44% 39%
26	BC	94	72% 76% 21%
27	BD	123	48% 65% 26% 7%
28	BE	144	67% 60% 30% 8%
29	BF	136	57% 65% 25% 7%
30	BG	127	35% 64% 30% 5%

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Mol	Chain	Length	Quality of chain
31	BH	117	57% 73% 21% 6%
32	BI	115	48% 58% 33% 8%
33	BJ	118	84% 69% 19% 9%
34	BK	103	92% 64% 27% 6%
35	BL	110	42% 72% 24% 5%
36	BM	99	69% 69% 23% 7%
37	BN	270	54% 61% 31% 6%
38	BO	103	99% 62% 30% 6%
39	BP	85	27% 59% 34% 5%
40	BQ	63	51% 65% 27% 8%
41	BR	59	58% 71% 20% 5%
42	BS	70	67% 71% 24%
43	BT	57	46% 49% 32% 16%
44	BU	54	80% 65% 30% 6%
45	BV	46	46% 67% 22% 9%
46	BW	64	73% 66% 19% 16%
47	BX	38	68% 68% 18% 11%
48	BY	209	33% 61% 29% 9%
49	BZ	213	96% 77% 21%
50	B1	201	71% 65% 25% 8%
51	B2	178	29% 61% 30% 7%
52	B3	177	81% 76% 18% 6%
53	B4	149	92% 76% 23%
54	B5	142	53% 80% 15%
55	B6	140	45% 71% 19% 9%

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 149248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called A/T, P and E-site tRNAs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	75	1600	715	288	523	74	0	0
1	AP	75	1600	715	288	523	74	0	0
1	AE	76	1622	725	293	529	75	0	0

- Molecule 2 is a RNA chain called mRNA model.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AM	20	397	180	40	158	19	0	0

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A1	1530	32828	14642	6024	10633	1529	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AC	117	876	540	174	159	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AD	123	954	590	196	164	4	0	0

- Molecule 7 is a protein called 30S ribosomal protein S13.

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

- Molecule 8 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AG	96	773	483	160	127	3	0	0

- Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AH	88	715	440	146	128	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AI	82	648	406	128	113	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S17.

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

- Molecule 12 is a protein called 30S ribosomal protein S18.

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

- Molecule 13 is a protein called 30S ribosomal protein S19.

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

- Molecule 14 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AN	85	664	411	137	113	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S3.

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

- Molecule 16 is a protein called 30S ribosomal protein S21.

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

- Molecule 17 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AR	205	1642	1026	315	297	4	0	0

- Molecule 18 is a protein called 30S ribosomal protein S5.

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

- Molecule 19 is a protein called 30S ribosomal protein S6.

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

- Molecule 20 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AU	150	1174	730	226	214	4	0	0

- Molecule 21 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AV	129	978	616	173	183	6	0	0

- Molecule 22 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	AW	127	1021	634	206	178	3	0	0

- Molecule 23 is a protein called 30S ribosomal protein S10.

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

- Molecule 24 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	BA	117	2504	1116	459	813	116	0	0

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	BB	2903	62317	27801	11467	20147	2902	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	BC	94	752	479	137	133	3	0	0

- Molecule 27 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BD	121	930	582	179	164	5	0	0

- Molecule 28 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BE	144	1052	654	207	189	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BF	136	1073	686	205	176	6	0	0

- Molecule 30 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BG	127	1007	621	204	177	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BH	117	899	557	179	162	1	0	0

- Molecule 32 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BI	114	916	574	179	162	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	BJ	117	946	604	192	150	0	0

- Molecule 34 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	BK	103	815	516	153	144	2	0	0

- Molecule 35 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BL	110	856	532	166	155	3	0	0

- Molecule 36 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BM	99	777	491	145	139	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BN	267	2053	1271	416	359	7	0	0

- Molecule 38 is a protein called 50S ribosomal protein L24.

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

- Molecule 39 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	BP	84	633	391	129	112	1	0	0

- Molecule 40 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BQ	63	508	313	99	94	2	0	0

- Molecule 41 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BR	58	448	281	87	78	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BS	70	548	339	104	99	6	0	0

- Molecule 43 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BT	56	443	269	94	79	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	BU	54	440	284	81	75	0	0

- Molecule 45 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BV	46	376	228	90	56	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BW	64	503	323	105	73	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BX	38	301	185	65	47	4	0	0

- Molecule 48 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BY	209	1564	979	288	293	4	0	0

- Molecule 49 is a protein called 50S ribosomal protein L1P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BZ	213	1687	1078	300	308	1	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BZ	1	MET	-	insertion	UNP P35024
BZ	?	-	MET	deletion	UNP P35024
BZ	70	SER	PHE	conflict	UNP P35024
BZ	82	LYS	ASN	conflict	UNP P35024
BZ	?	-	MET	deletion	UNP P35024
BZ	?	-	MET	deletion	UNP P35024
BZ	?	-	MET	deletion	UNP P35024

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	B1	201	1551	974	283	289	5	0	0

- Molecule 51 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	B2	178	1419	905	251	257	6	0	0

- Molecule 52 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	B3	176	1322	832	243	245	2	0	0

- Molecule 53 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	B4	149	1110	699	197	213	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	B5	141	1031	651	179	195	6	0	0

- Molecule 55 is a protein called 50S ribosomal protein L13.

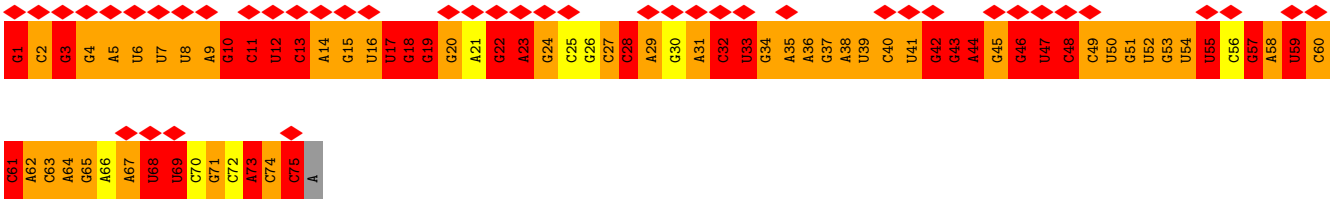
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	B6	140	1112	704	210	194	4	0	0

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.

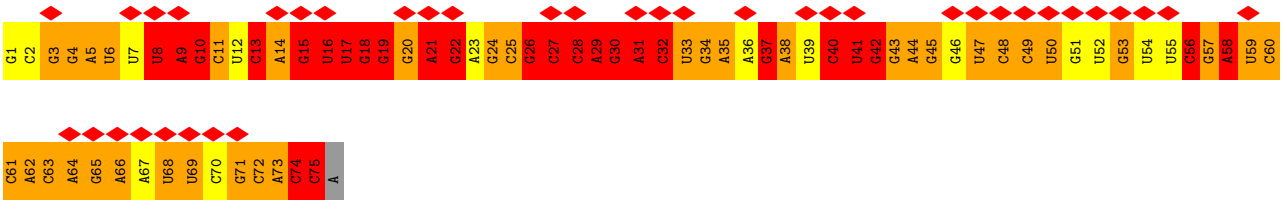
- Molecule 1: A/T, P and E-site tRNAs

Chain AA:



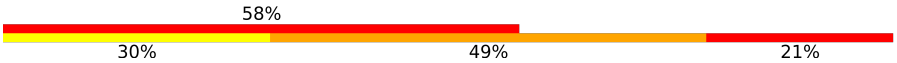
- Molecule 1: A/T, P and E-site tRNAs

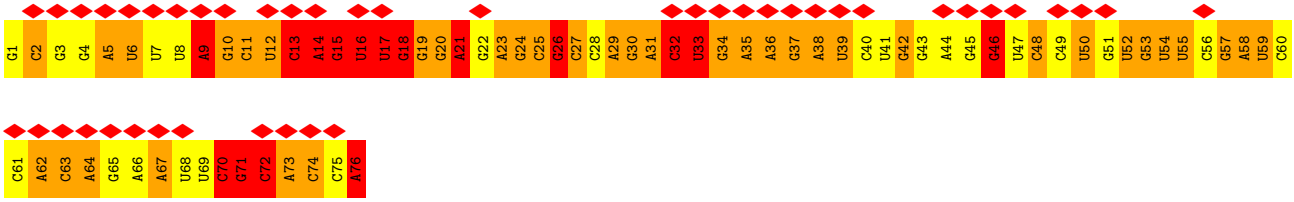
Chain AP:



- Molecule 1: A/T, P and E-site tRNAs

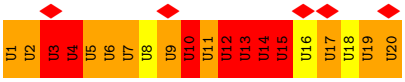
Chain AE:





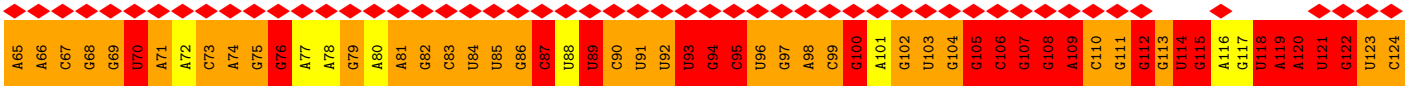
- Molecule 2: mRNA model

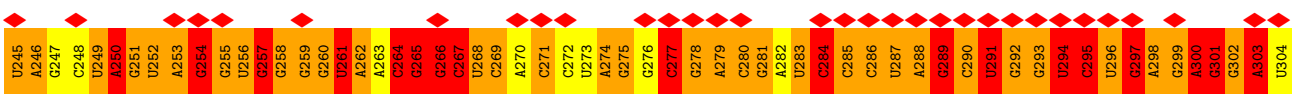
Chain AM:

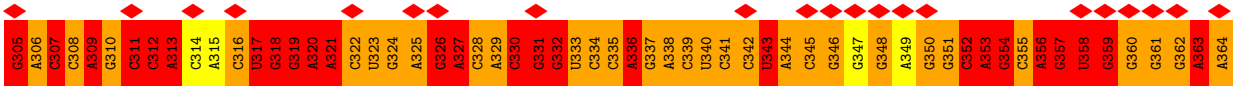


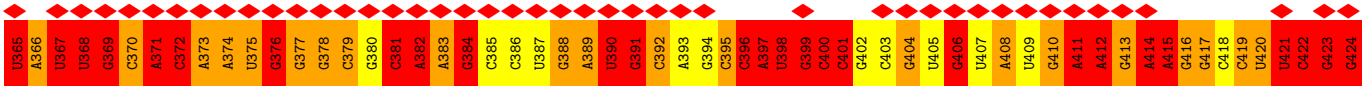
- Molecule 3: 16S rRNA

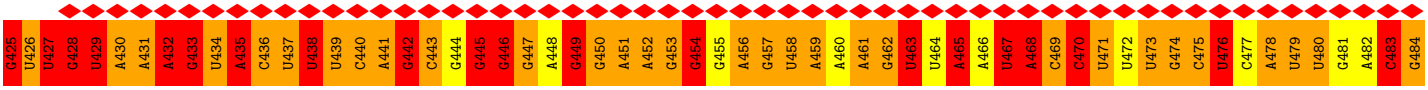
Chain A1:

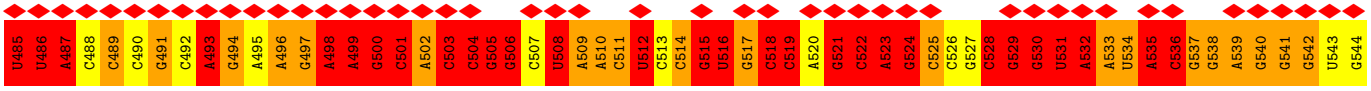


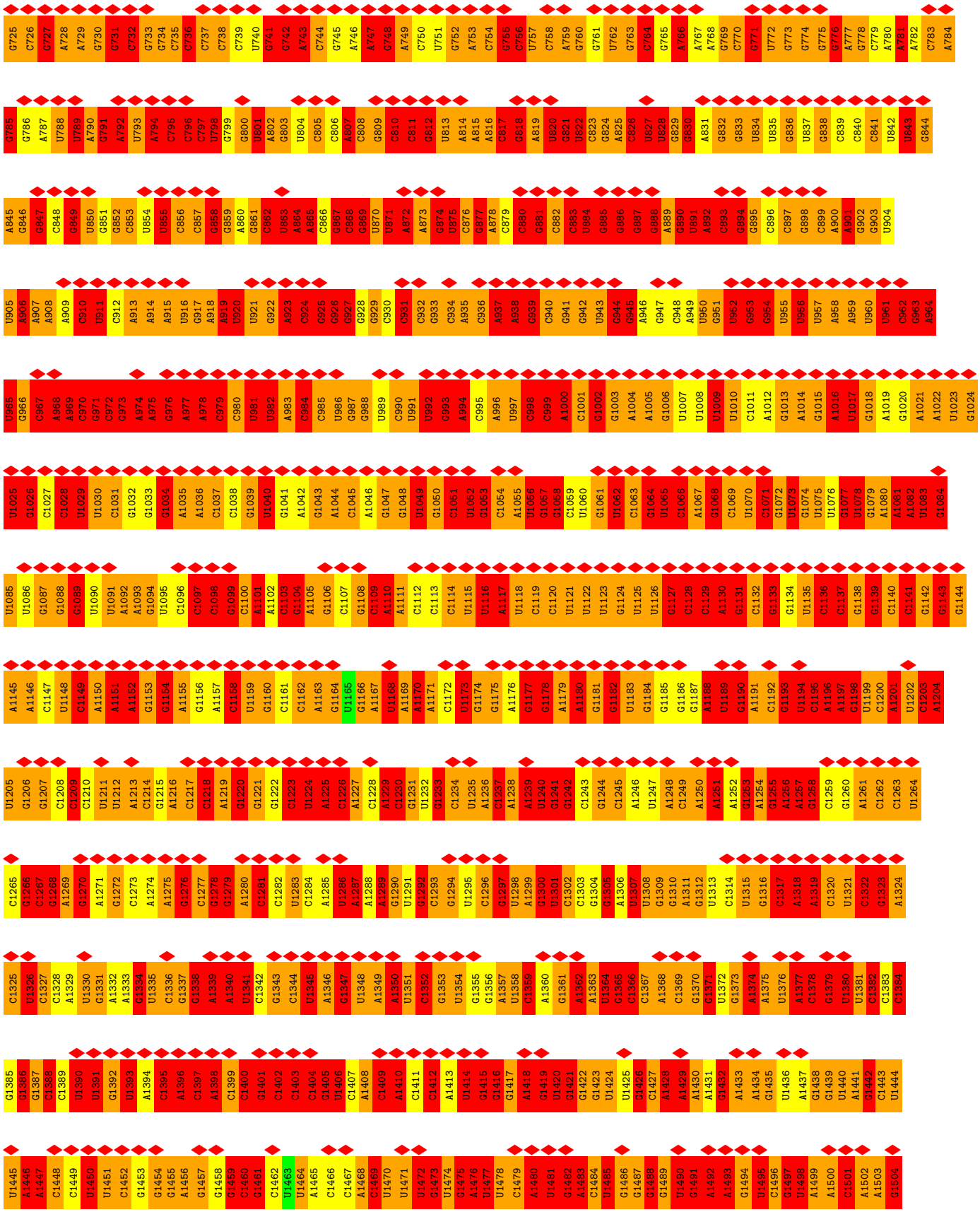








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- Molecule 4: 30S ribosomal protein S2

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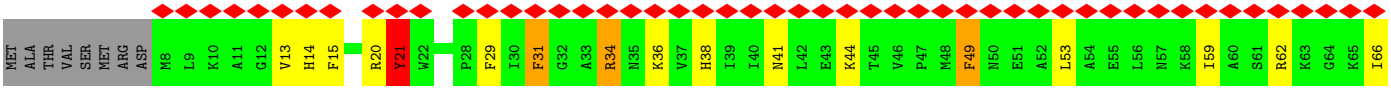

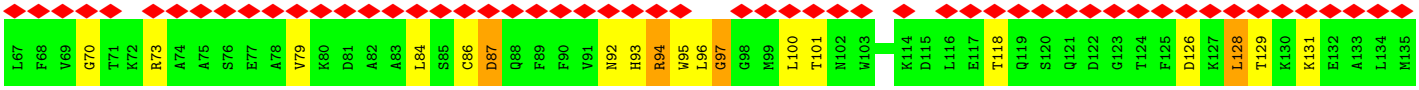

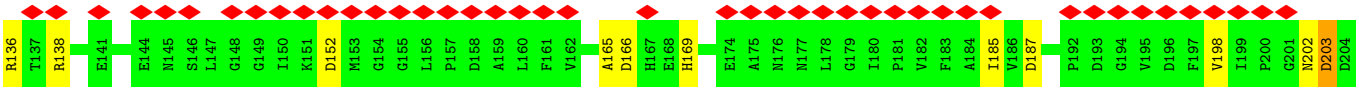

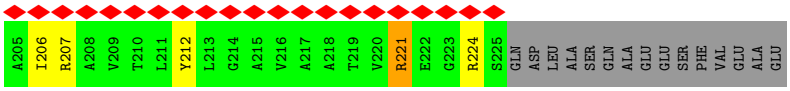

- Molecule 5: 30S ribosomal protein S11

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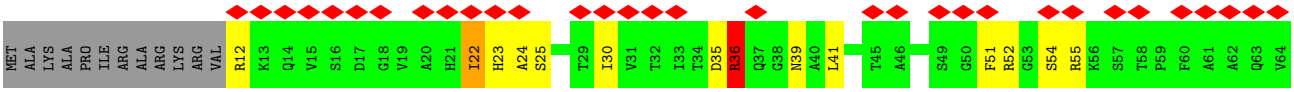
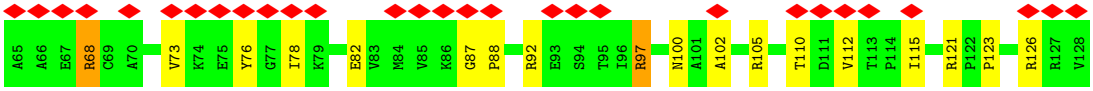
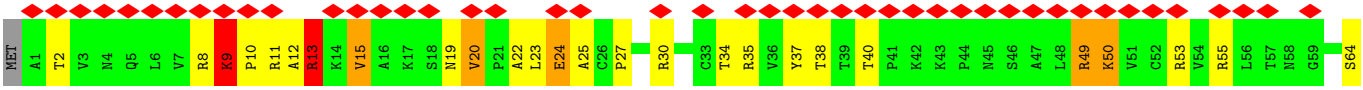
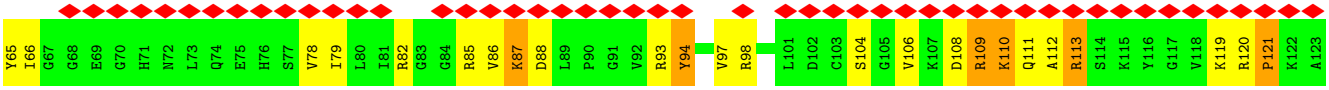




- Molecule 6: 30S ribosomal protein S12

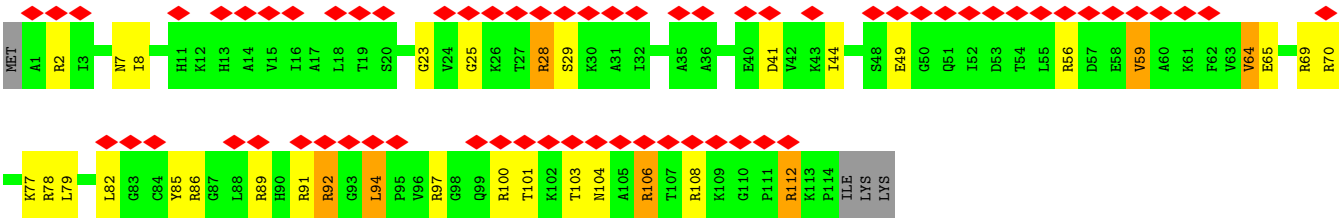
Chain AD:





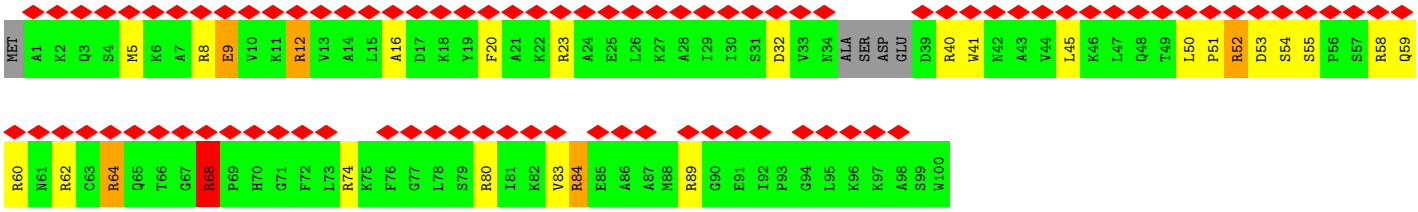
- Molecule 7: 30S ribosomal protein S13

Chain AF:



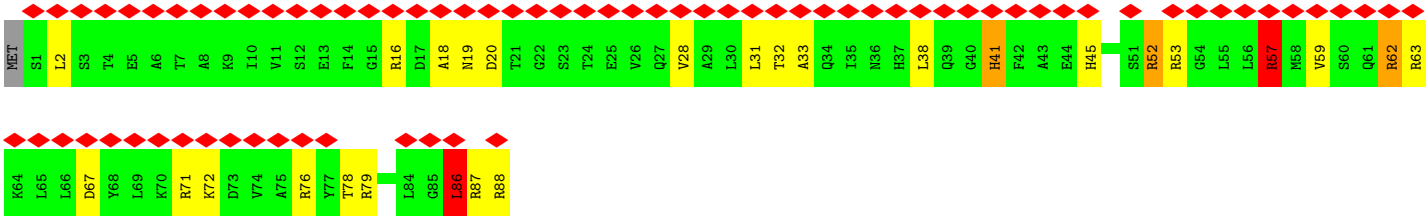
- Molecule 8: 30S ribosomal protein S14

Chain AG:



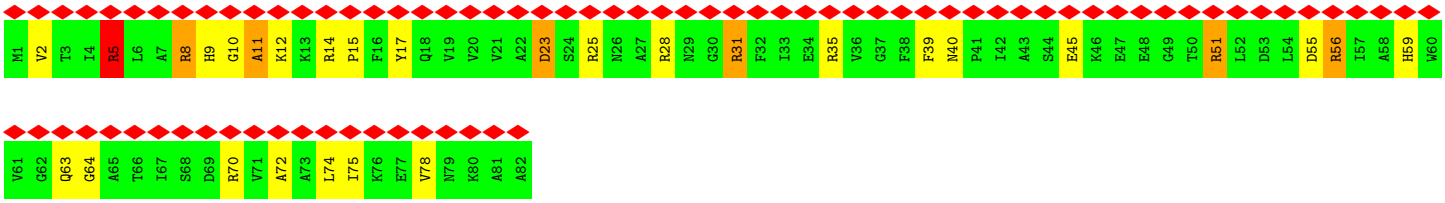
- Molecule 9: 30S ribosomal protein S15

Chain AH:



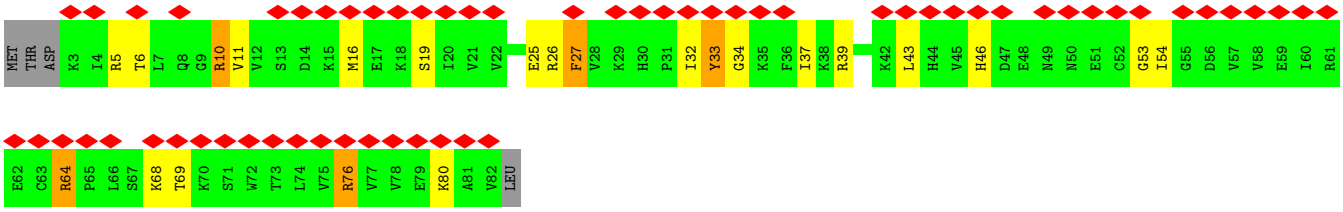
- Molecule 10: 30S ribosomal protein S16

Chain AI:



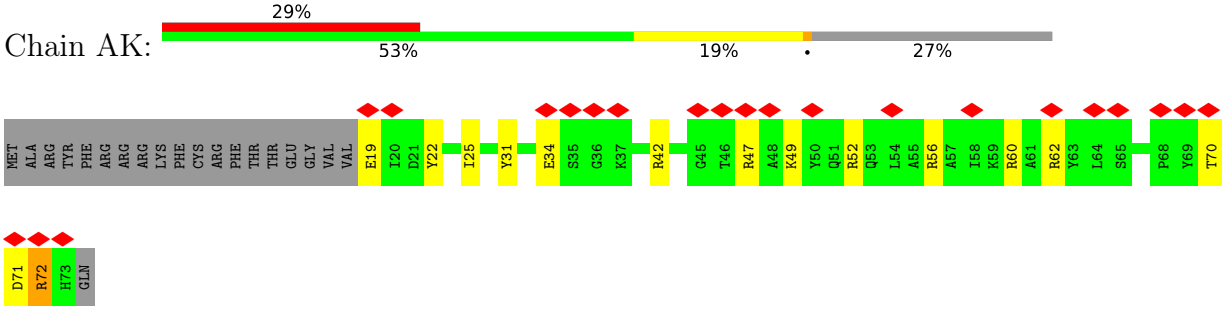
- Molecule 11: 30S ribosomal protein S17

Chain AJ:



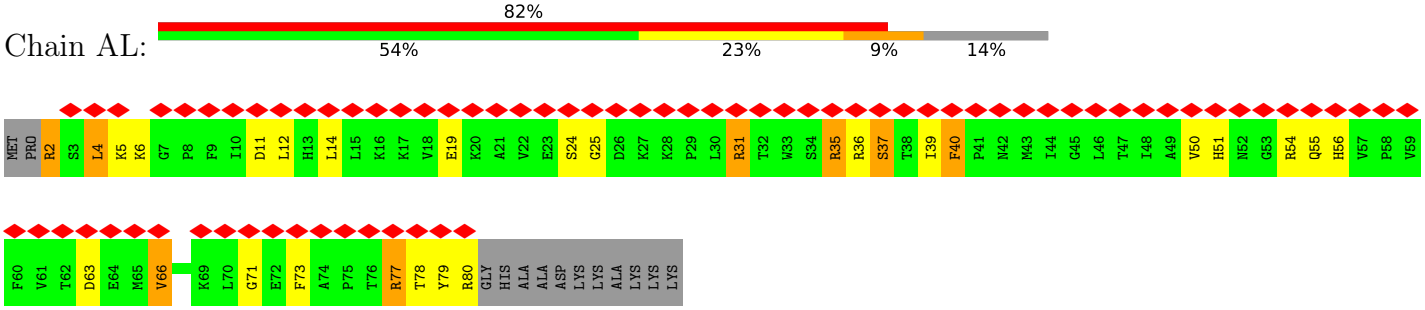
- Molecule 12: 30S ribosomal protein S18

Chain AK:



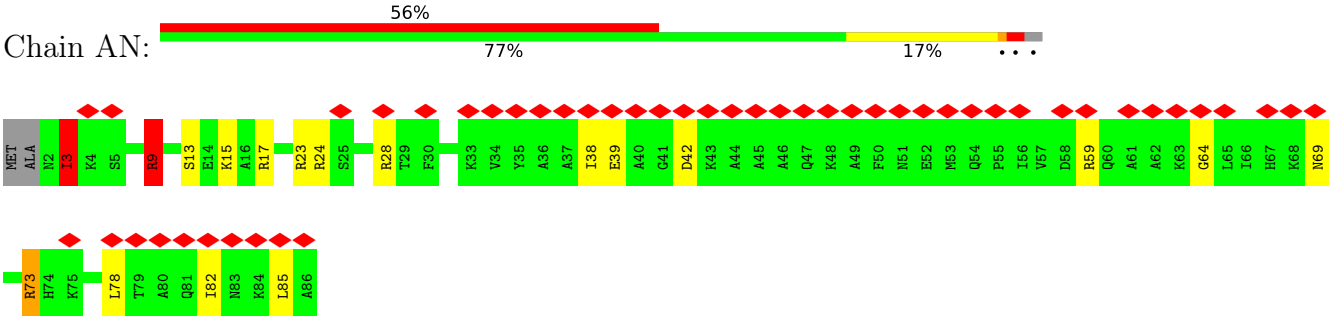
- Molecule 13: 30S ribosomal protein S19

Chain AL:



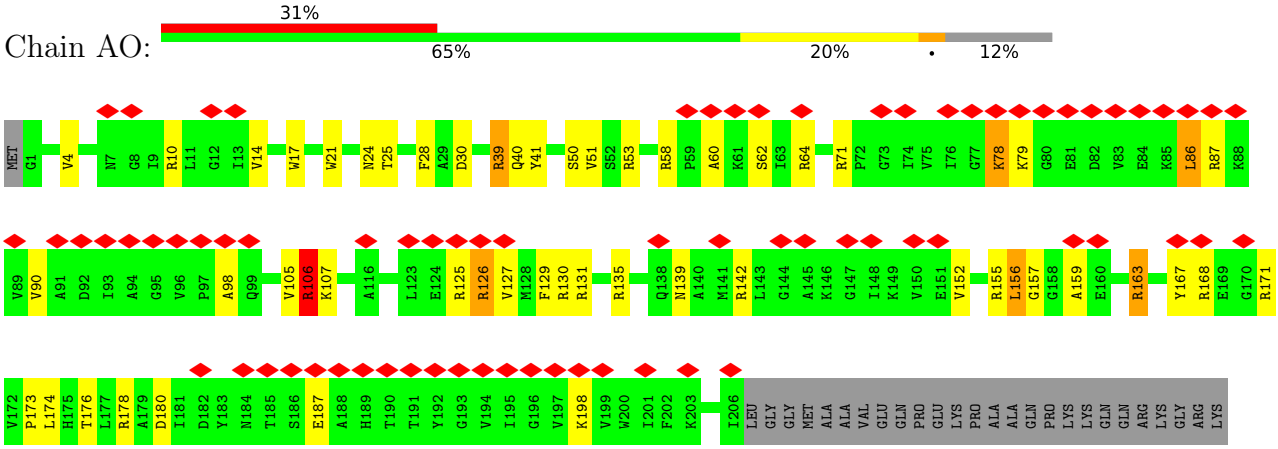
- Molecule 14: 30S ribosomal protein S20

Chain AN:



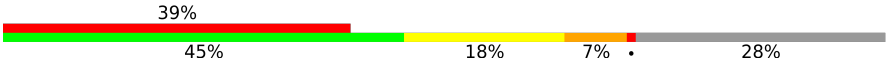
- Molecule 15: 30S ribosomal protein S3

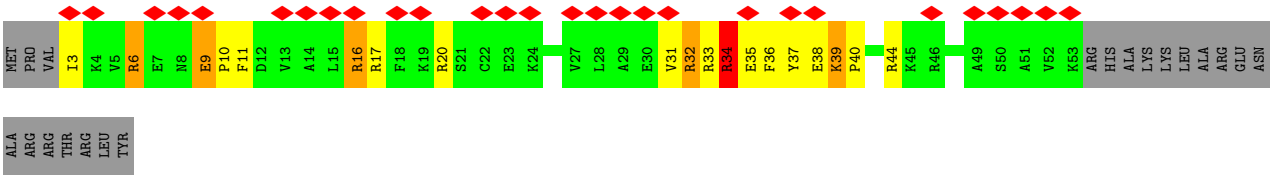
Chain AO:



- Molecule 16: 30S ribosomal protein S21

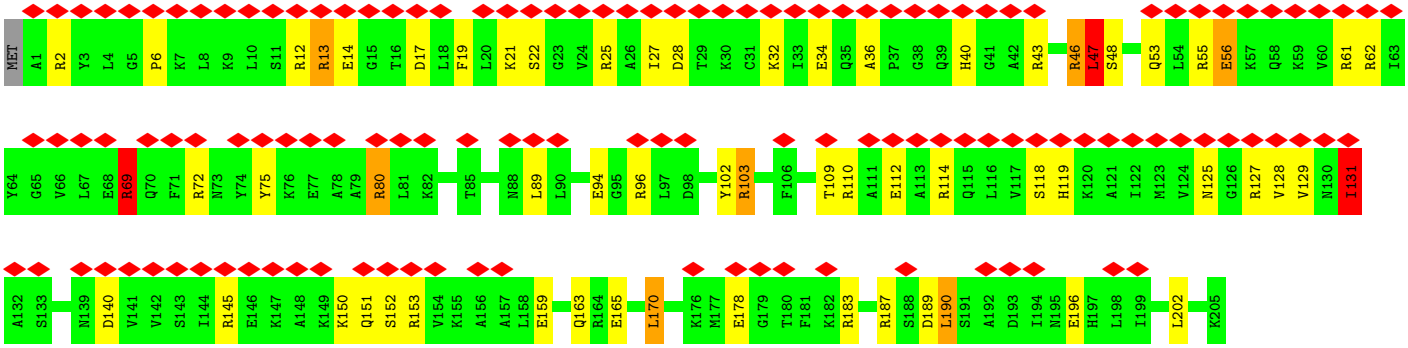
Chain AQ:





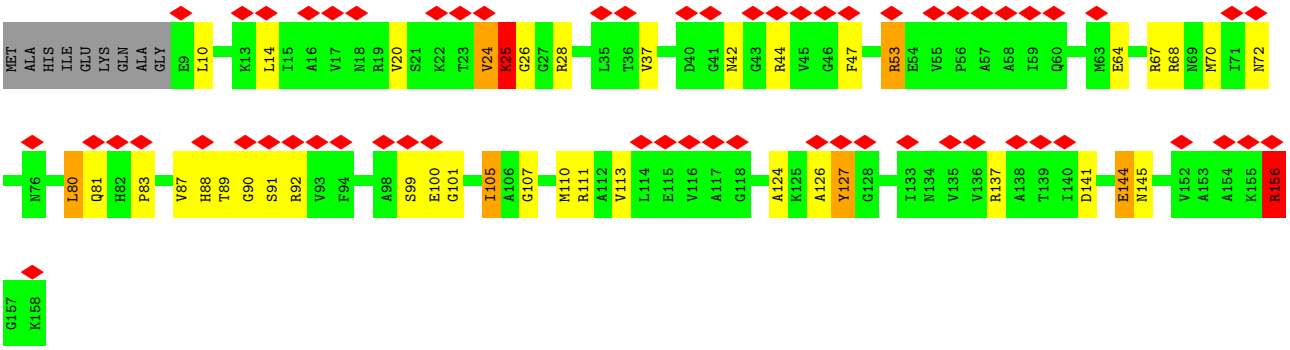
- Molecule 17: 30S ribosomal protein S4

Chain AR:



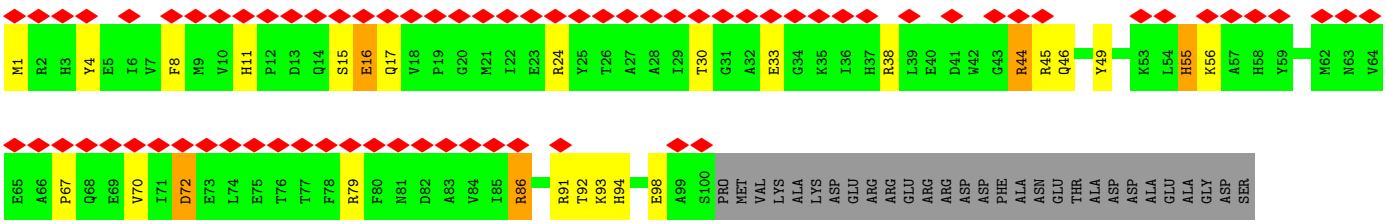
- Molecule 18: 30S ribosomal protein S5

Chain AS:



- Molecule 19: 30S ribosomal protein S6

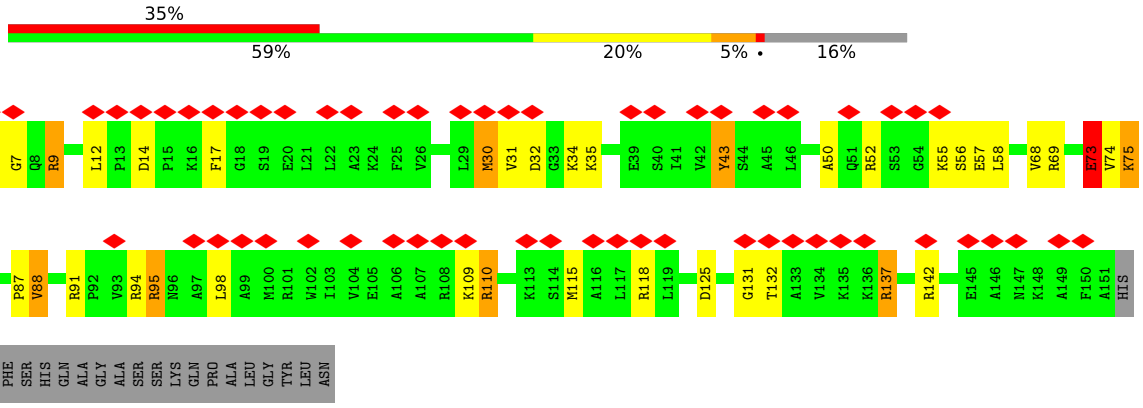
Chain AT:



GLU GLU GLU GLU GLU GLU

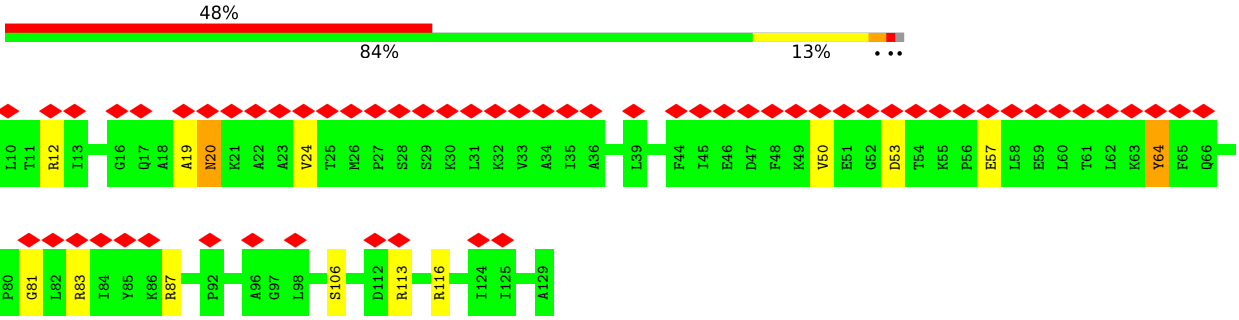
- Molecule 20: 30S ribosomal protein S7

Chain AU:



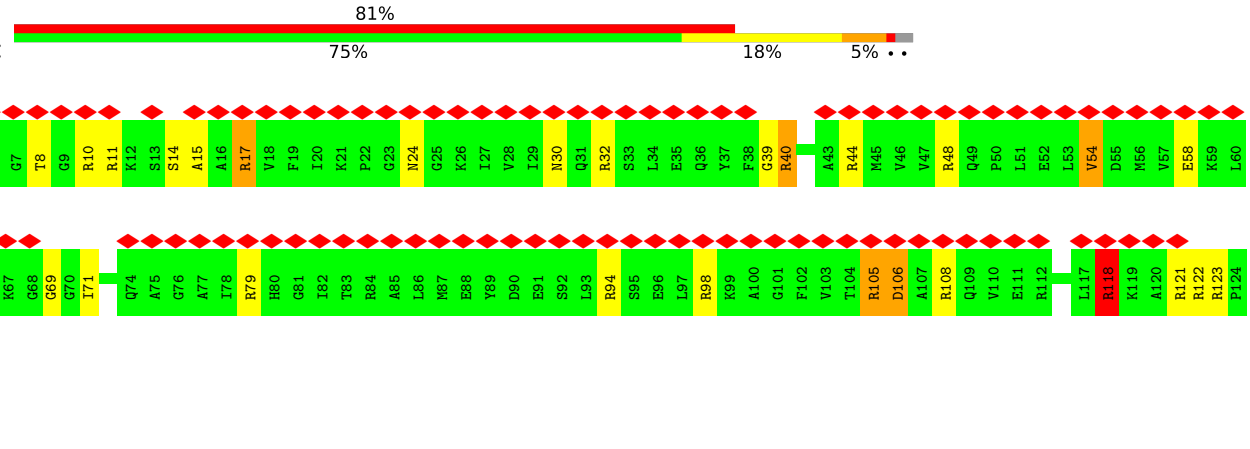
- Molecule 21: 30S ribosomal protein S8

Chain AV:



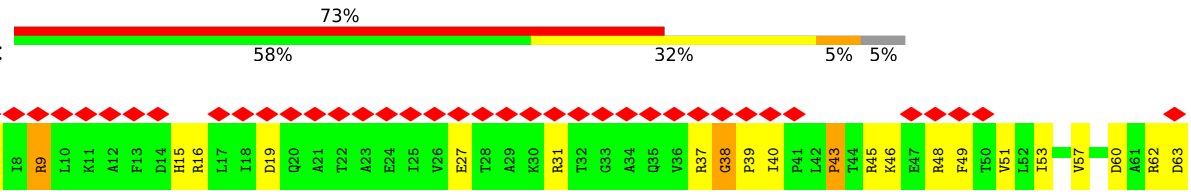
- Molecule 22: 30S ribosomal protein S9

Chain AW:



- Molecule 23: 30S ribosomal protein S10

Chain AX:



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- Molecule 24: 5S rRNA

Chain BA: 71% 25% 49% 26%

G2 C3 C4 U5 G6 G7 C8 G9 G10 C11 C12 G13 U14 A15 G16 C17 G18 C19 G20 G21 U22 G23 G24 U25 C26 C27 C28 A29 C30 C31 U32 G33 A34 C35 C36 C37 C38 A39 U40 G41 C42 C43 G44 A45 A46 C47 U48 C49 A50 G51 A52 A53 G54 U55 G56 A57 A58 A59 C60 G61

C62 C63 G64 U65 A66 G67 C68 G69 C70 C71 G72 A73 U74 G75 G76 U77 A78 G79 U80 G81 U82 G83 G84 G85 G86 U87 C88 U89 C90 C91 C92 C93 A94 U95 G96 C97 G98 A99 G100 A101 G102 U103 A104 G105 G106 G107 A108 A109 C110 U111 G112 C113 C114 A115 G116 G117 C118

- Molecule 25: 23S rRNA

Chain BB: 52% 17% 44% 39%

G1 G2 U3 U4 A5 A6 G7 C8 G9 A10 C11 U12 A13 A14 G15 C16 G17 U18 A19 C20 A21 C22 G23 G24 U25 G26 G27 A28 U29 G30 C31 C32 C33 U34 G35 G36 C37 A38 G39 U40 C41 A42 G43 A44 G45 G46 C47 G48 A49 U50 G51 A52 A53 G54 G55 A56 C57 G58 U59 G60

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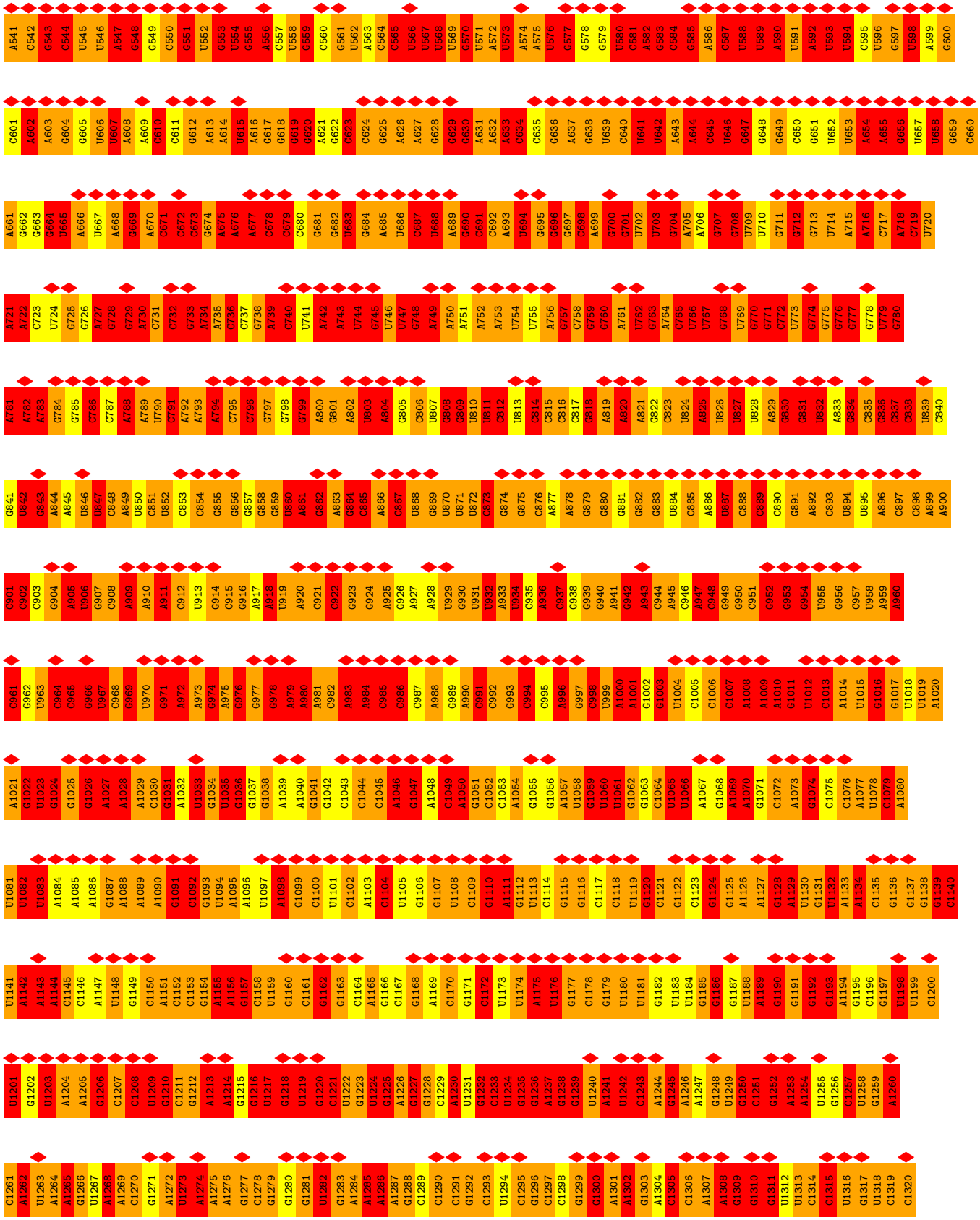
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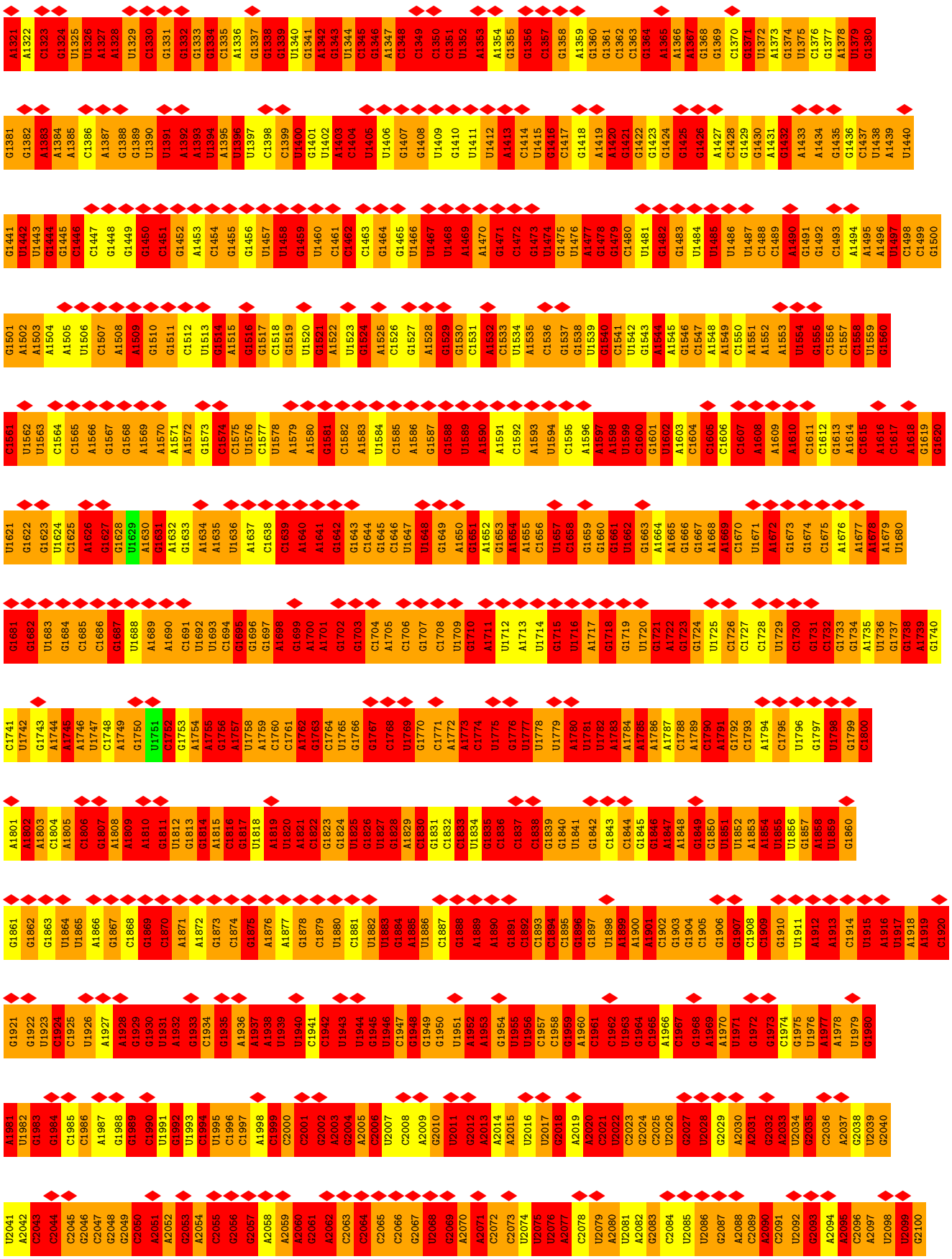
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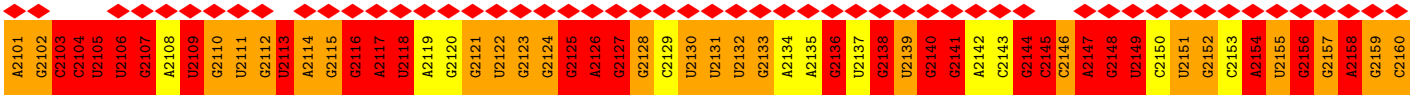
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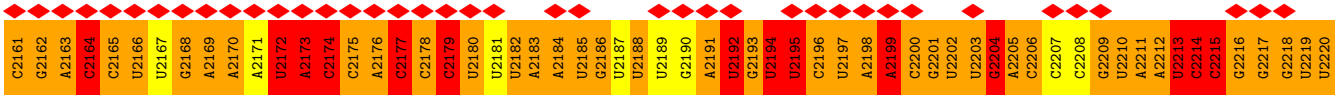
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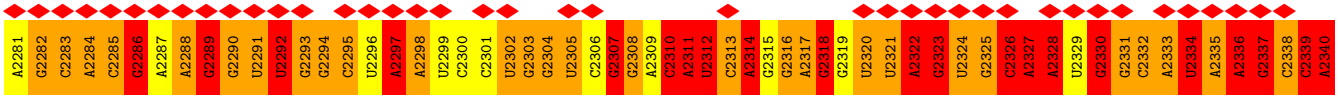
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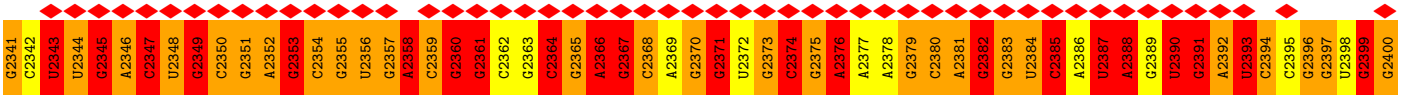
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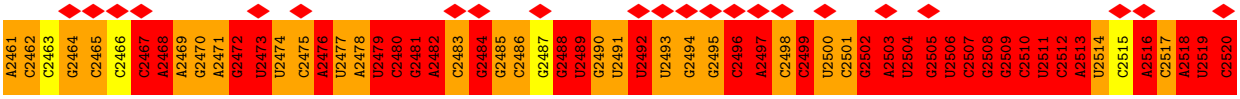
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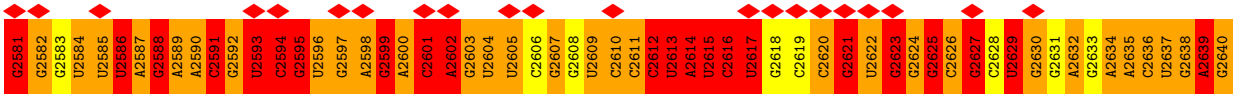
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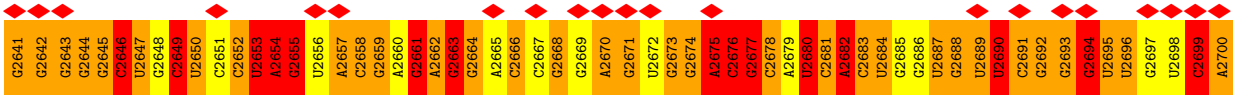
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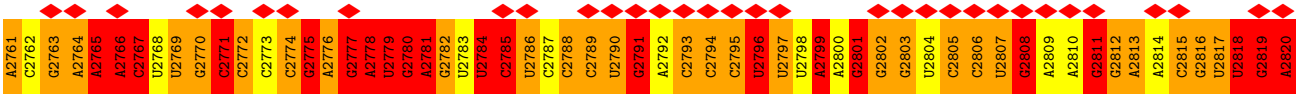
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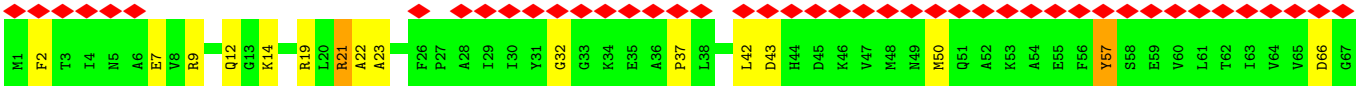
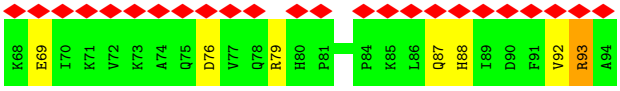
A2821 G2822 A2823 C2824 G2825 A2826 C2827 G2828 A2829 C2830 G2831 U2832 U2833 G2834 A2835 U2836 A2837 G2838 G2839 C2840 C2841 G2842 G2843 G2844 U2845 G2846 U2847 G2848 U2849 A2850 A2851 G2852 C2853 G2854 C2855 A2856 G2857 C2858 G2859 A2860 U2861 G2862 C2863 G2864 U2865 U2866 G2867 A2868 G2869 C2870 U2871 A2872 A2873 C2874 C2875 G2876 G2877 U2878 A2879 C2880

• Molecule 26: 50S ribosomal protein L25

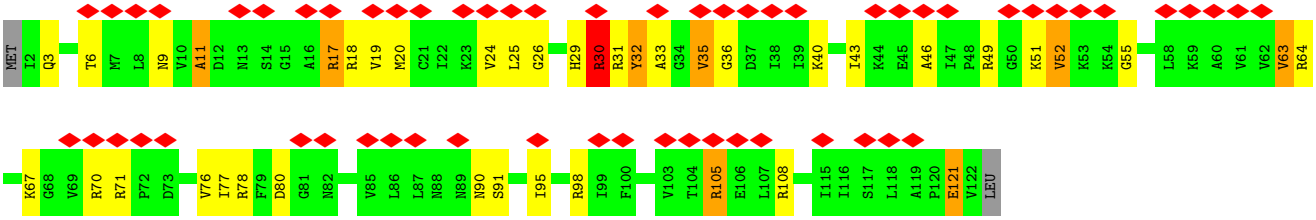
Chain BC:





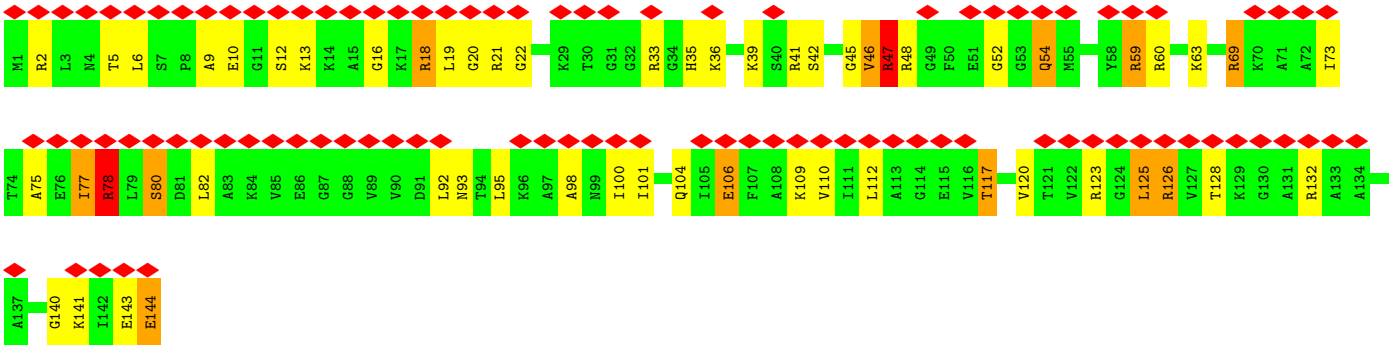
• Molecule 27: 50S ribosomal protein L14

Chain BD:



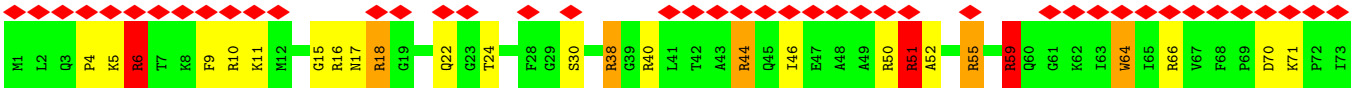
• Molecule 28: 50S ribosomal protein L15

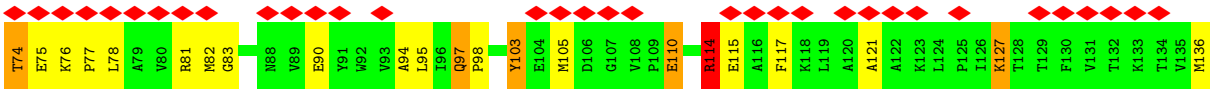
Chain BE:



• Molecule 29: 50S ribosomal protein L16

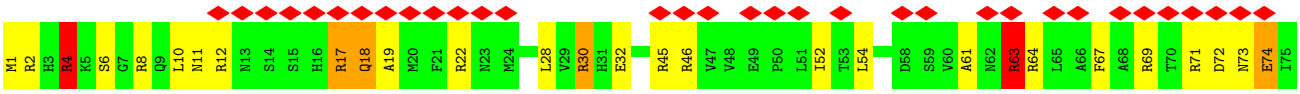
Chain BF:

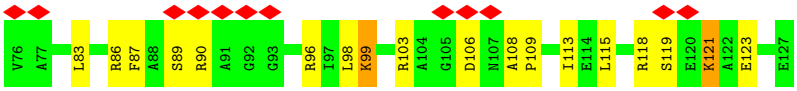




- Molecule 30: 50S ribosomal protein L17

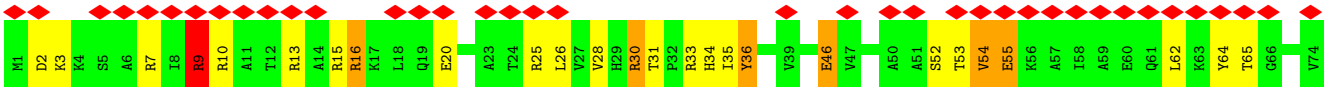
Chain BG:

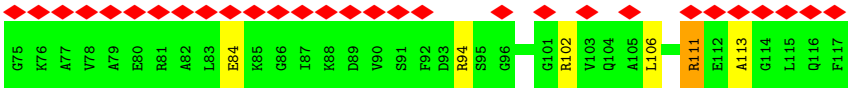




- Molecule 31: 50S ribosomal protein L18

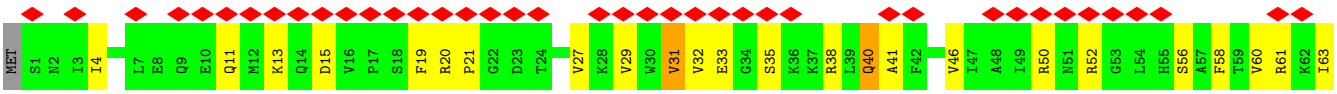
Chain BH:

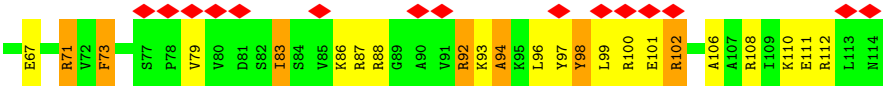




- Molecule 32: 50S ribosomal protein L19

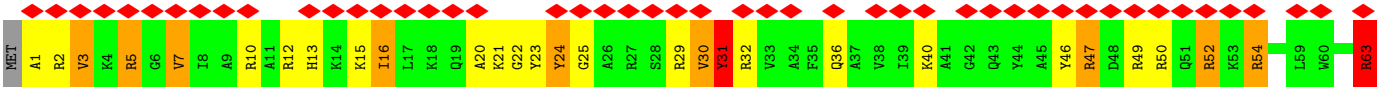
Chain BI:

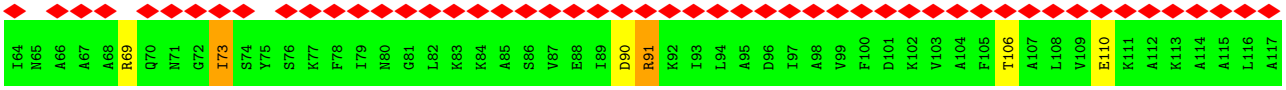




- Molecule 33: 50S ribosomal protein L20

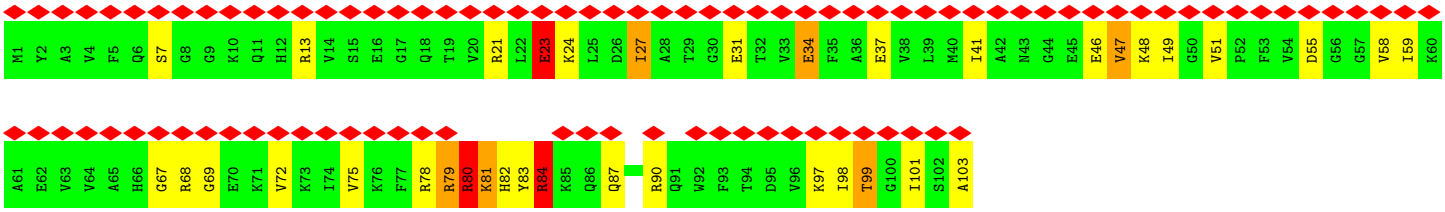
Chain BJ:





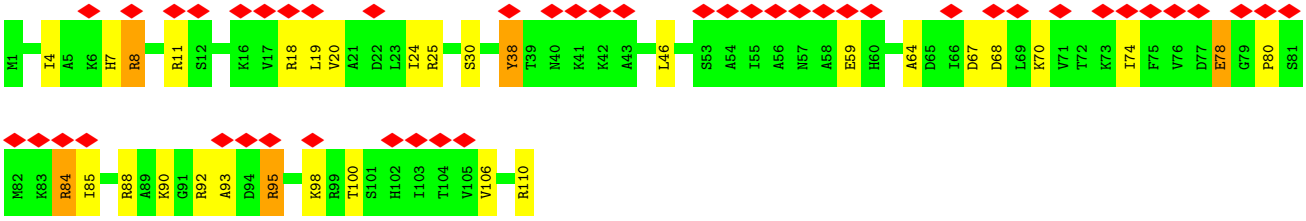
- Molecule 34: 50S ribosomal protein L21

Chain BK: 92% 64% 27% 6%



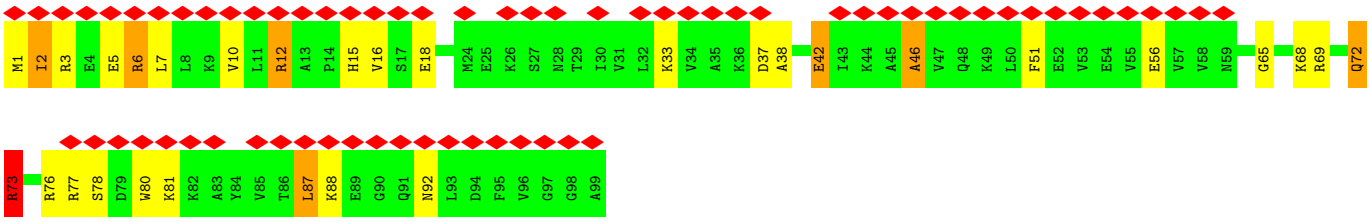
- Molecule 35: 50S ribosomal protein L22

Chain BL: 42% 72% 24% 5%



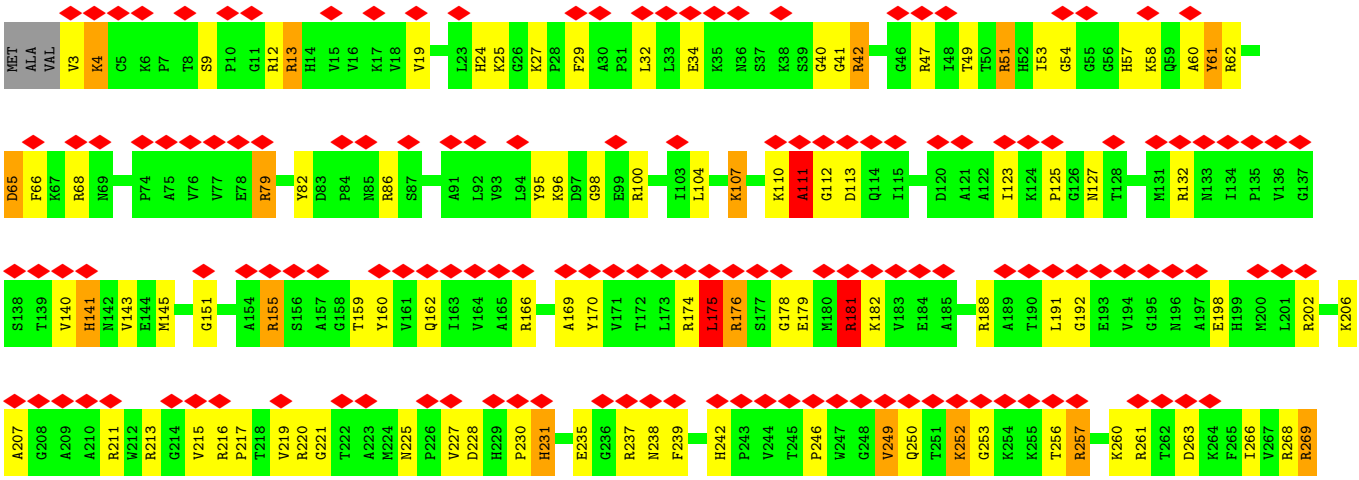
- Molecule 36: 50S ribosomal protein L23

Chain BM: 69% 69% 23% 7%



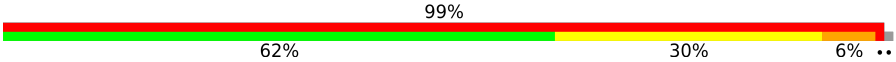
- Molecule 37: 50S ribosomal protein L2

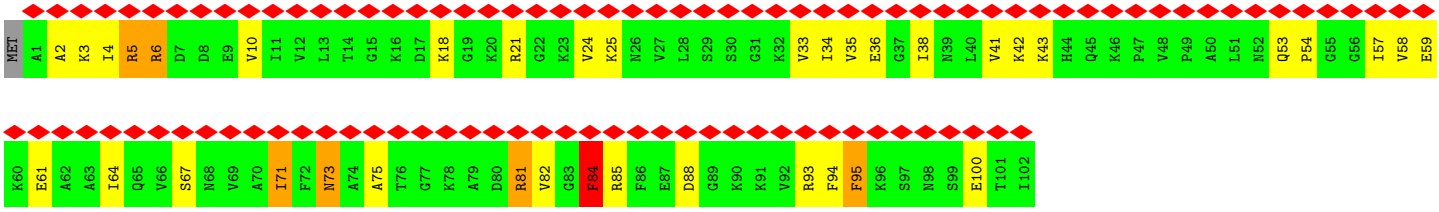
Chain BN: 54% 61% 31% 6%



- Molecule 38: 50S ribosomal protein L24

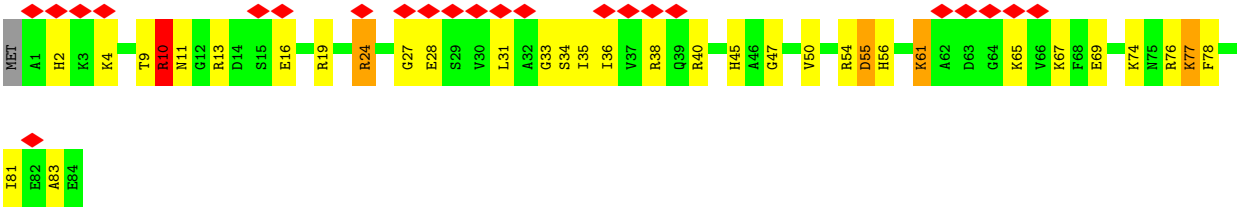
Chain BO:





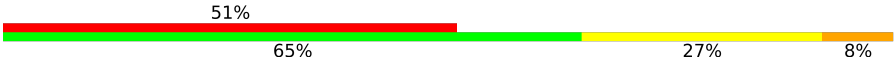
- Molecule 39: 50S ribosomal protein L27

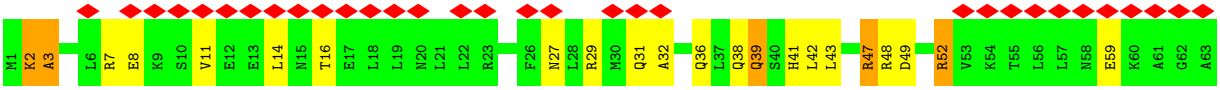
Chain BP:



- Molecule 40: 50S ribosomal protein L29

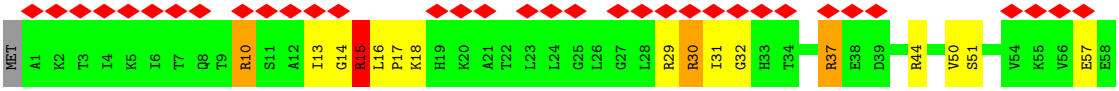
Chain BQ:





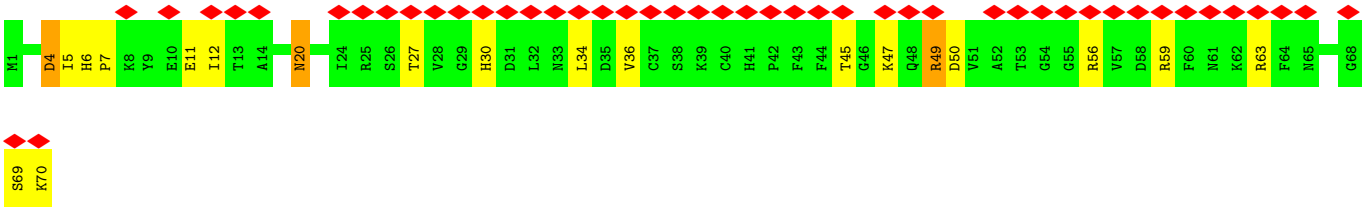
- Molecule 41: 50S ribosomal protein L30

Chain BR:



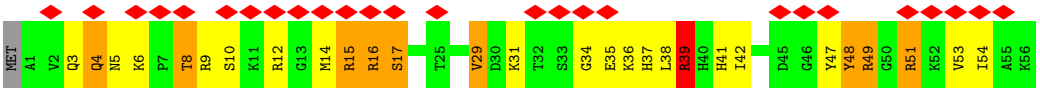
- Molecule 42: 50S ribosomal protein L31

Chain BS:



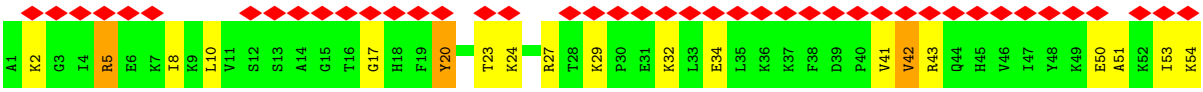
- Molecule 43: 50S ribosomal protein L32

Chain BT: 46% 49% 32% 16%



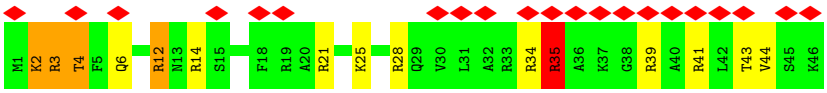
- Molecule 44: 50S ribosomal protein L33

Chain BU: 80% 65% 30% 6%



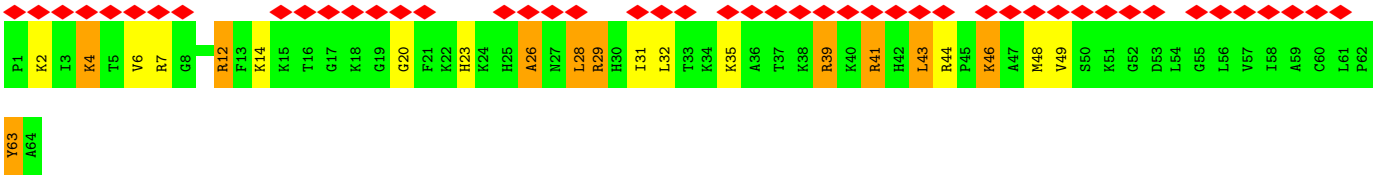
- Molecule 45: 50S ribosomal protein L34

Chain BV: 46% 67% 22% 9%



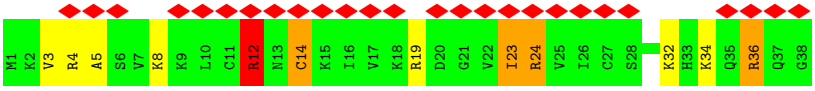
- Molecule 46: 50S ribosomal protein L35

Chain BW: 73% 66% 19% 16%



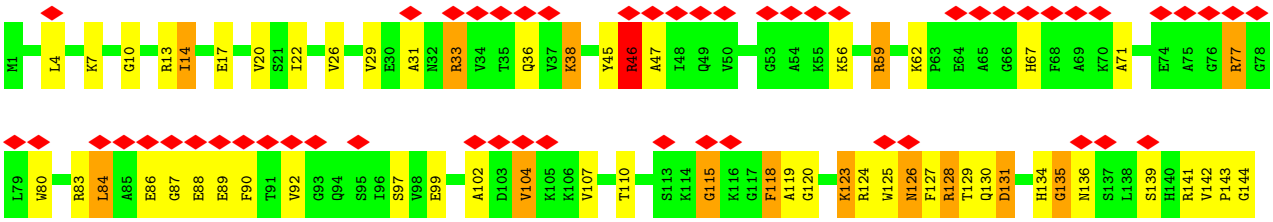
- Molecule 47: 50S ribosomal protein L36

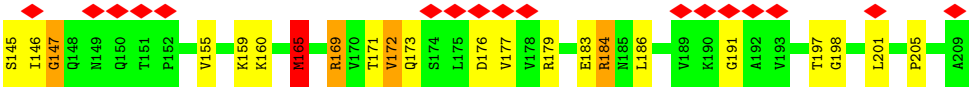
Chain BX: 68% 68% 18% 11%



- Molecule 48: 50S ribosomal protein L3

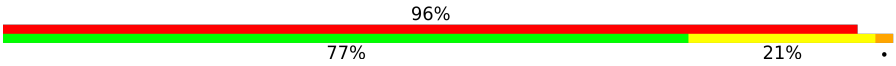
Chain BY: 33% 61% 29% 9%

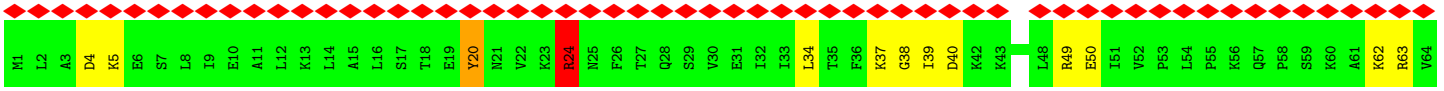


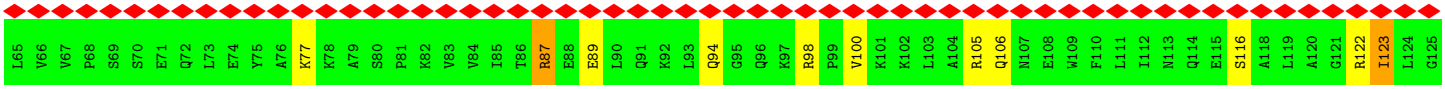


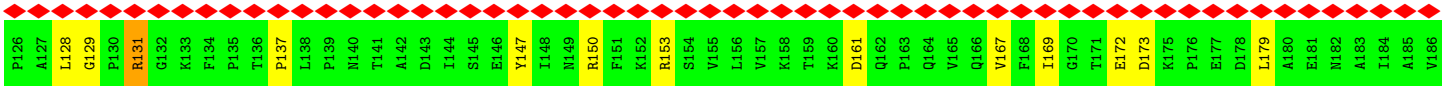
- Molecule 49: 50S ribosomal protein L1P

Chain BZ:



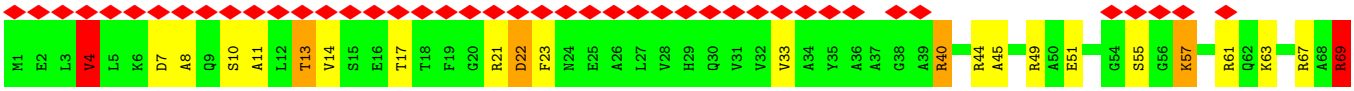


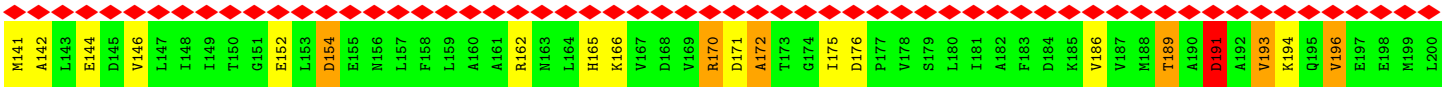




- Molecule 50: 50S ribosomal protein L4

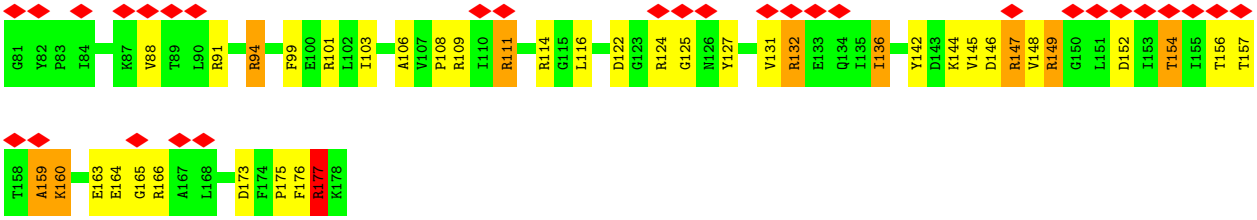
Chain B1:





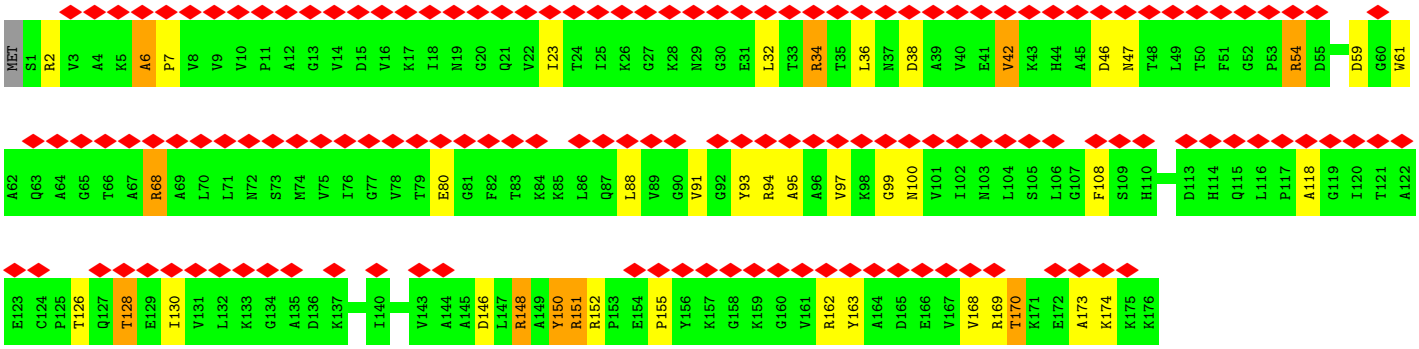
- Molecule 51: 50S ribosomal protein L5

Chain B2:



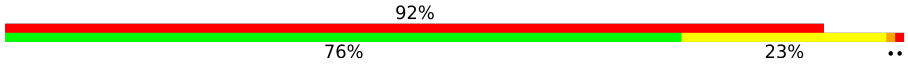
• Molecule 52: 50S ribosomal protein L6

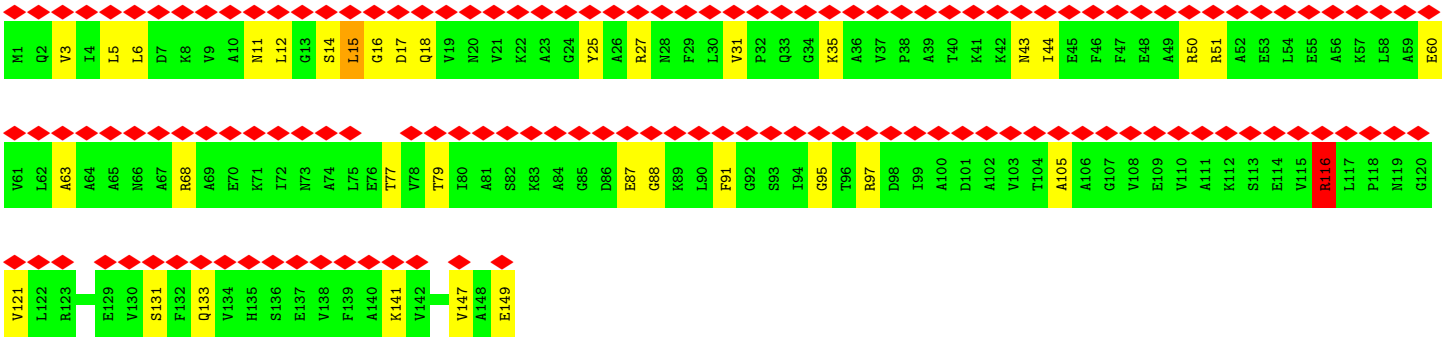
Chain B3:



• Molecule 53: 50S ribosomal protein L9

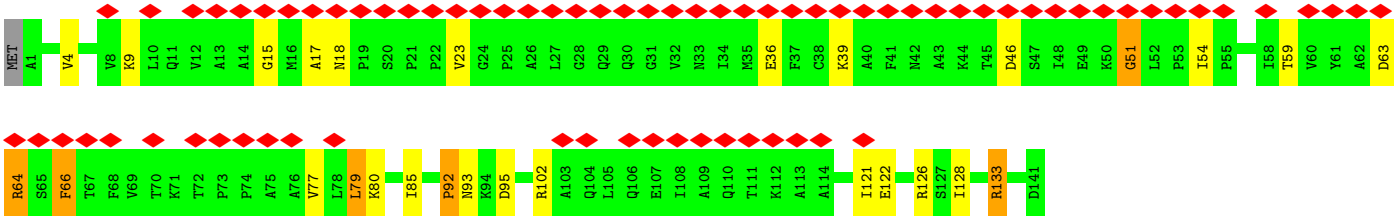
Chain B4:





• Molecule 54: 50S ribosomal protein L11

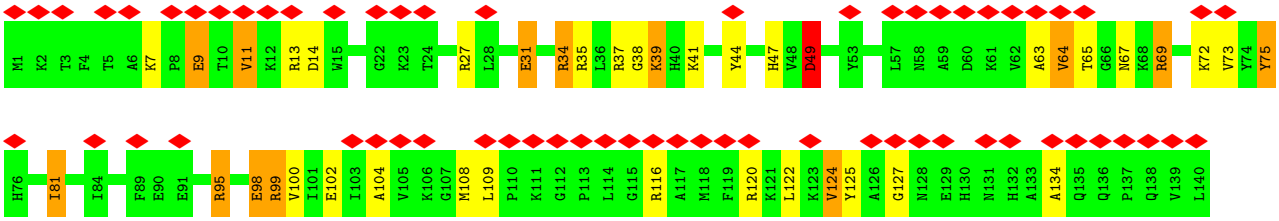
Chain B5:



• Molecule 55: 50S ribosomal protein L13

Chain B6:

45%
71%
19%
9%


M1 K2 T3 F4 T5 A6 K7 P8 E9 T10 V11 K12 R13 D14 W15 G22 K23 T24 R27 L28 E31 R34 R35 L36 R37 G38 K39 H40 K41 Y44 H47 V48 D49 Y53 L57 N58 A59 D60 K61 V62 A63 V64 T65 G66 N67 K68 R69 K72 V73 Y74 Y75
H76 I81 I84 F89 E90 E91 R95 E98 R99 V100 I101 E102 I103 A104 V105 K106 G107 M108 L109 P110 K111 G112 P113 L114 G115 R116 A117 M118 F119 R120 K121 L122 K123 V124 Y125 A126 G127 N128 E129 H130 N131 H132 A133 A134 Q135 Q136 P137 Q138 V139 L140

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75996	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	250.984	Depositor
Minimum map value	-85.859	Depositor
Average map value	4.444	Depositor
Map value standard deviation	25.344	Depositor
Recommended contour level	57.2	Depositor
Map size (Å)	366.6, 366.6, 366.6	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.82, 2.82, 2.82	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	AA	2.55	109/1789 (6.1%)	3.85	439/2788 (15.7%)
1	AE	2.27	78/1814 (4.3%)	3.60	403/2827 (14.3%)
1	AP	3.55	99/1789 (5.5%)	3.96	389/2788 (14.0%)
2	AM	2.44	19/436 (4.4%)	3.59	99/672 (14.7%)
3	A1	2.55	1627/36759 (4.4%)	3.68	8418/57346 (14.7%)
4	AB	0.97	2/1735 (0.1%)	1.84	41/2338 (1.8%)
5	AC	1.10	5/892 (0.6%)	1.74	19/1205 (1.6%)
6	AD	1.14	2/968 (0.2%)	2.24	38/1300 (2.9%)
7	AF	1.16	7/892 (0.8%)	2.21	32/1193 (2.7%)
8	AG	1.13	3/785 (0.4%)	2.22	33/1046 (3.2%)
9	AH	1.13	5/723 (0.7%)	2.18	30/966 (3.1%)
10	AI	1.17	4/658 (0.6%)	2.16	20/884 (2.3%)
11	AJ	0.99	2/657 (0.3%)	1.87	11/881 (1.2%)
12	AK	1.19	5/462 (1.1%)	1.98	15/621 (2.4%)
13	AL	1.08	2/652 (0.3%)	1.96	14/877 (1.6%)
14	AN	1.03	4/670 (0.6%)	1.87	14/888 (1.6%)
15	AO	1.08	6/1651 (0.4%)	1.94	43/2225 (1.9%)
16	AQ	1.23	2/430 (0.5%)	2.26	19/570 (3.3%)
17	AR	1.08	2/1664 (0.1%)	1.94	46/2227 (2.1%)
18	AS	1.02	2/1118 (0.2%)	1.70	19/1504 (1.3%)
19	AT	1.03	1/835 (0.1%)	1.81	13/1128 (1.2%)
20	AU	1.12	4/1187 (0.3%)	1.97	33/1591 (2.1%)
21	AV	0.95	1/988 (0.1%)	1.65	14/1326 (1.1%)
22	AW	1.13	1/1033 (0.1%)	1.98	27/1375 (2.0%)
23	AX	1.03	2/796 (0.3%)	2.11	28/1077 (2.6%)
24	BA	2.22	97/2800 (3.5%)	3.50	592/4367 (13.6%)
25	BB	2.24	2712/69795 (3.9%)	3.62	15539/108884 (14.3%)
26	BC	1.01	1/765 (0.1%)	1.78	11/1025 (1.1%)
27	BD	1.11	4/939 (0.4%)	2.36	28/1258 (2.2%)
28	BE	1.13	2/1061 (0.2%)	1.97	25/1413 (1.8%)
29	BF	1.09	3/1092 (0.3%)	2.16	36/1460 (2.5%)
30	BG	1.16	6/1020 (0.6%)	2.13	43/1364 (3.2%)
31	BH	1.11	1/909 (0.1%)	2.12	33/1219 (2.7%)
32	BI	1.15	4/928 (0.4%)	2.04	30/1242 (2.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BJ	1.18	4/959 (0.4%)	1.97	27/1278 (2.1%)
34	BK	1.05	1/828 (0.1%)	2.02	23/1107 (2.1%)
35	BL	0.98	0/863	1.86	17/1156 (1.5%)
36	BM	0.99	2/784 (0.3%)	1.93	18/1048 (1.7%)
37	BN	1.10	9/2092 (0.4%)	1.99	65/2813 (2.3%)
38	BO	1.03	1/787 (0.1%)	1.87	18/1051 (1.7%)
39	BP	1.05	1/641 (0.2%)	2.02	17/848 (2.0%)
40	BQ	1.02	0/509	2.09	13/677 (1.9%)
41	BR	0.99	2/452 (0.4%)	2.05	14/605 (2.3%)
42	BS	1.04	0/558	1.99	13/745 (1.7%)
43	BT	1.10	0/449	2.22	16/599 (2.7%)
44	BU	1.08	0/447	1.81	8/594 (1.3%)
45	BV	1.16	0/379	2.33	18/498 (3.6%)
46	BW	0.99	0/512	1.74	9/676 (1.3%)
47	BX	1.07	1/302 (0.3%)	2.23	8/397 (2.0%)
48	BY	0.99	3/1585 (0.2%)	1.98	42/2134 (2.0%)
49	BZ	0.98	3/1711 (0.2%)	1.64	26/2305 (1.1%)
50	B1	1.01	0/1570	1.86	35/2113 (1.7%)
51	B2	1.07	2/1443 (0.1%)	1.88	40/1937 (2.1%)
52	B3	1.01	0/1342	1.81	32/1816 (1.8%)
53	B4	0.97	1/1121 (0.1%)	1.74	16/1515 (1.1%)
54	B5	0.94	0/1045	1.71	11/1410 (0.8%)
55	B6	1.02	1/1135 (0.1%)	1.95	28/1529 (1.8%)
All	All	2.08	4855/162206 (3.0%)	3.29	27108/242726 (11.2%)

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
1	AA	0	55
1	AE	0	49
1	AP	2	50
2	AM	0	9
3	A1	4	945
4	AB	0	3
5	AC	0	3
6	AD	0	7
7	AF	0	5
8	AG	0	4
9	AH	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	AI	0	3
11	AJ	0	4
13	AL	0	8
14	AN	1	1
15	AO	0	3
16	AQ	0	4
17	AR	0	7
18	AS	0	3
19	AT	0	4
20	AU	0	4
21	AV	0	2
22	AW	0	4
23	AX	0	4
24	BA	0	66
25	BB	3	1717
26	BC	0	3
27	BD	0	6
28	BE	0	6
29	BF	0	4
30	BG	0	4
31	BH	0	1
32	BI	0	4
33	BJ	0	4
34	BK	0	5
35	BL	0	5
36	BM	0	1
37	BN	0	12
38	BO	0	4
39	BP	0	3
40	BQ	0	3
41	BR	0	3
42	BS	0	3
43	BT	0	2
44	BU	0	5
45	BV	0	2
46	BW	0	4
47	BX	0	2
48	BY	0	9
49	BZ	0	2
50	B1	0	9
51	B2	0	6
52	B3	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	B4	0	4
54	B5	0	3
55	B6	0	8
All	All	10	3101

The worst 5 of 4855 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A1	1429	A	P-O5'	178.16	3.38	1.59
3	A1	1340	A	C3'-O3'	99.95	2.82	1.42
1	AP	31	A	C4'-C3'	53.26	2.11	1.53
1	AP	31	A	C2'-C1'	45.01	2.02	1.53
1	AP	31	A	C4'-O4'	44.63	2.03	1.45

The worst 5 of 27108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AP	74	C	P-O3'-C3'	-78.58	25.40	119.70
1	AP	74	C	O3'-P-O5'	-40.02	27.95	104.00
25	BB	2376	A	N1-C6-N6	-29.09	101.15	118.60
3	A1	1225	A	N1-C6-N6	-28.97	101.22	118.60
3	A1	1250	A	N1-C6-N6	-27.68	101.99	118.60

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AP	31	A	C2',C1'
3	A1	13	U	C2',C1'
3	A1	1198	G	C4'
3	A1	1483	A	C2'
14	AN	13	SER	CA

5 of 3101 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1	G	Sidechain
1	AA	3	G	Sidechain
1	AA	4	G	Sidechain
1	AA	5	A	Sidechain
1	AA	6	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1600	0	760	11	0
1	AE	1622	0	769	7	0
1	AP	1600	0	755	42	0
2	AM	397	0	202	6	0
3	A1	32828	0	15511	162	0
4	AB	1704	0	1732	9	0
5	AC	876	0	887	3	0
6	AD	954	0	1019	4	0
7	AF	883	0	944	1	0
8	AG	773	0	825	2	0
9	AH	715	0	742	2	0
10	AI	648	0	666	5	0
11	AJ	648	0	691	3	0
12	AK	455	0	478	0	0
13	AL	637	0	665	0	0
14	AN	664	0	714	4	0
15	AO	1624	0	1699	5	0
16	AQ	425	0	449	1	0
17	AR	1642	0	1710	9	0
18	AS	1105	0	1148	4	0
19	AT	817	0	808	2	0
20	AU	1174	0	1230	3	0
21	AV	978	0	1034	0	0
22	AW	1021	0	1070	1	0
23	AX	786	0	828	4	0
24	BA	2504	0	1208	11	0
25	BB	62317	0	29633	224	0
26	BC	752	0	780	4	0
27	BD	930	0	1000	5	0
28	BE	1052	0	1129	9	0
29	BF	1073	0	1157	8	0
30	BG	1007	0	1045	4	0
31	BH	899	0	935	2	0
32	BI	916	0	965	6	0
33	BJ	946	0	1022	8	0
34	BK	815	0	839	4	0
35	BL	856	0	922	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BM	777	0	840	2	0
37	BN	2053	0	2122	9	0
38	BO	779	0	834	2	0
39	BP	633	0	656	1	0
40	BQ	508	0	543	3	0
41	BR	448	0	491	2	0
42	BS	548	0	552	2	0
43	BT	443	0	461	2	0
44	BU	440	0	485	2	0
45	BV	376	0	418	2	0
46	BW	503	0	574	7	0
47	BX	301	0	343	1	0
48	BY	1564	0	1616	7	0
49	BZ	1687	0	1814	3	0
50	B1	1551	0	1619	7	0
51	B2	1419	0	1460	8	0
52	B3	1322	0	1374	3	0
53	B4	1110	0	1148	2	0
54	B5	1031	0	1088	4	0
55	B6	1112	0	1147	2	0
All	All	149248	0	97556	534	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 534 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)
25:BB:1687:G:C2'	25:BB:1687:G:C3'	1.91	1.47
25:BB:1687:G:C2'	25:BB:1687:G:C1'	1.93	1.45
1:AP:31:A:C2'	3:A1:1340:A:H3'	1.45	1.44
25:BB:1687:G:C3'	25:BB:1687:G:C4'	1.96	1.43
1:AP:31:A:C2'	1:AP:31:A:C3'	2.01	1.39

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	
4	AB	216/241 (90%)	178 (82%)	33 (15%)	5 (2%)	6	34
5	AC	115/129 (89%)	91 (79%)	17 (15%)	7 (6%)	1	17
6	AD	121/124 (98%)	78 (64%)	28 (23%)	15 (12%)	0	5
7	AF	112/118 (95%)	80 (71%)	24 (21%)	8 (7%)	1	14
8	AG	94/101 (93%)	69 (73%)	20 (21%)	5 (5%)	2	19
9	AH	86/89 (97%)	73 (85%)	11 (13%)	2 (2%)	6	34
10	AI	80/82 (98%)	55 (69%)	15 (19%)	10 (12%)	0	5
11	AJ	78/84 (93%)	52 (67%)	18 (23%)	8 (10%)	0	8
12	AK	53/75 (71%)	44 (83%)	7 (13%)	2 (4%)	3	24
13	AL	77/92 (84%)	51 (66%)	19 (25%)	7 (9%)	1	11
14	AN	83/87 (95%)	66 (80%)	13 (16%)	4 (5%)	2	21
15	AO	204/233 (88%)	151 (74%)	38 (19%)	15 (7%)	1	14
16	AQ	49/71 (69%)	35 (71%)	8 (16%)	6 (12%)	0	6
17	AR	203/206 (98%)	161 (79%)	29 (14%)	13 (6%)	1	16
18	AS	148/159 (93%)	114 (77%)	20 (14%)	14 (10%)	0	10
19	AT	98/135 (73%)	80 (82%)	13 (13%)	5 (5%)	2	19
20	AU	148/179 (83%)	118 (80%)	19 (13%)	11 (7%)	1	14
21	AV	127/130 (98%)	103 (81%)	19 (15%)	5 (4%)	3	23
22	AW	125/130 (96%)	95 (76%)	23 (18%)	7 (6%)	2	19
23	AX	96/103 (93%)	78 (81%)	9 (9%)	9 (9%)	0	10
26	BC	92/94 (98%)	74 (80%)	14 (15%)	4 (4%)	2	22
27	BD	119/123 (97%)	90 (76%)	16 (13%)	13 (11%)	0	8
28	BE	142/144 (99%)	91 (64%)	30 (21%)	21 (15%)	0	3
29	BF	134/136 (98%)	73 (54%)	40 (30%)	21 (16%)	0	3
30	BG	125/127 (98%)	84 (67%)	32 (26%)	9 (7%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	115/117 (98%)	72 (63%)	32 (28%)	11 (10%)	0	10
32	BI	112/115 (97%)	63 (56%)	32 (29%)	17 (15%)	0	4
33	BJ	115/118 (98%)	77 (67%)	27 (24%)	11 (10%)	0	10
34	BK	101/103 (98%)	59 (58%)	33 (33%)	9 (9%)	1	11
35	BL	108/110 (98%)	72 (67%)	27 (25%)	9 (8%)	1	12
36	BM	97/99 (98%)	69 (71%)	18 (19%)	10 (10%)	0	8
37	BN	265/270 (98%)	165 (62%)	61 (23%)	39 (15%)	0	4
38	BO	100/103 (97%)	60 (60%)	22 (22%)	18 (18%)	0	3
39	BP	82/85 (96%)	44 (54%)	21 (26%)	17 (21%)	0	2
40	BQ	61/63 (97%)	42 (69%)	14 (23%)	5 (8%)	1	12
41	BR	56/59 (95%)	38 (68%)	13 (23%)	5 (9%)	1	11
42	BS	68/70 (97%)	38 (56%)	22 (32%)	8 (12%)	0	6
43	BT	54/57 (95%)	32 (59%)	11 (20%)	11 (20%)	0	2
44	BU	52/54 (96%)	33 (64%)	14 (27%)	5 (10%)	0	10
45	BV	44/46 (96%)	33 (75%)	6 (14%)	5 (11%)	0	7
46	BW	62/64 (97%)	35 (56%)	20 (32%)	7 (11%)	0	7
47	BX	36/38 (95%)	23 (64%)	8 (22%)	5 (14%)	0	4
48	BY	207/209 (99%)	113 (55%)	54 (26%)	40 (19%)	0	2
49	BZ	211/213 (99%)	163 (77%)	33 (16%)	15 (7%)	1	14
50	B1	199/201 (99%)	111 (56%)	53 (27%)	35 (18%)	0	3
51	B2	176/178 (99%)	123 (70%)	26 (15%)	27 (15%)	0	3
52	B3	174/177 (98%)	149 (86%)	20 (12%)	5 (3%)	4	29
53	B4	147/149 (99%)	103 (70%)	33 (22%)	11 (8%)	1	13
54	B5	139/142 (98%)	113 (81%)	17 (12%)	9 (6%)	1	16
55	B6	138/140 (99%)	79 (57%)	41 (30%)	18 (13%)	0	5
All	All	5844/6172 (95%)	4093 (70%)	1173 (20%)	578 (10%)	1	9

5 of 578 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AB	36	LYS
4	AB	97	GLY
4	AB	169	HIS

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Mol	Chain	Res	Type
6	AD	9	LYS
6	AD	15	VAL

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	
4	AB	180/199 (90%)	164 (91%)	16 (9%)	9	30
5	AC	90/99 (91%)	81 (90%)	9 (10%)	7	26
6	AD	103/104 (99%)	87 (84%)	16 (16%)	2	14
7	AF	92/96 (96%)	84 (91%)	8 (9%)	10	31
8	AG	79/84 (94%)	75 (95%)	4 (5%)	24	48
9	AH	76/77 (99%)	73 (96%)	3 (4%)	32	56
10	AI	65/65 (100%)	61 (94%)	4 (6%)	18	43
11	AJ	74/78 (95%)	69 (93%)	5 (7%)	16	41
12	AK	48/66 (73%)	44 (92%)	4 (8%)	11	34
13	AL	70/79 (89%)	59 (84%)	11 (16%)	2	14
14	AN	65/66 (98%)	59 (91%)	6 (9%)	9	29
15	AO	170/190 (90%)	158 (93%)	12 (7%)	14	39
16	AQ	44/61 (72%)	40 (91%)	4 (9%)	9	29
17	AR	172/173 (99%)	156 (91%)	16 (9%)	9	28
18	AS	113/119 (95%)	98 (87%)	15 (13%)	4	18
19	AT	87/116 (75%)	77 (88%)	10 (12%)	5	21
20	AU	123/147 (84%)	108 (88%)	15 (12%)	5	20
21	AV	104/105 (99%)	98 (94%)	6 (6%)	20	45
22	AW	105/107 (98%)	98 (93%)	7 (7%)	16	41
23	AX	86/90 (96%)	78 (91%)	8 (9%)	9	28
26	BC	78/78 (100%)	74 (95%)	4 (5%)	24	48
27	BD	102/104 (98%)	98 (96%)	4 (4%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	BE	103/103 (100%)	84 (82%)	19 (18%)	1	9
29	BF	109/109 (100%)	95 (87%)	14 (13%)	4	18
30	BG	103/103 (100%)	90 (87%)	13 (13%)	4	19
31	BH	87/87 (100%)	81 (93%)	6 (7%)	15	40
32	BI	99/100 (99%)	96 (97%)	3 (3%)	41	63
33	BJ	89/90 (99%)	78 (88%)	11 (12%)	4	19
34	BK	84/84 (100%)	73 (87%)	11 (13%)	4	18
35	BL	93/93 (100%)	83 (89%)	10 (11%)	6	23
36	BM	83/83 (100%)	69 (83%)	14 (17%)	2	12
37	BN	213/215 (99%)	189 (89%)	24 (11%)	6	21
38	BO	83/84 (99%)	76 (92%)	7 (8%)	11	33
39	BP	62/63 (98%)	55 (89%)	7 (11%)	6	21
40	BQ	55/55 (100%)	47 (86%)	8 (14%)	3	15
41	BR	48/49 (98%)	46 (96%)	2 (4%)	30	54
42	BS	62/62 (100%)	58 (94%)	4 (6%)	17	42
43	BT	47/48 (98%)	35 (74%)	12 (26%)	0	3
44	BU	48/48 (100%)	45 (94%)	3 (6%)	18	43
45	BV	38/38 (100%)	34 (90%)	4 (10%)	7	24
46	BW	51/51 (100%)	43 (84%)	8 (16%)	2	14
47	BX	34/34 (100%)	30 (88%)	4 (12%)	5	20
48	BY	164/164 (100%)	145 (88%)	19 (12%)	5	21
49	BZ	187/187 (100%)	174 (93%)	13 (7%)	15	40
50	B1	165/165 (100%)	147 (89%)	18 (11%)	6	23
51	B2	149/149 (100%)	130 (87%)	19 (13%)	4	18
52	B3	137/138 (99%)	125 (91%)	12 (9%)	10	31
53	B4	114/114 (100%)	104 (91%)	10 (9%)	10	31
54	B5	109/110 (99%)	102 (94%)	7 (6%)	17	42
55	B6	114/114 (100%)	107 (94%)	7 (6%)	18	44
All	All	4856/5043 (96%)	4380 (90%)	476 (10%)	11	26

5 of 476 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	BG	115	LEU
52	B3	42	VAL
36	BM	80	TRP
51	B2	160	LYS
55	B6	81	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
34	BK	91	GLN
43	BT	4	GLN
40	BQ	41	HIS
44	BU	45	HIS
10	AI	26	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	75/76 (98%)	20 (26%)	8 (10%)
1	AE	75/76 (98%)	11 (14%)	1 (1%)
1	AP	74/76 (97%)	15 (20%)	6 (8%)
2	AM	20/20 (100%)	9 (45%)	7 (35%)
24	BA	116/117 (99%)	37 (31%)	11 (9%)
25	BB	2901/2903 (99%)	1516 (52%)	511 (17%)
3	A1	1529/1530 (99%)	753 (49%)	280 (18%)
All	All	4790/4798 (99%)	2361 (49%)	824 (17%)

5 of 2361 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	C
1	AA	3	G
1	AA	10	G
1	AA	13	C
1	AA	17	U

5 of 824 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BB	914	G
25	BB	1567	G

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Mol	Chain	Res	Type
25	BB	2711	A
25	BB	974	G
25	BB	908	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BB	1
1	AP	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BB	1959:G	O3'	1960:A	P	3.50
1	AP	74:C	O3'	75:C	P	1.08

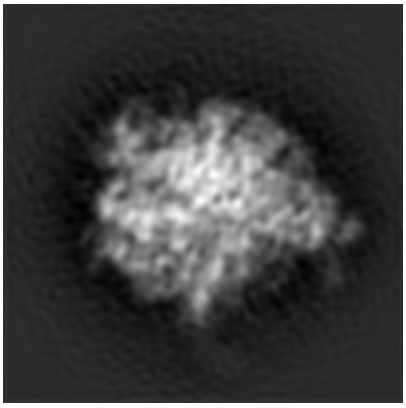
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1055. These allow visual inspection of the internal detail of the map and identification of artifacts.

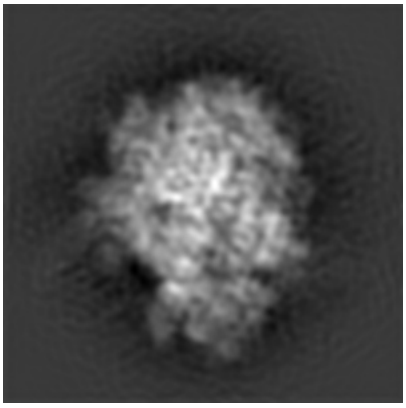
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

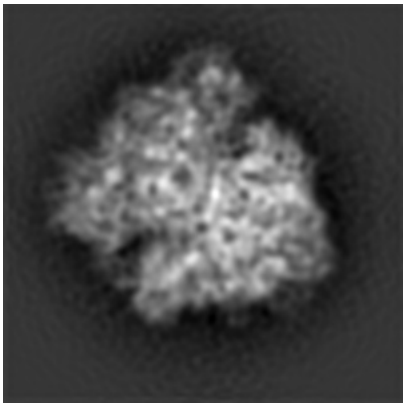
6.1.1 Primary map



X



Y

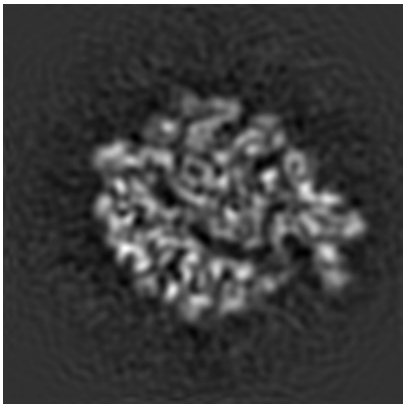


Z

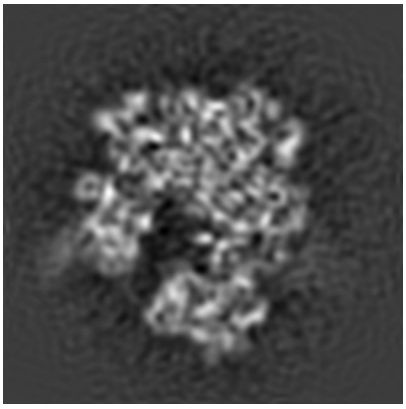
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

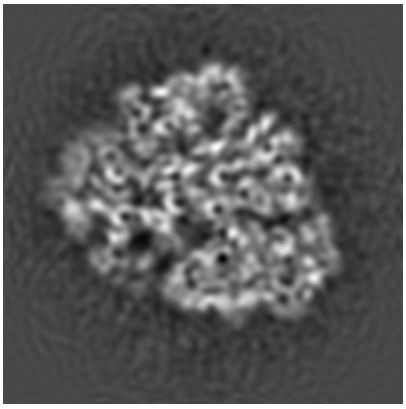
6.2.1 Primary map



X Index: 65



Y Index: 65

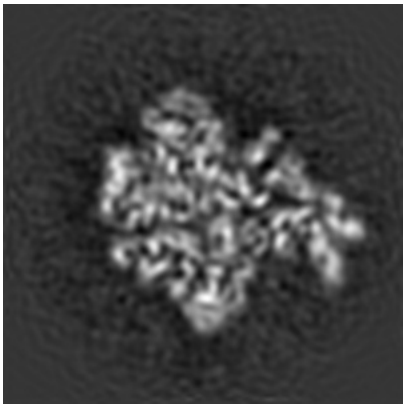


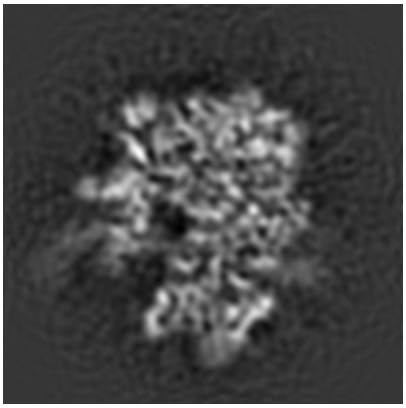
Z Index: 65

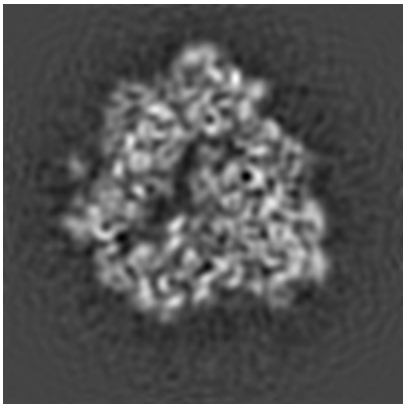
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 68

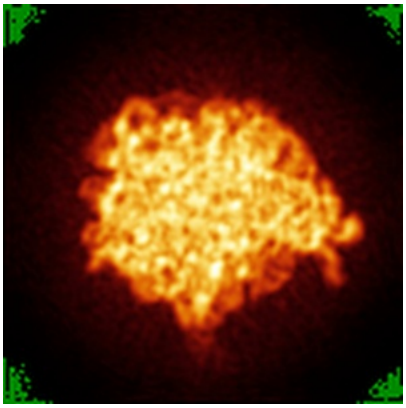

Y Index: 68

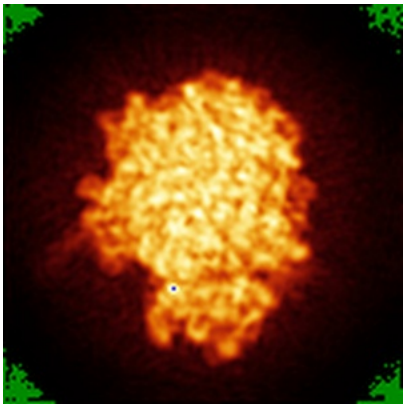

Z Index: 59

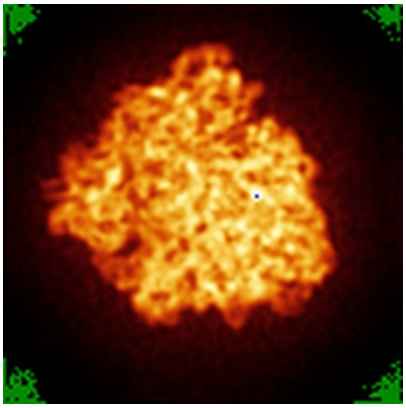
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

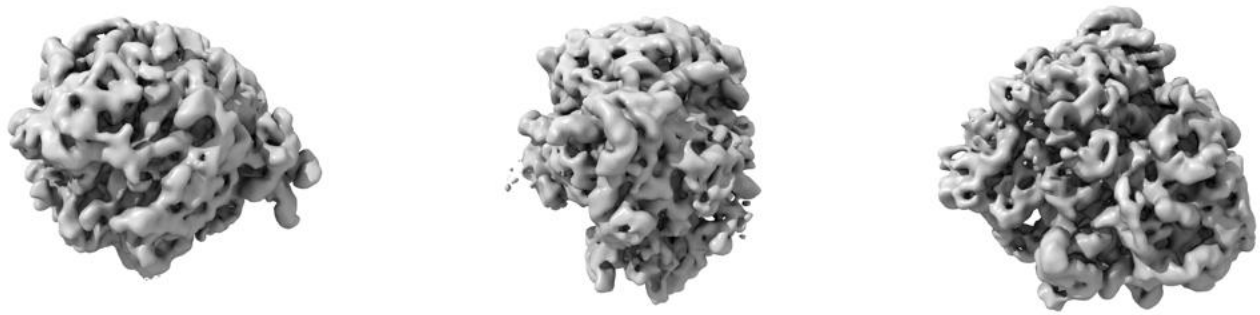

Y


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

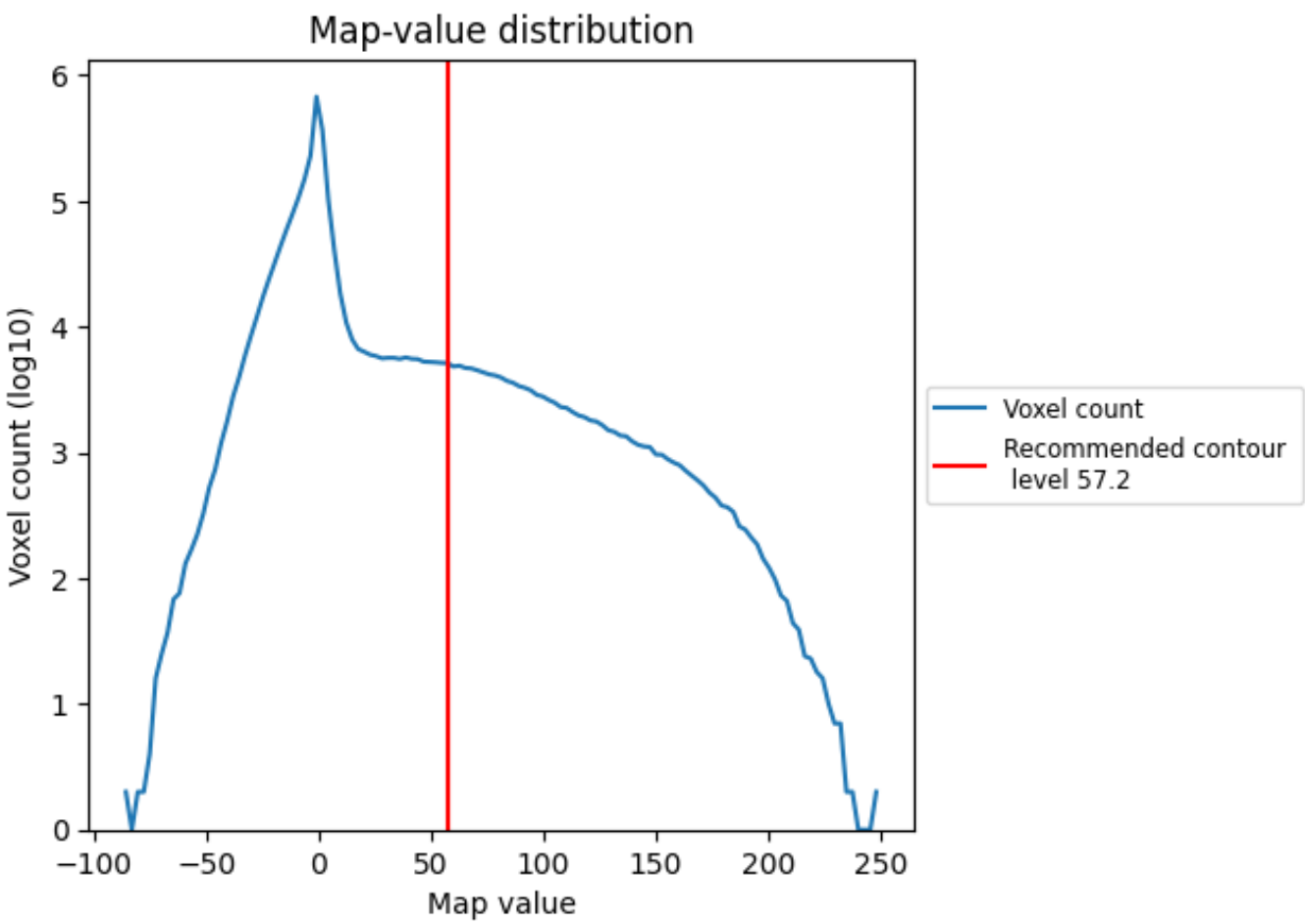
6.6 Mask visualisation (i)

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

7 Map analysis (i)

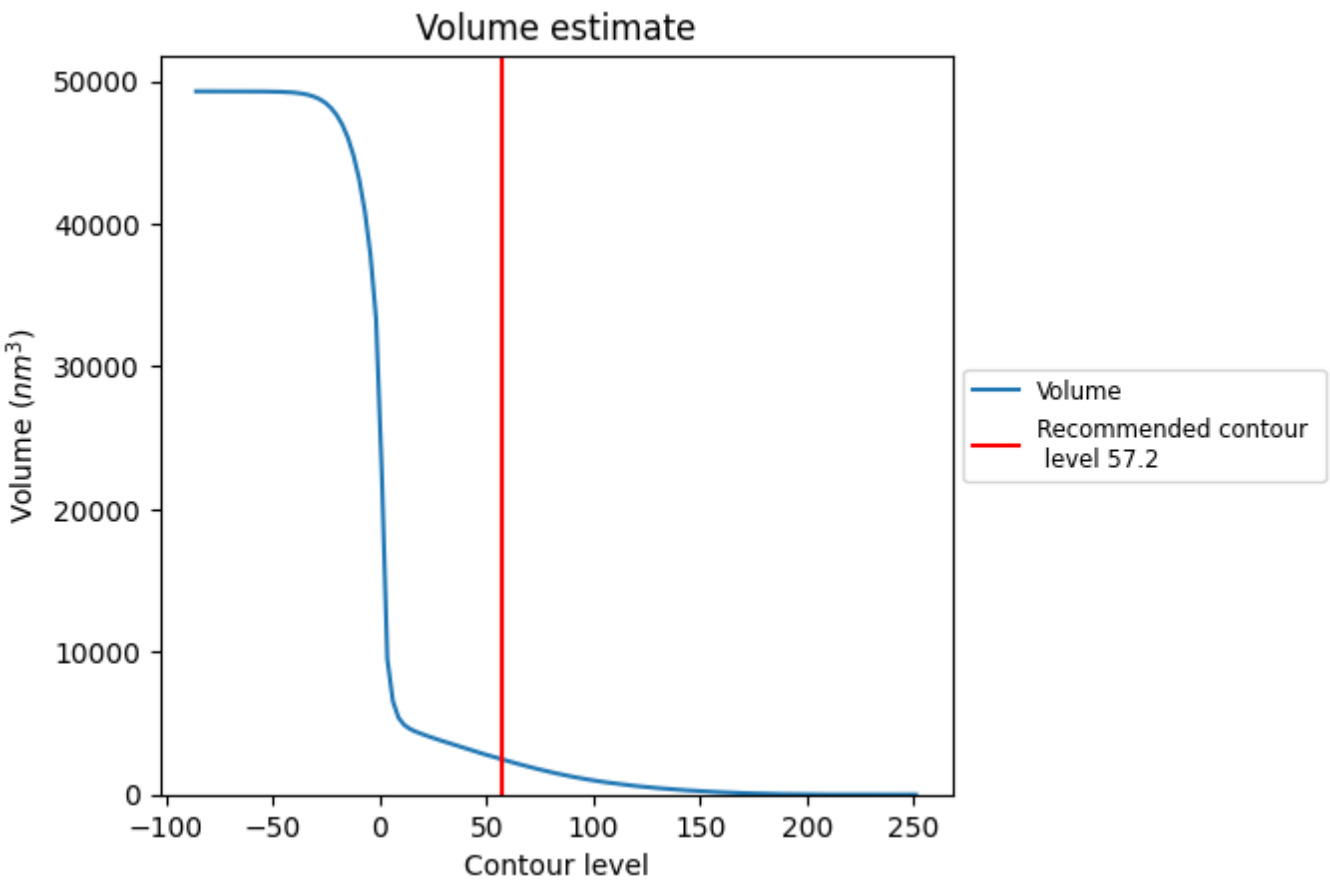
This section contains the results of statistical analysis of the map.

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.

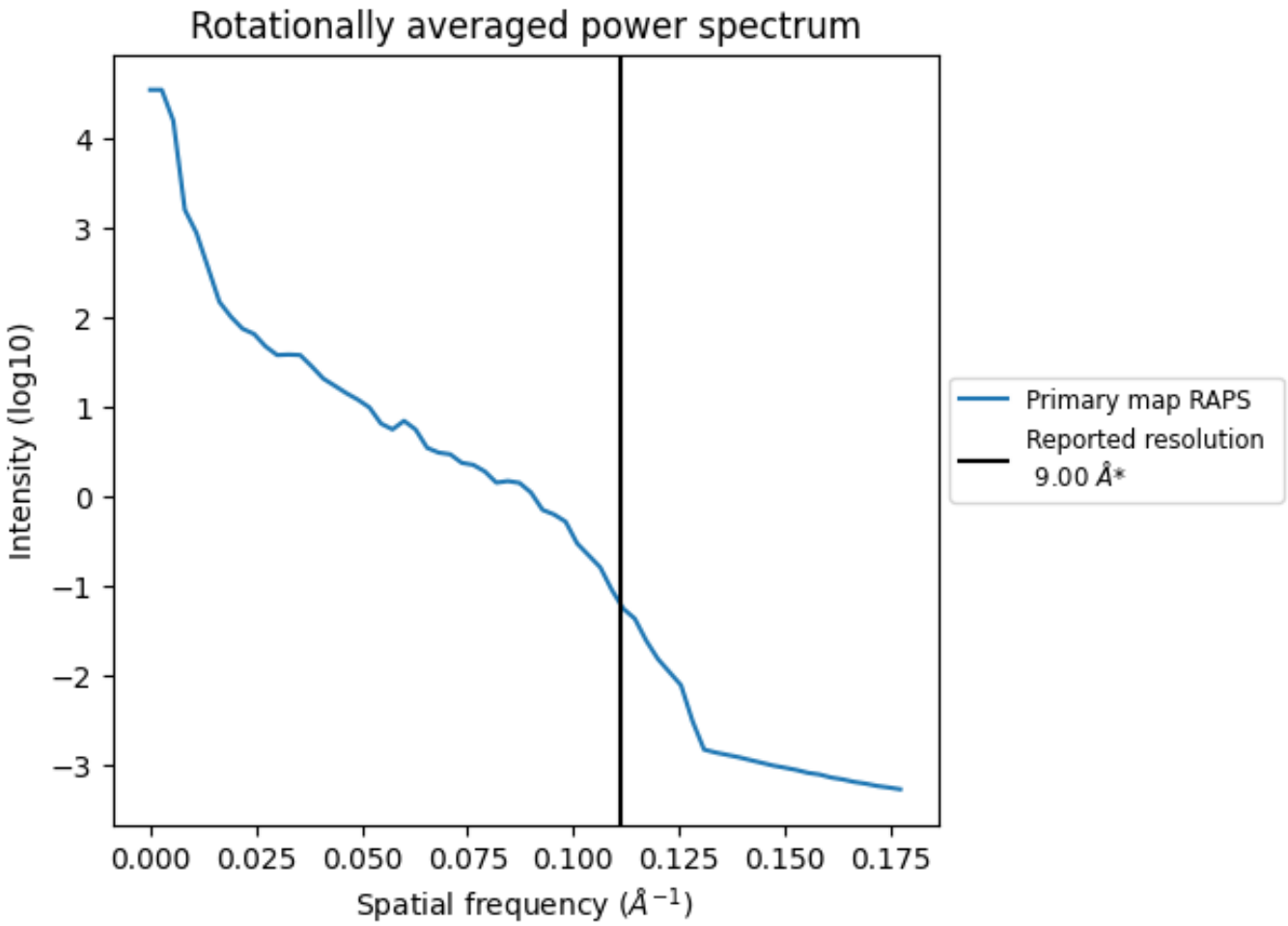
7.2 Volume estimate (i)



The volume at the recommended contour level is 2467 nm^3; this corresponds to an approximate mass of 2228 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 0.111 Å^{-1}

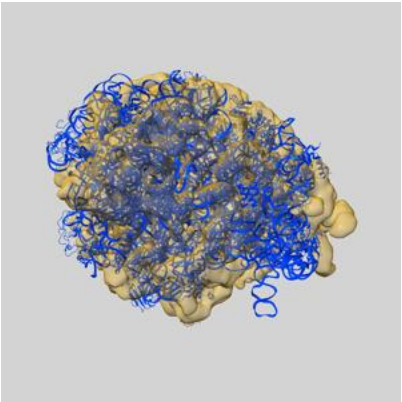
8 Fourier-Shell correlation (i)

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

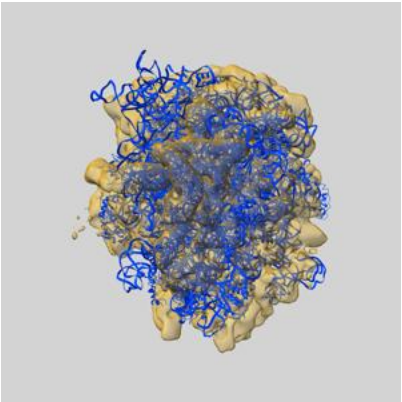
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1055 and PDB model 4V65. Per-residue inclusion information can be found in section 3 on page 14.

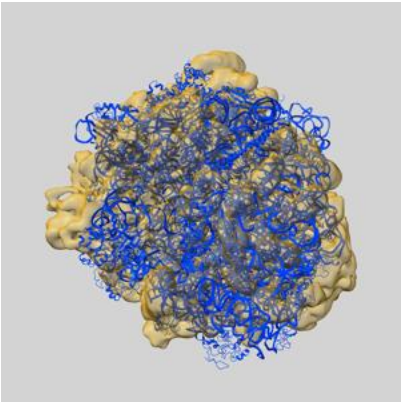
9.1 Map-model overlay (i)



X



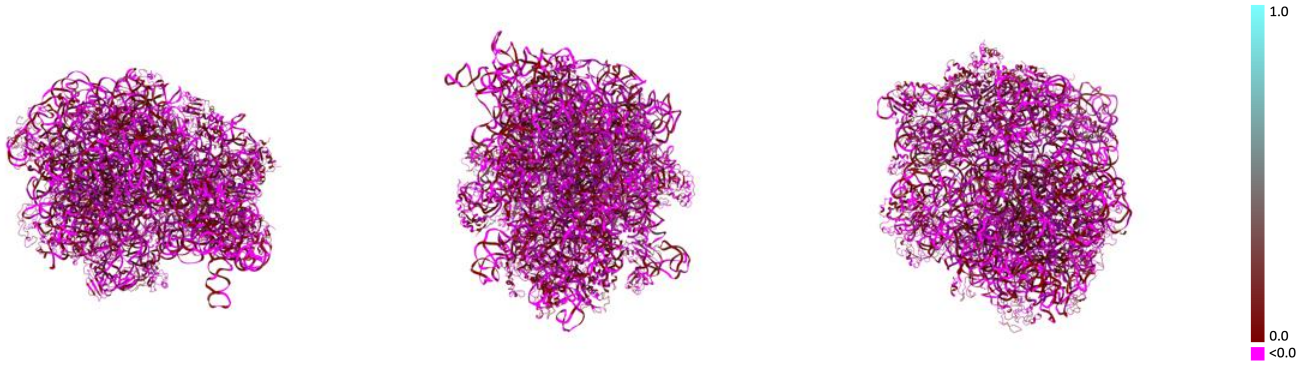
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 57.2 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.

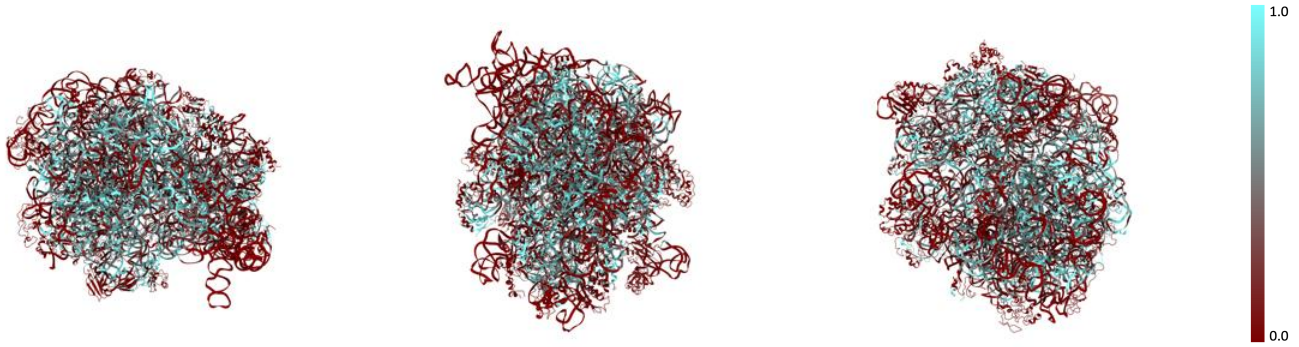
9.2 Q-score mapped to coordinate model (i)



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.

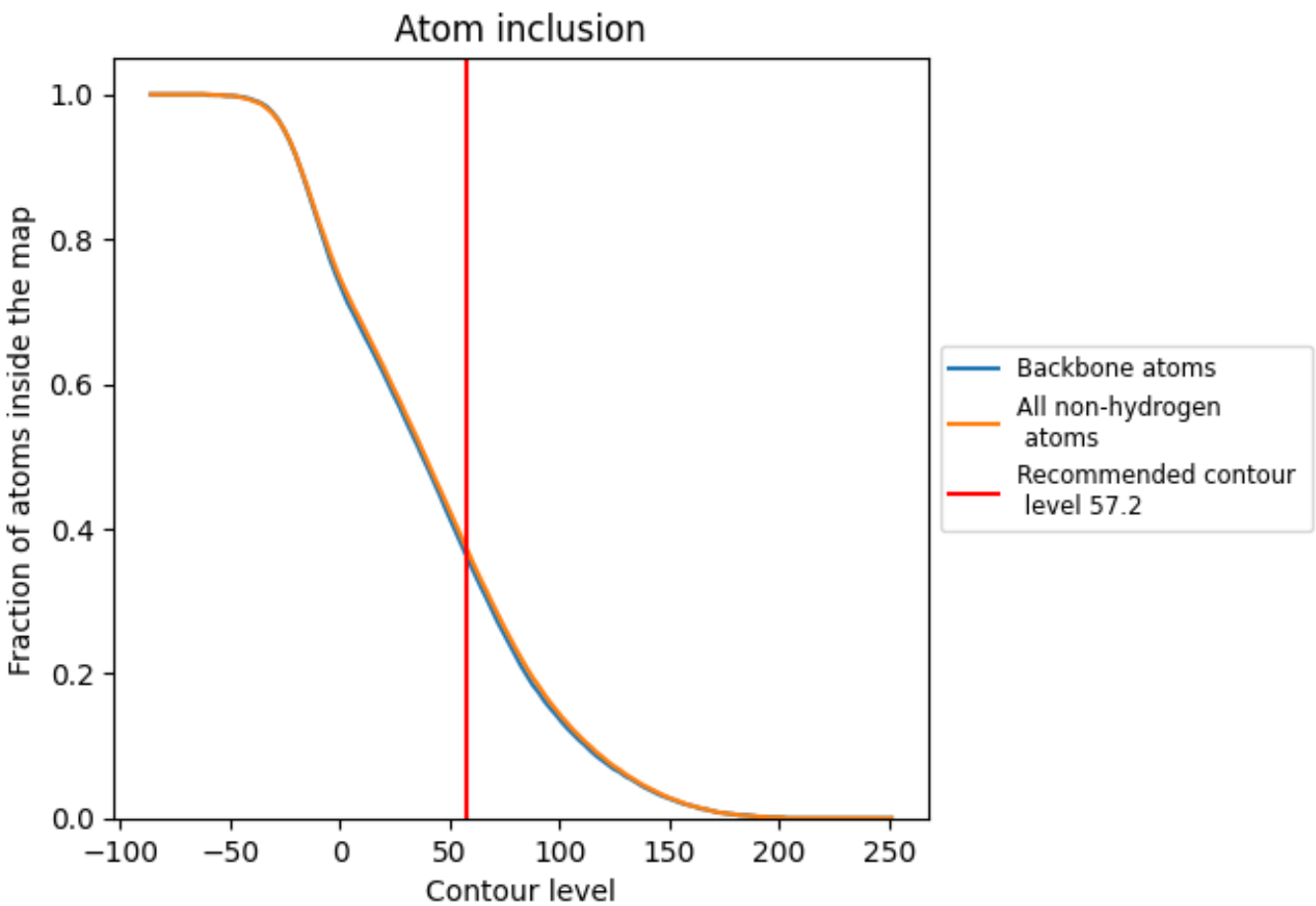
9.3 Atom inclusion mapped to coordinate model (i)



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 (57.2).

9.4 Atom inclusion (i)



At the recommended contour level, 37% of all backbone atoms, 38% 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 (57.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3760	-0.0070
A1	0.3220	-0.0130
AA	0.3780	-0.0130
AB	0.2190	-0.0010
AC	0.4260	-0.0050
AD	0.2170	-0.0200
AE	0.4110	-0.0070
AF	0.4210	-0.0010
AG	0.0860	-0.0290
AH	0.1550	-0.0100
AI	0.0000	-0.0440
AJ	0.2480	-0.0170
AK	0.5960	0.0120
AL	0.0340	-0.0240
AM	0.6420	0.0200
AN	0.4280	0.0120
AO	0.6140	0.0210
AP	0.4060	-0.0080
AQ	0.3970	-0.0520
AR	0.3640	-0.0030
AS	0.5510	-0.0110
AT	0.2370	-0.0150
AU	0.5410	0.0030
AV	0.4380	0.0190
AW	0.1440	0.0260
AX	0.2300	0.0050
B1	0.2650	0.0020
B2	0.6520	0.0280
B3	0.1800	-0.0280
B4	0.0720	-0.0250
B5	0.4570	-0.0390
B6	0.5180	0.0080
BA	0.2920	-0.0240
BB	0.4270	-0.0050
BC	0.2500	-0.0150

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Chain	Atom inclusion	Q-score
BD	0.4830	0.0040
BE	0.3080	-0.0030
BF	0.3510	-0.0060
BG	0.5990	-0.0100
BH	0.3760	-0.0030
BI	0.4390	-0.0430
BJ	0.1550	-0.0360
BK	0.0730	-0.0250
BL	0.5110	0.0130
BM	0.2860	-0.0330
BN	0.4240	-0.0100
BO	0.0000	-0.0070
BP	0.6370	0.0410
BQ	0.4540	0.0330
BR	0.4200	-0.0110
BS	0.3110	-0.0130
BT	0.4940	-0.0230
BU	0.1760	-0.0250
BV	0.5110	0.0300
BW	0.2590	-0.0140
BX	0.3060	-0.0010
BY	0.5940	0.0050
BZ	0.0400	0.0080