wwPDB EM Validation Summary Report

Apr 29, 2024 – 06:38 am BST

PDB ID	:	4V5H
EMDB ID	:	EMD-1657
Title	:	E.Coli 70s Ribosome Stalled During Translation Of Tnac Leader Peptide.
Authors	:	Seidelt, B.; Innis, C.A.; Wilson, D.N.; Gartmann, M.; Armache, J.; Villa, E.; Trabuco, L.G.; Becker, T.; Mielke, T.; Schulten, K.; Steitz, T.A.; Beckmann, R.
Deposited on	:	2009-10-26
Resolution	:	5.80 Å(reported)
Based on initial models	:	3FIH, 3FIK

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:

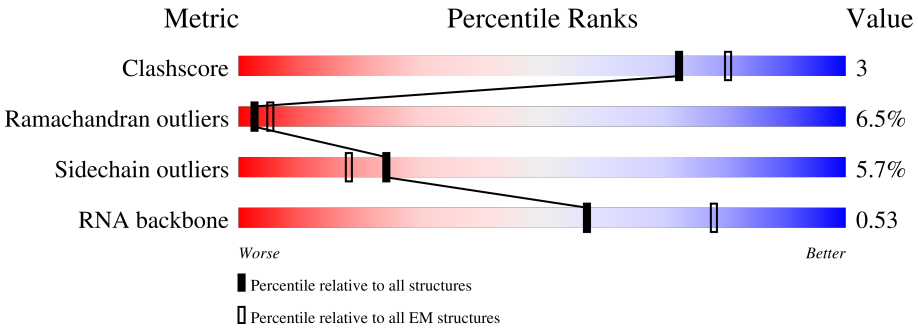
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 5.80 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	1530	35% 47% 18%
2	AB	218	54% 68% 28%
3	AC	206	37% 65% 25% 9%
4	AD	205	43% 67% 24% 8%
5	AE	150	29% 65% 28% 7%
6	AF	100	21% 65% 28% 6%
7	AG	150	39% 67% 25% 7%

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Mol	Chain	Length	Quality of chain
8	AH	129	29% 71% 26%
9	AI	127	38% 59% 33% 7%
10	AJ	98	65% 54% 42%
11	AK	117	30% 70% 26%
12	AL	123	37% 66% 25% 8%
13	AM	113	28% 60% 28% 9%
14	AN	96	27% 64% 27% 9%
15	AO	88	28% 67% 25% 7%
16	AP	80	39% 64% 32%
17	AQ	80	25% 65% 26% 8%
18	AR	55	20% 64% 27% 9%
19	AS	79	25% 59% 30% 10%
20	AT	85	31% 73% 22%
21	AU	51	57% 65% 27% 8%
22	AV	77	26% 58% 29% 13%
23	AX	11	64% 9% 18% 27% 45%
24	AZ	20	55% 80% 20%
25	B0	77	26% 70% 25% 5%
26	B1	63	25% 65% 32%
27	B2	58	22% 76% 24%
28	B3	56	32% 66% 25% 7%
29	B4	50	26% 66% 30%
30	B5	234	99% 77% 20%
31	B6	46	37% 59% 20% 20%
32	B7	64	23% 59% 39%

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Mol	Chain	Length	Quality of chain
33	B8	38	21% 76% 24%
34	BA	117	42% 43% 14%
35	BB	2903	38% 45% 17%
36	BC	271	27% 68% 25% 6%
37	BD	209	20% 67% 23% 8%
38	BE	201	39% 66% 27% 6%
39	BF	178	22% 63% 26% 10%
40	BG	176	14% 72% 22% 6%
41	BH	149	71% 74% 21% 5%
42	BI	141	75% 35% 59% 6%
43	BJ	142	18% 69% 21% 8%
44	BK	121	33% 64% 26% 8%
45	BL	143	30% 67% 29%
46	BM	136	24% 68% 29%
47	BN	120	26% 67% 27% 7%
48	BO	116	20% 74% 22%
49	BP	114	27% 68% 25% 7%
50	BQ	117	22% 60% 31% 7%
51	BR	103	17% 59% 32% 7%
52	BS	110	25% 61% 27% 12%
53	BT	93	37% 56% 39% 5%
54	BU	102	19% 62% 26% 6%
55	BW	94	16% 61% 31% 7%
56	BY	79	32% 63% 27% 6%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 145960 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 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	113	Total	C	N	O	S	0	0
			876	541	177	155	3		

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	80	Total	C	N	O	S	0	0
			638	400	126	111	1		

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

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

- Molecule 22 is a RNA chain called P-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AX	11	Total	C	N	O	P	0	0
			236	106	46	73	11		

- Molecule 24 is a protein called POLY-ALA NASCENT CHAIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	AZ	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B1	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	B4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 34 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	115	Total	C	N	O	P	0	0
			2464	1097	451	801	115		

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BB	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BG	175	Total	C	N	O	S	0	0
			1316	827	242	245	2		

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BK	121	Total	C	N	O	S	0	0
			930	582	179	163	6		

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	BU	99	Total	C	N	O	0	0
			755	479	140	136		

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L27.

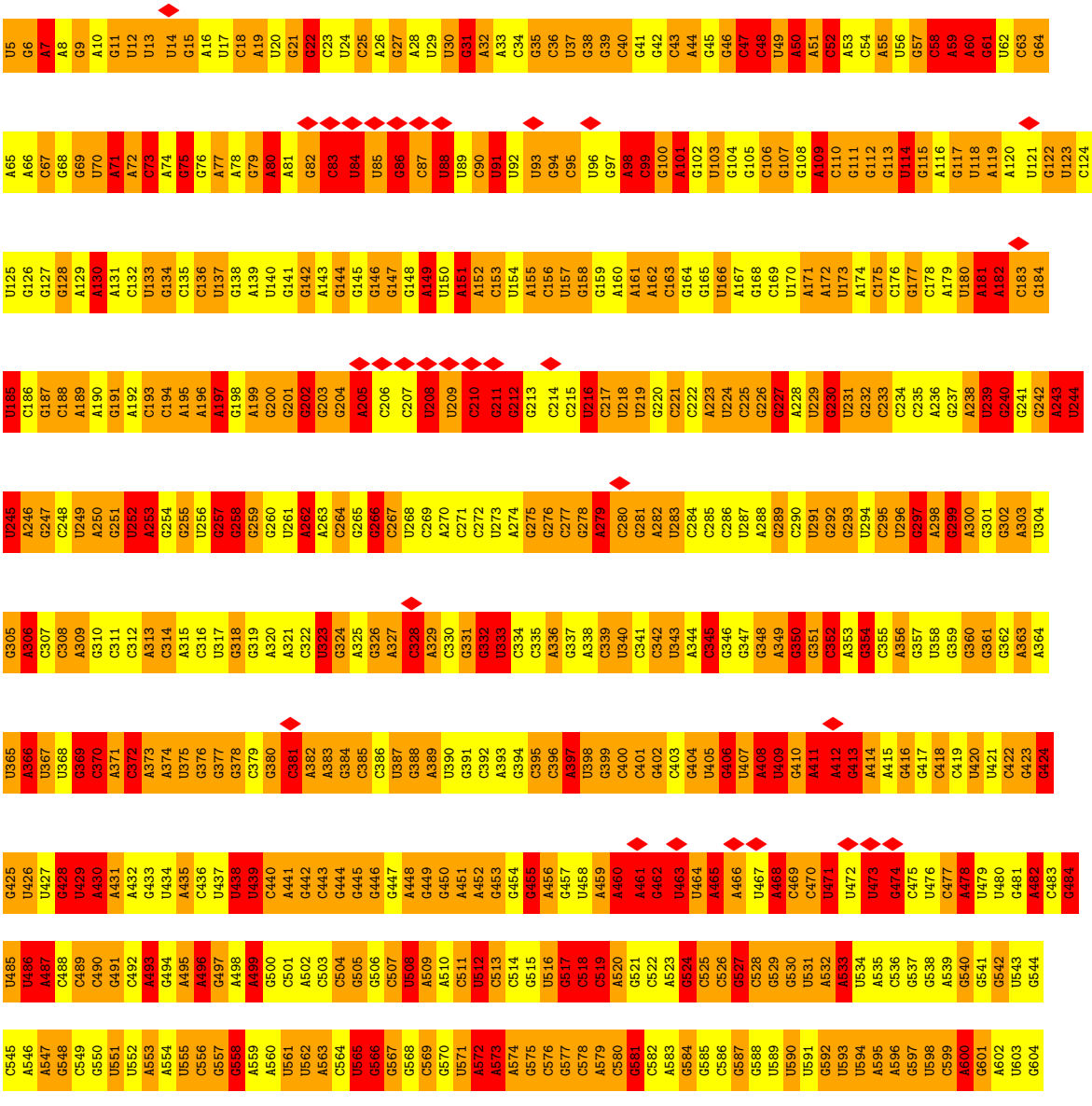
Mol	Chain	Residues	Atoms					AltConf	Trace
56	BY	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

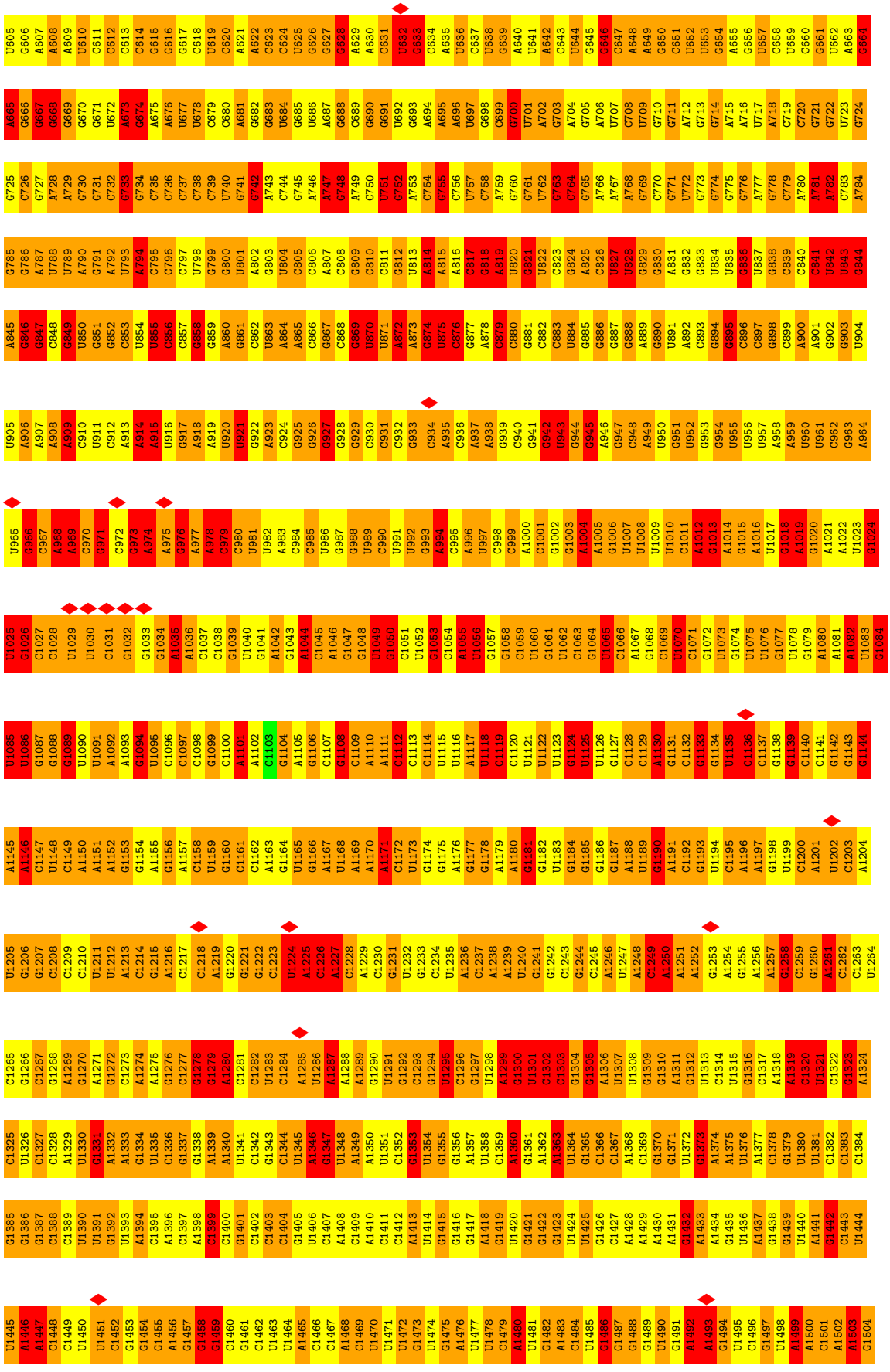
3 Residue-property plots (i)

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: 16S RIBOSOMAL RNA

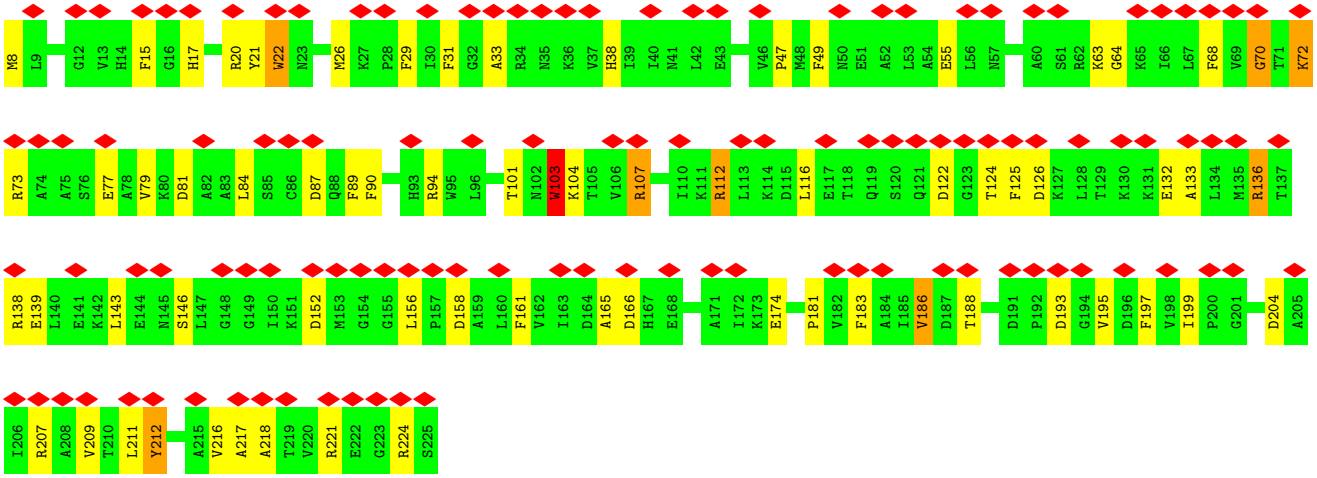
Chain AA:





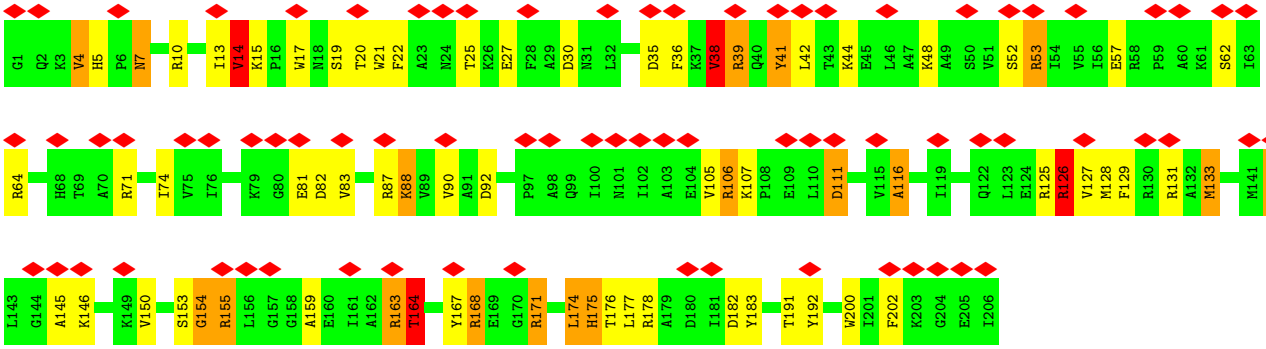
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



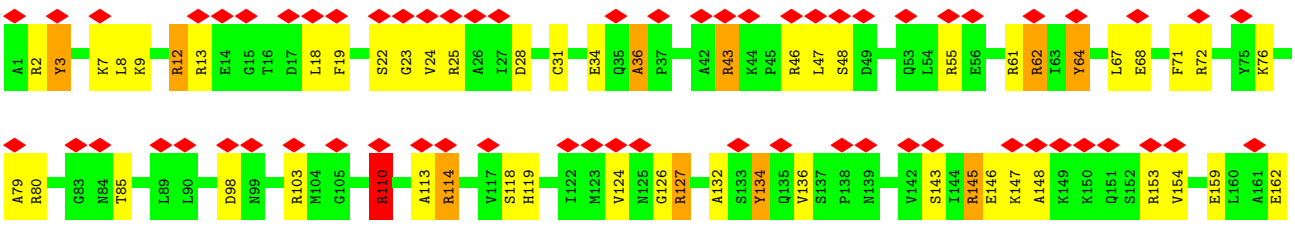
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

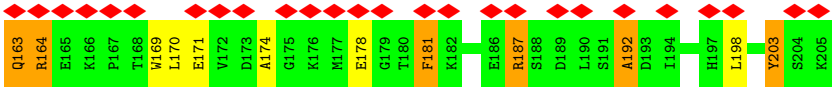
Chain AC:



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

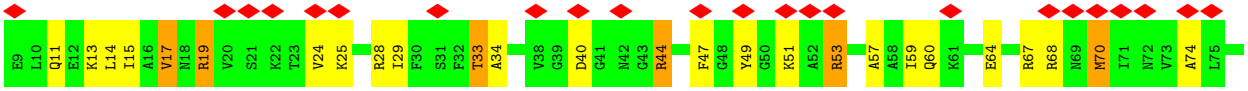
Chain AD:

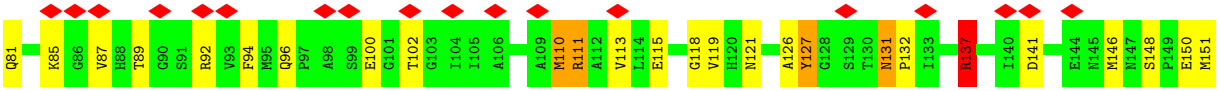




• Molecule 5: 30S RIBOSOMAL PROTEIN S5

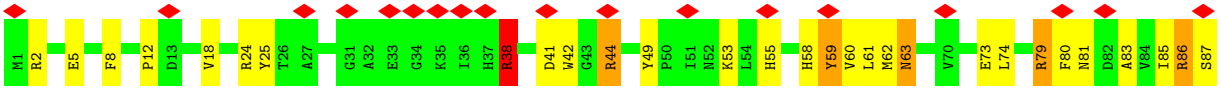
Chain AE:

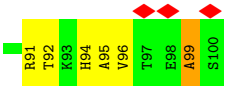




• Molecule 6: 30S RIBOSOMAL PROTEIN S6

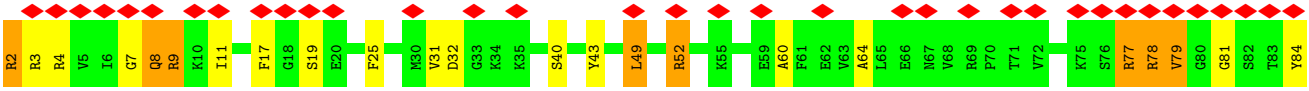
Chain AF:

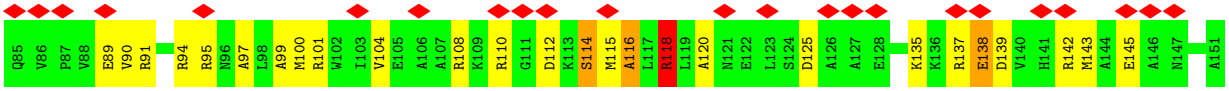




• Molecule 7: 30S RIBOSOMAL PROTEIN S7

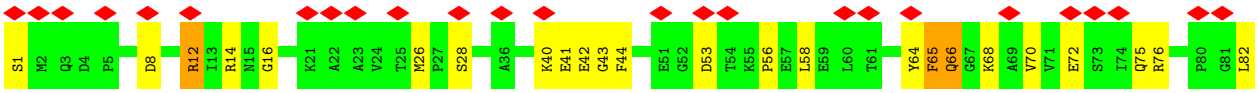
Chain AG:

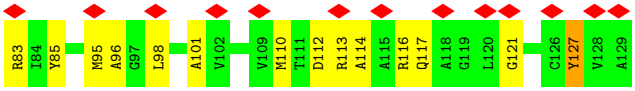




• Molecule 8: 30S RIBOSOMAL PROTEIN S8

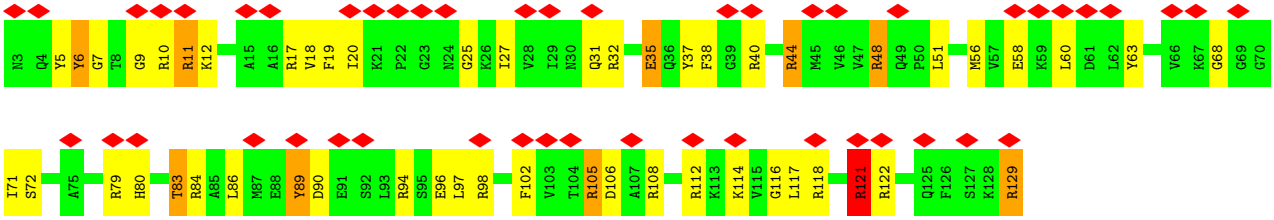
Chain AH:





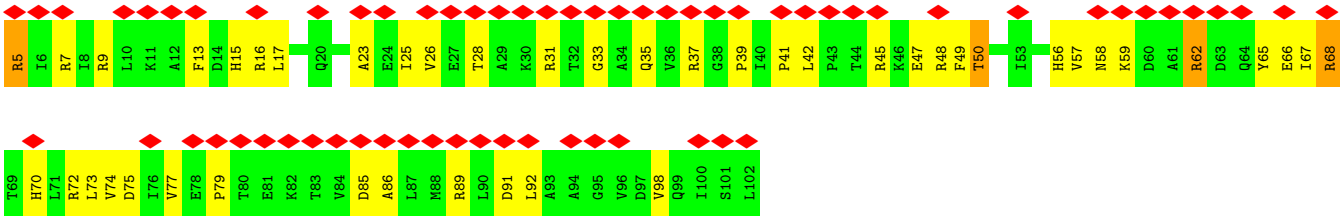
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



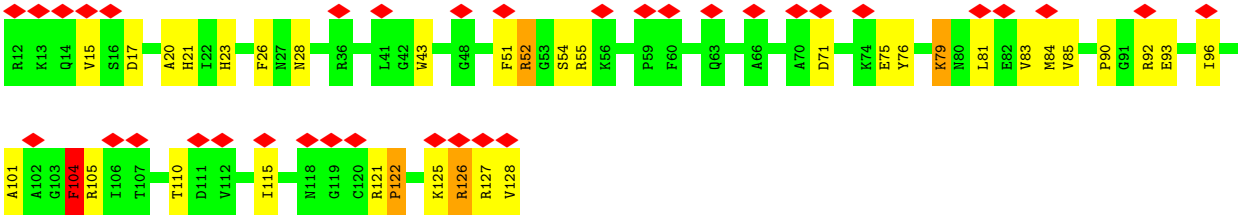
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



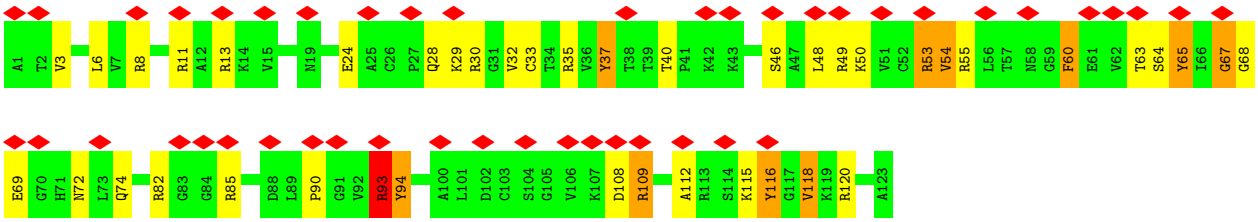
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



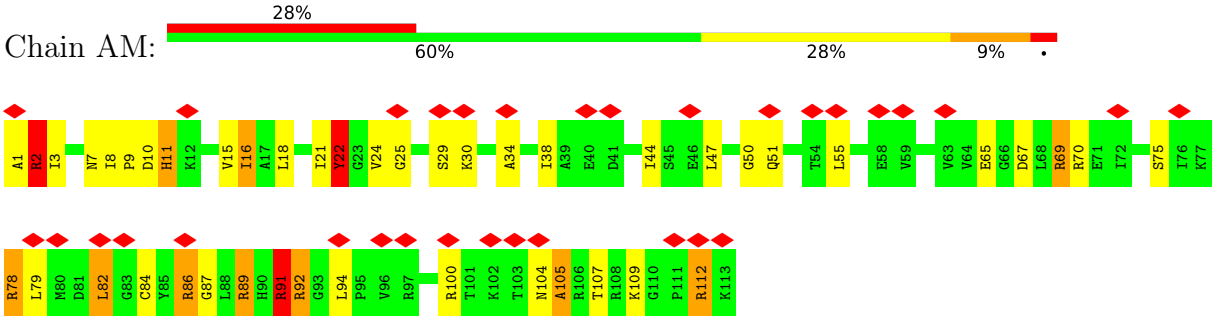
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



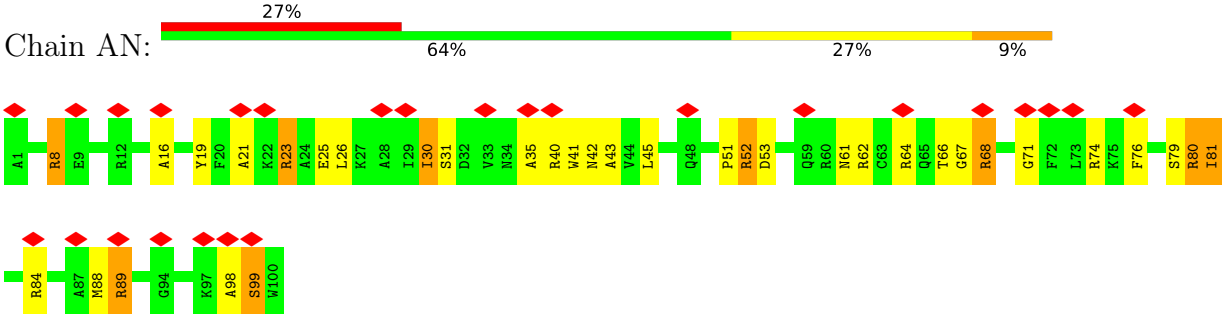
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



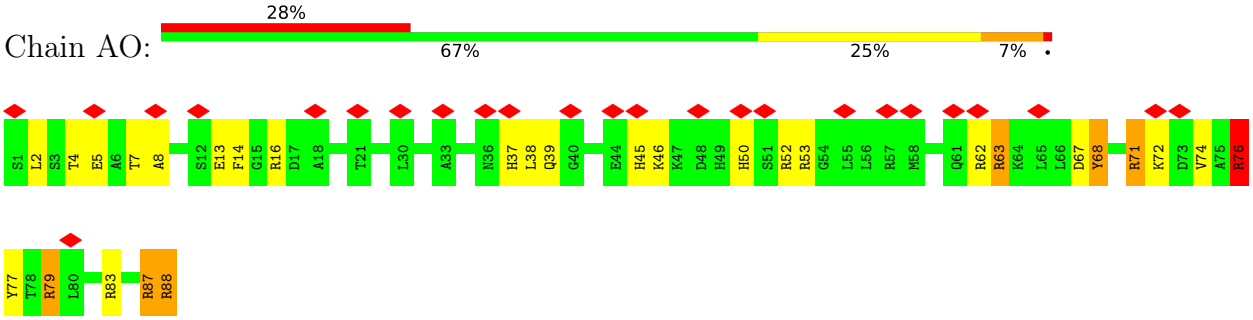
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



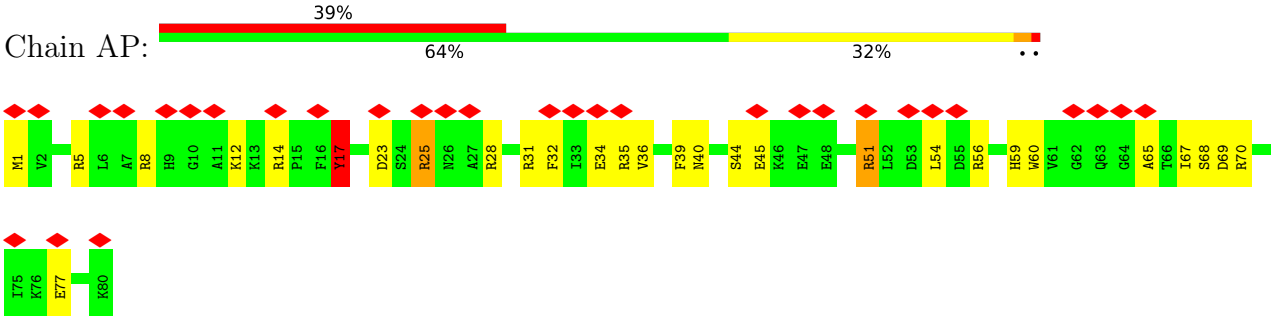
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



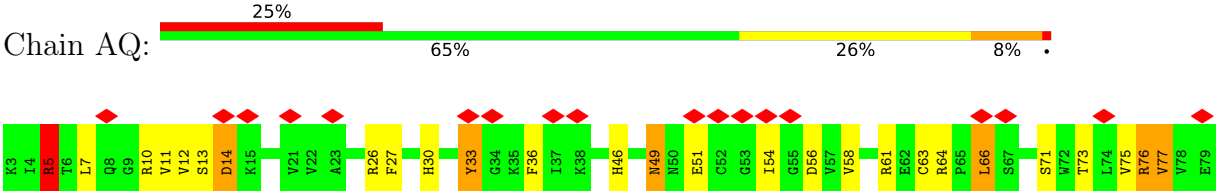
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



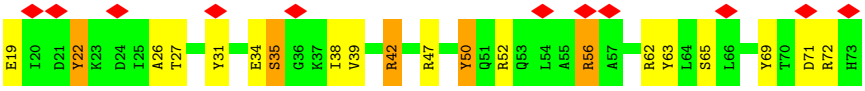
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



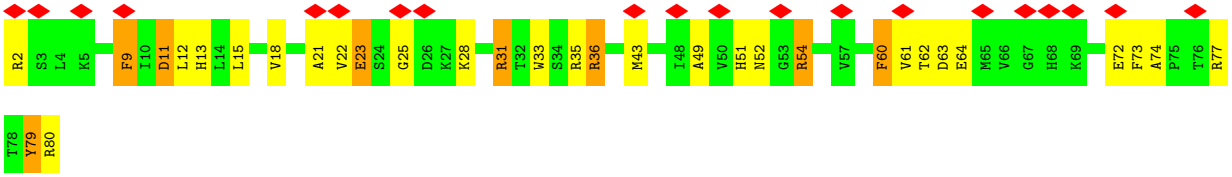
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



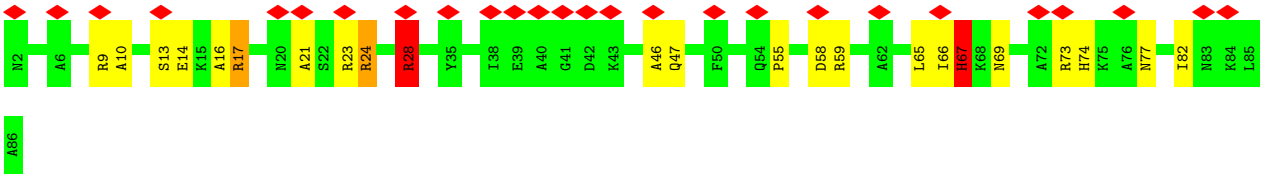
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



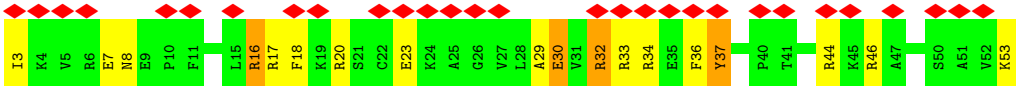
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



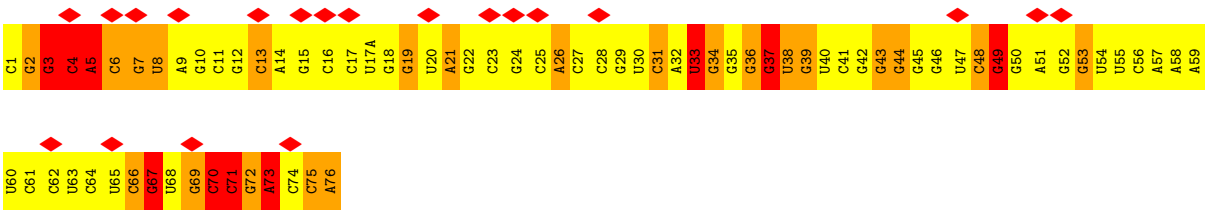
• Molecule 21: 30S RIBOSOMAL PROTEIN S21

Chain AU:



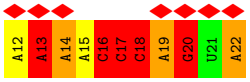
• Molecule 22: P-SITE TRNA

Chain AV:



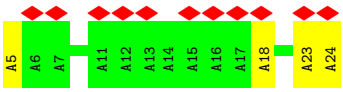
• Molecule 23: MRNA

Chain AX:



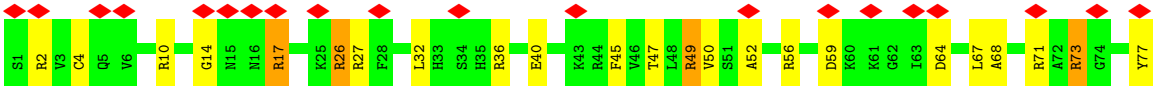
• Molecule 24: POLY-ALA NASCENT CHAIN

Chain AZ:



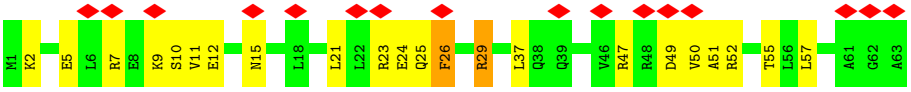
• Molecule 25: 50S RIBOSOMAL PROTEIN L28

Chain B0:



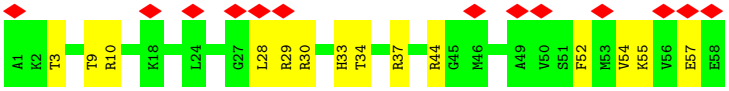
• Molecule 26: 50S RIBOSOMAL PROTEIN L29

Chain B1:



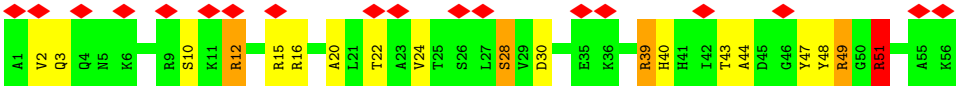
• Molecule 27: 50S RIBOSOMAL PROTEIN L30

Chain B2:



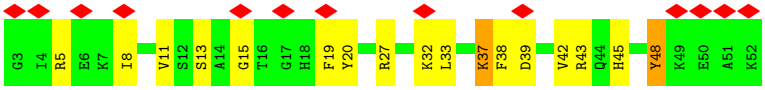
• Molecule 28: 50S RIBOSOMAL PROTEIN L32

Chain B3:



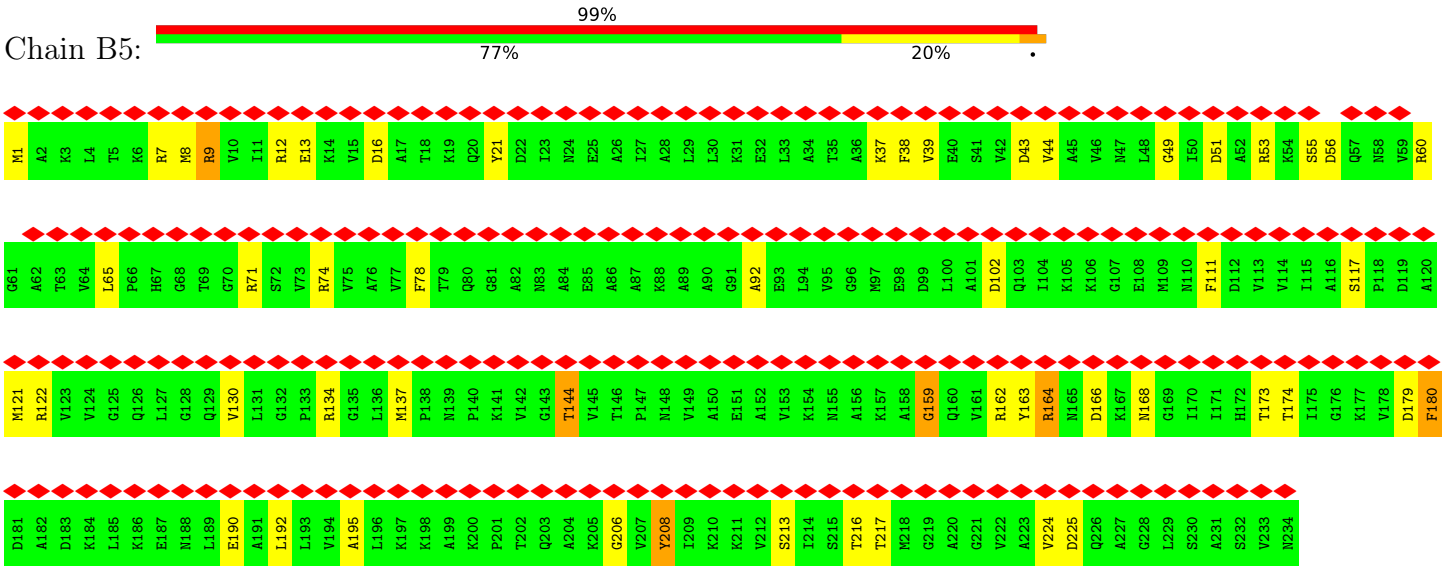
• Molecule 29: 50S RIBOSOMAL PROTEIN L33

Chain B4:



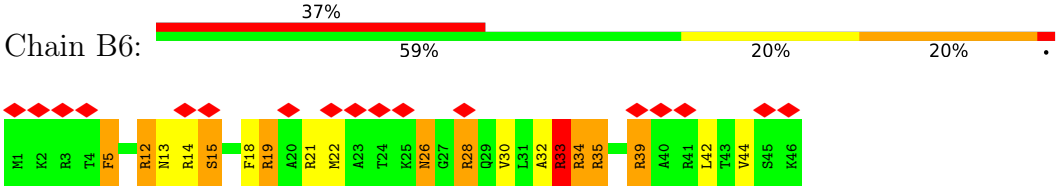
• Molecule 30: 50S RIBOSOMAL PROTEIN L1

Chain B5:



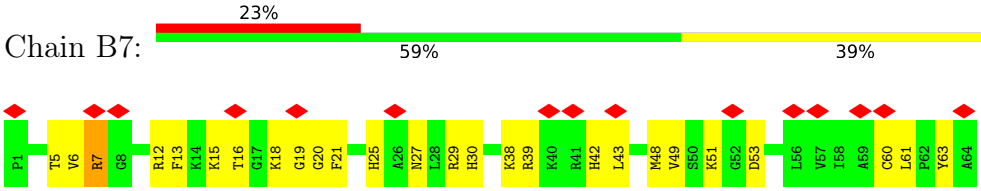
• Molecule 31: 50S RIBOSOMAL PROTEIN L34

Chain B6:



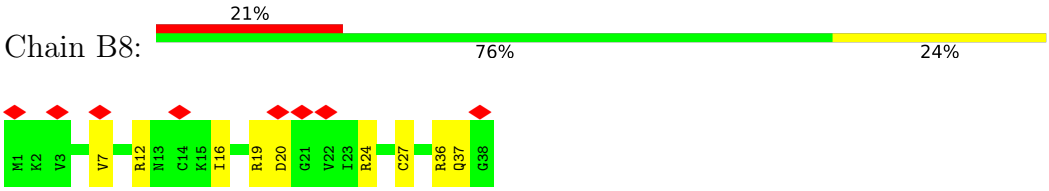
• Molecule 32: 50S RIBOSOMAL PROTEIN L35

Chain B7:



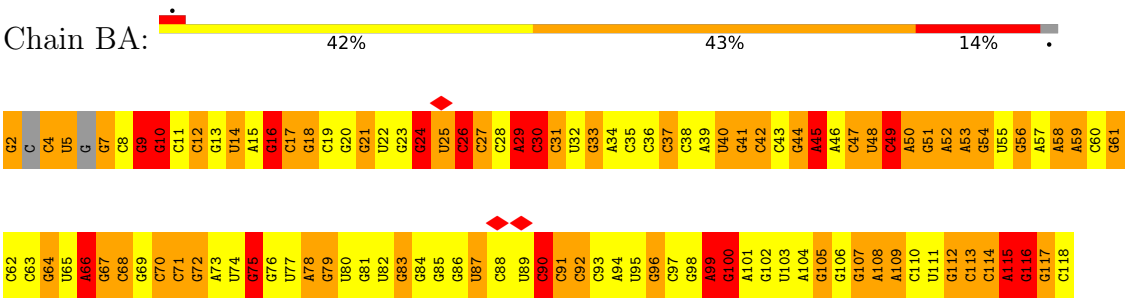
• Molecule 33: 50S RIBOSOMAL PROTEIN L36

Chain B8:



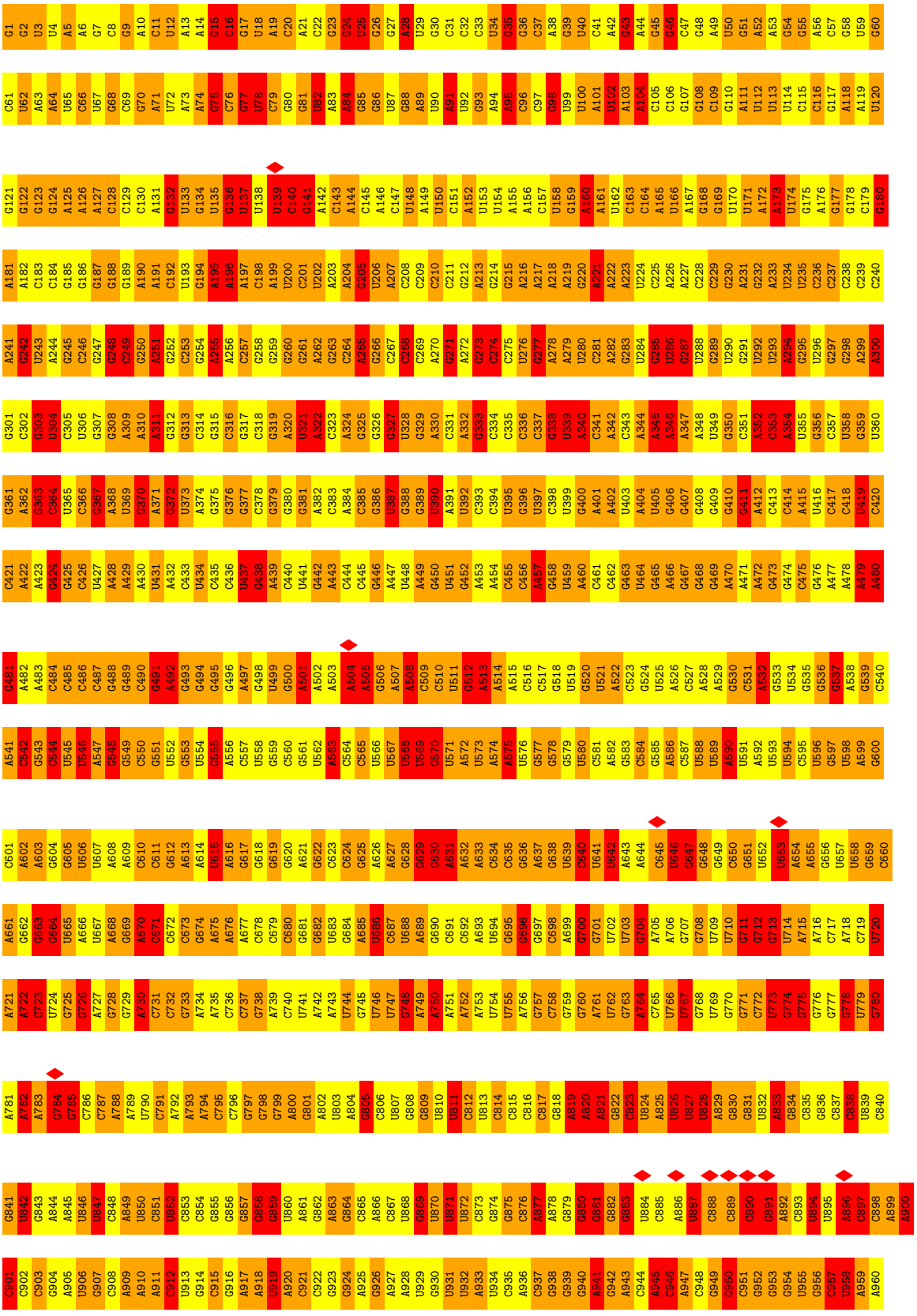
• Molecule 34: 5S RIBOSOMAL RNA

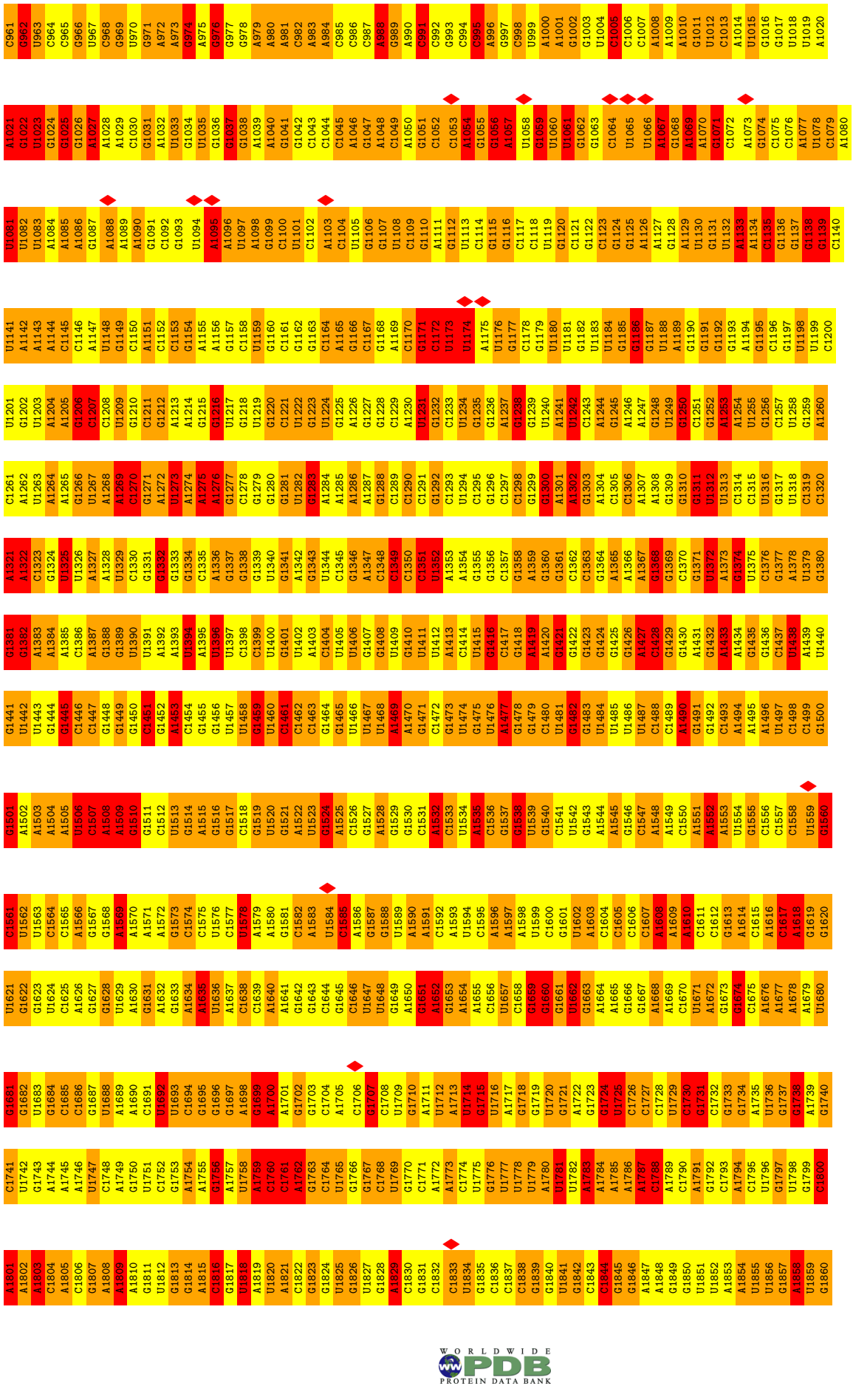
Chain BA:

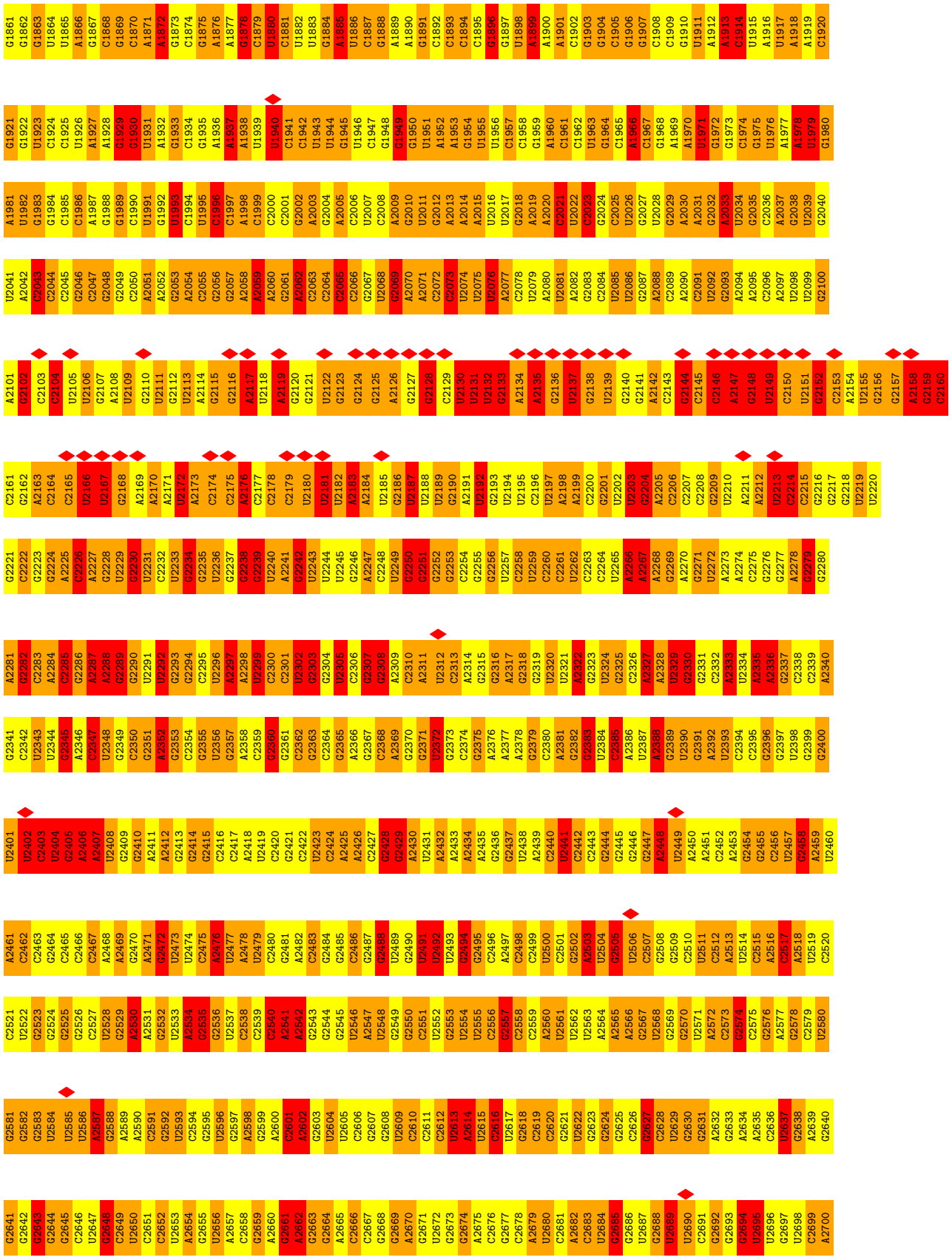


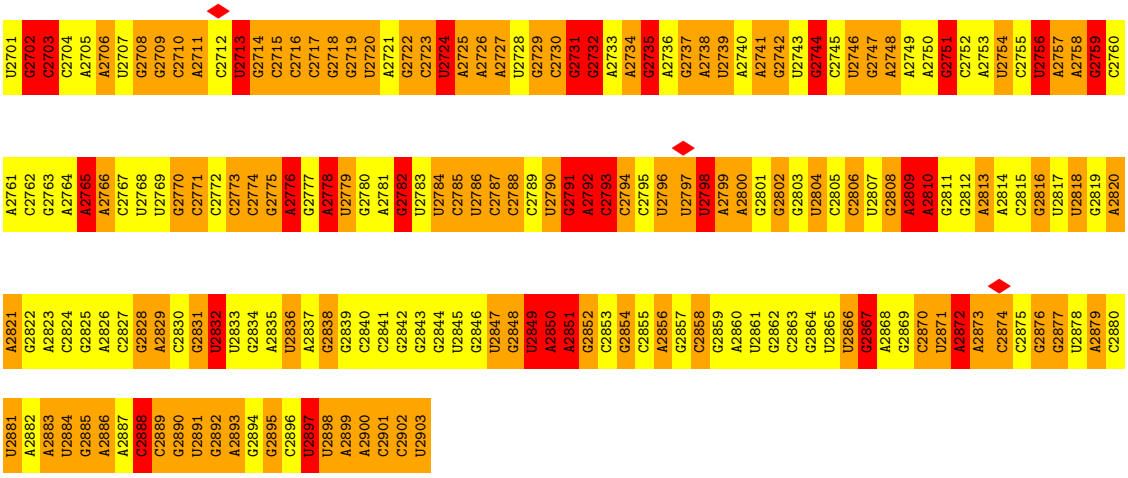
• Molecule 35: 23S RIBOSOMAL RNA

Chain BB:



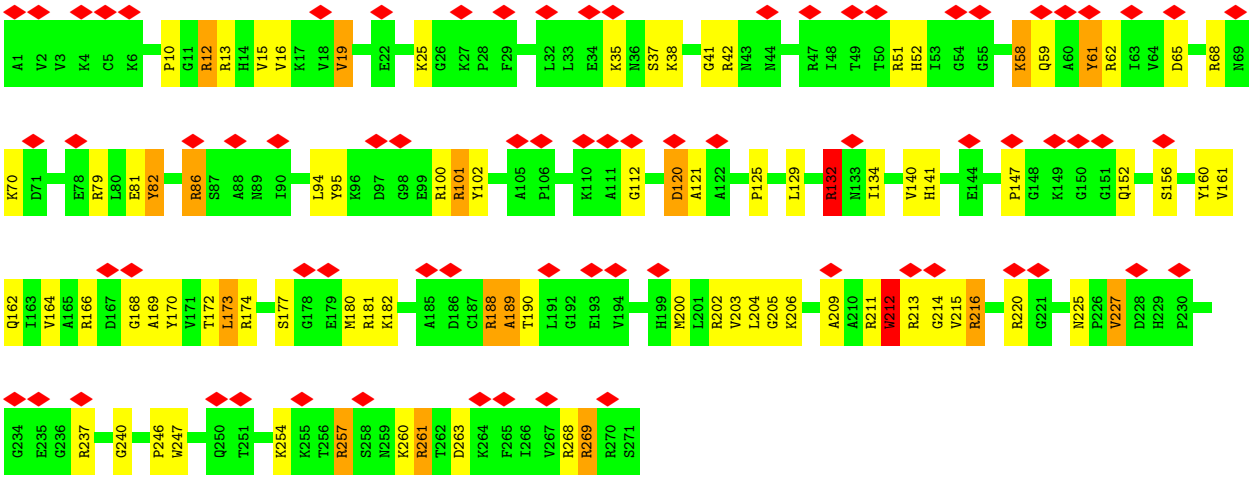






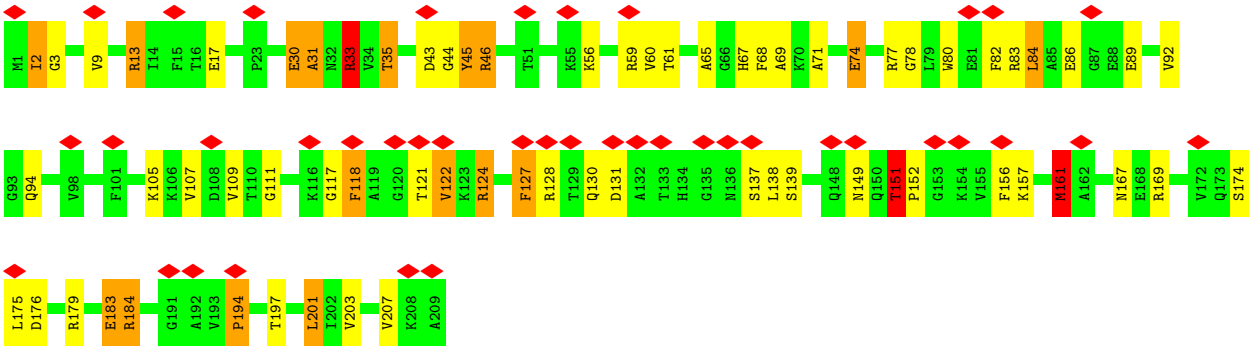
• Molecule 36: 50S RIBOSOMAL PROTEIN L2

Chain BC:



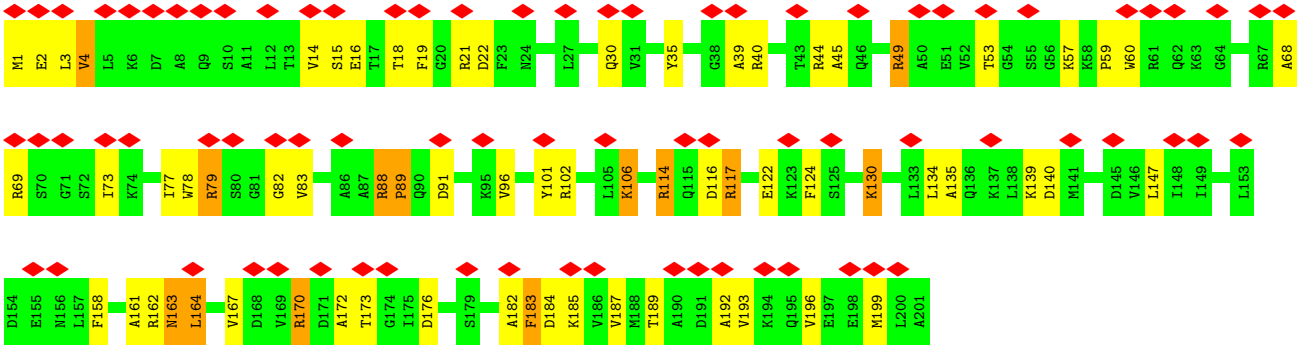
• Molecule 37: 50S RIBOSOMAL PROTEIN L3

Chain BD:



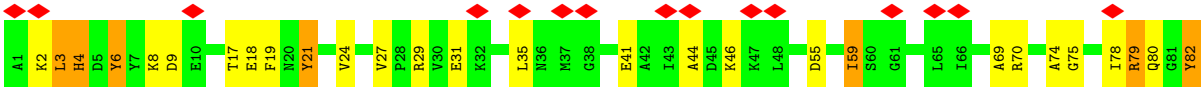
• Molecule 38: 50S RIBOSOMAL PROTEIN L4

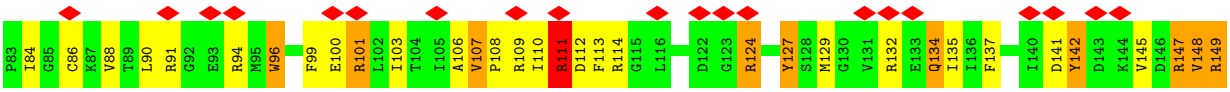
Chain BE:

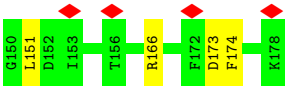


• Molecule 39: 50S RIBOSOMAL PROTEIN L5

Chain BF:

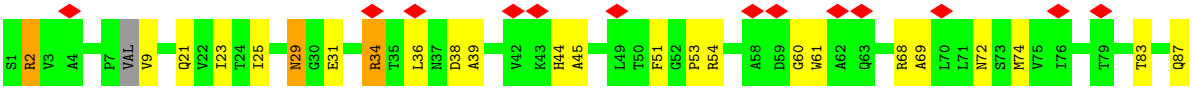


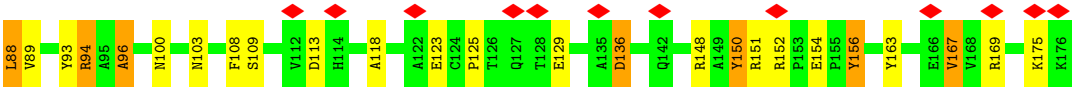




• Molecule 40: 50S RIBOSOMAL PROTEIN L6

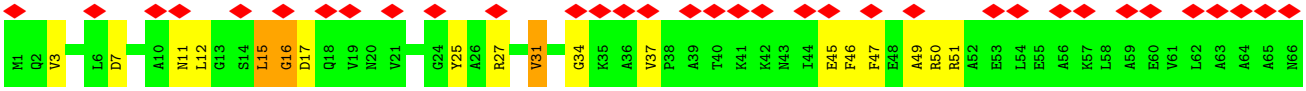
Chain BG:

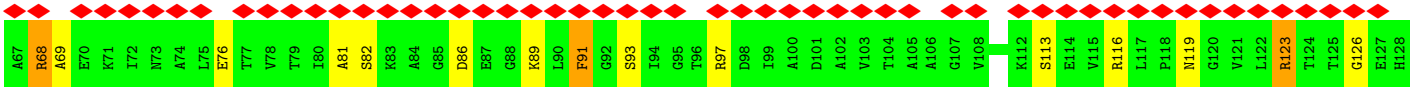


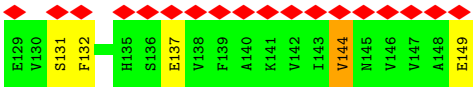


• Molecule 41: 50S RIBOSOMAL PROTEIN L9

Chain BH:

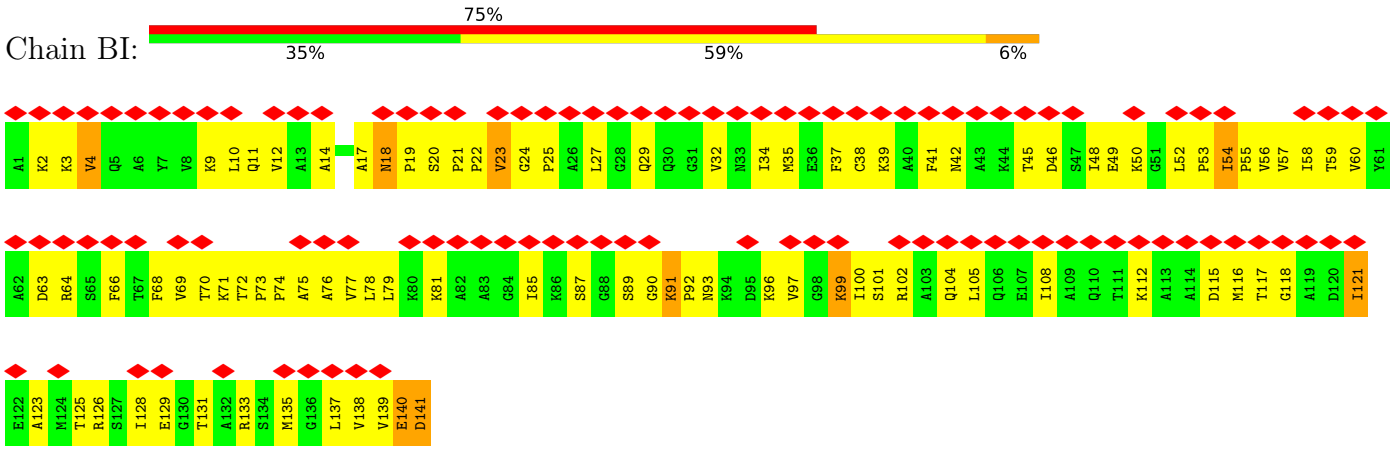






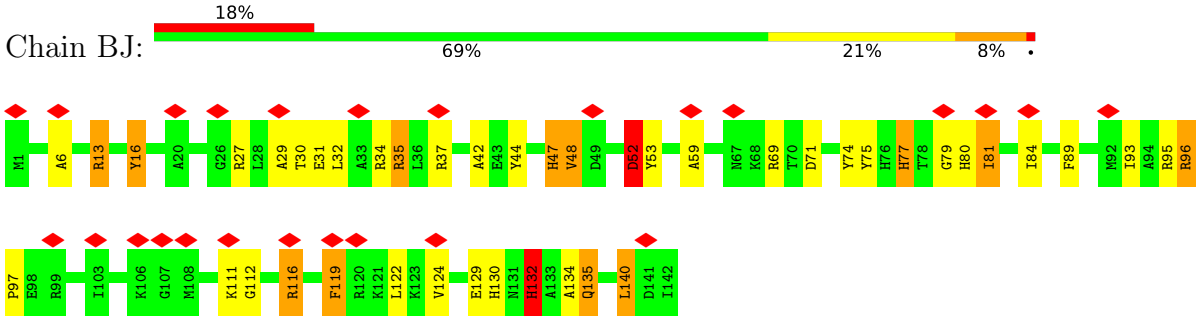
• Molecule 42: 50S RIBOSOMAL PROTEIN L11

Chain BI:



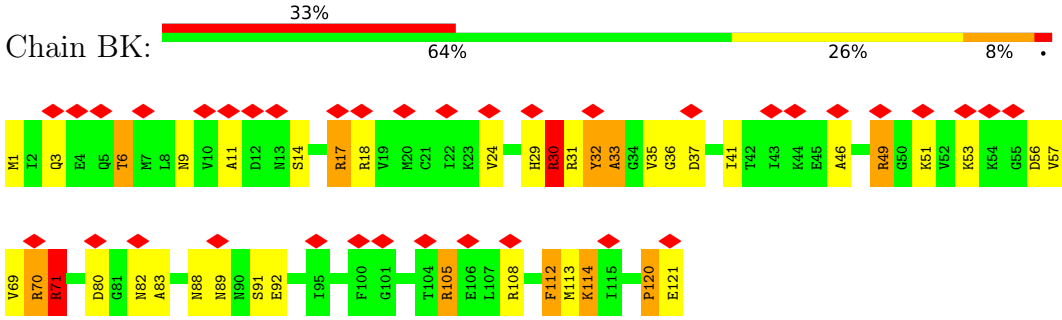
• Molecule 43: 50S RIBOSOMAL PROTEIN L13

Chain BJ:



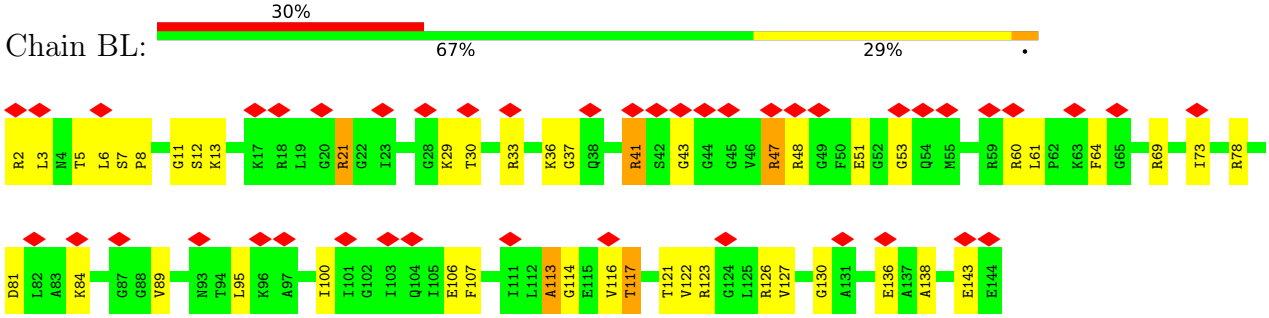
• Molecule 44: 50S RIBOSOMAL PROTEIN L14

Chain BK:



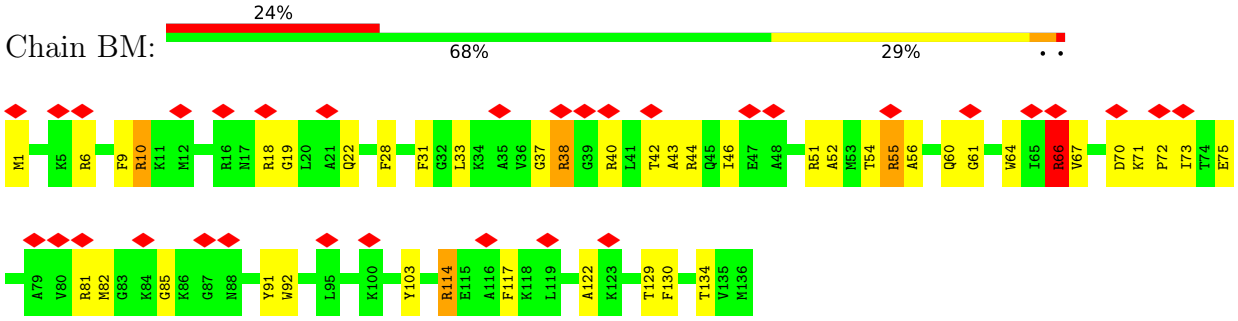
• Molecule 45: 50S RIBOSOMAL PROTEIN L15

Chain BL:



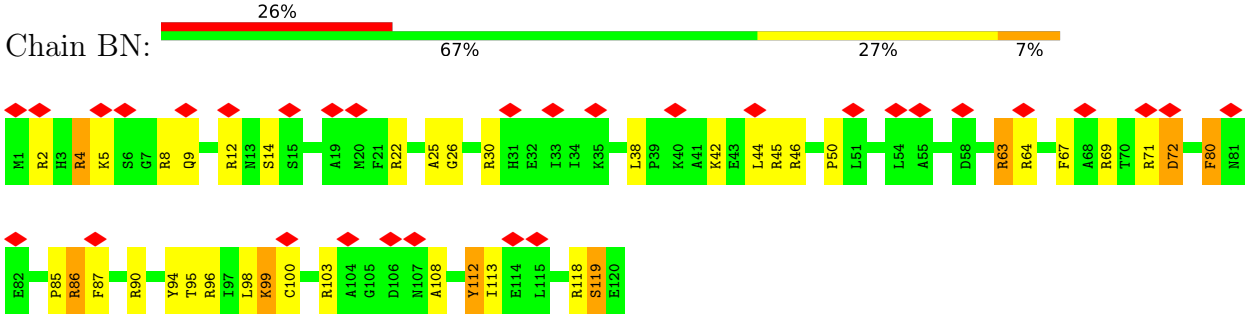
• Molecule 46: 50S RIBOSOMAL PROTEIN L16

Chain BM:



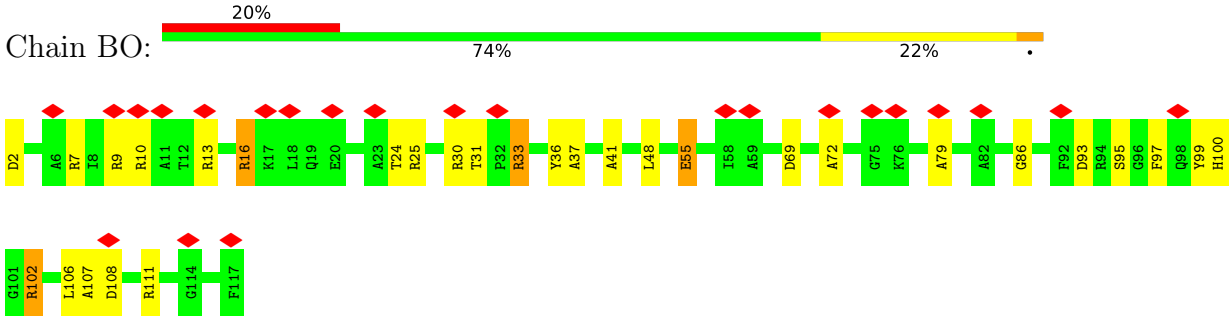
- Molecule 47: 50S RIBOSOMAL PROTEIN L17

Chain BN:



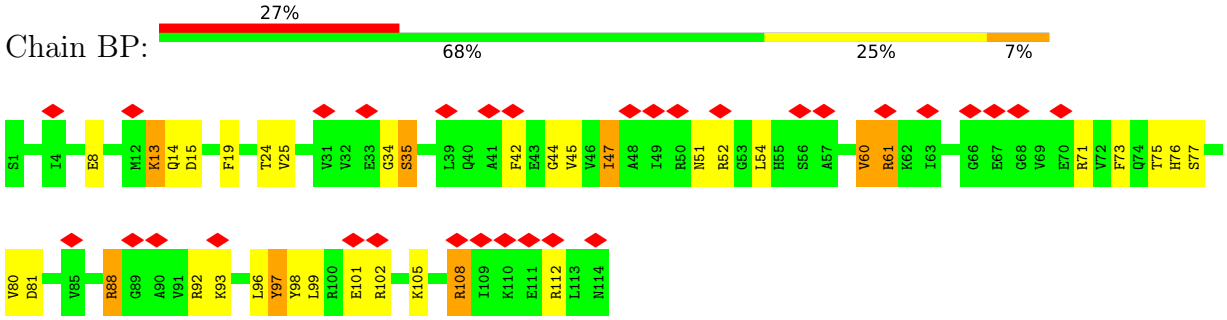
- Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain BO:



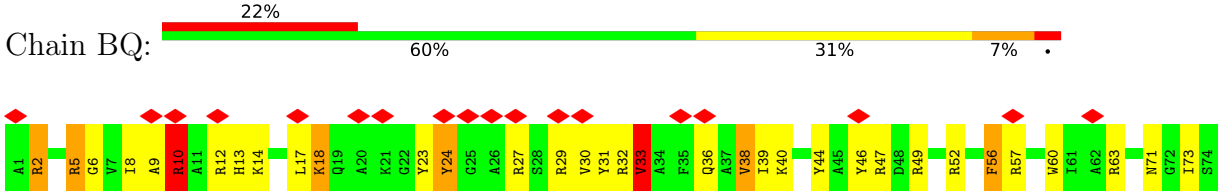
- Molecule 49: 50S RIBOSOMAL PROTEIN L19

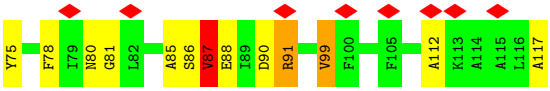
Chain BP:



- Molecule 50: 50S RIBOSOMAL PROTEIN L20

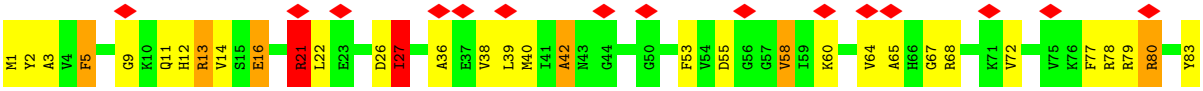
Chain BQ:

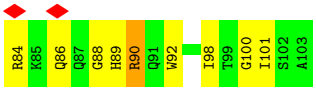




• Molecule 51: 50S RIBOSOMAL PROTEIN L21

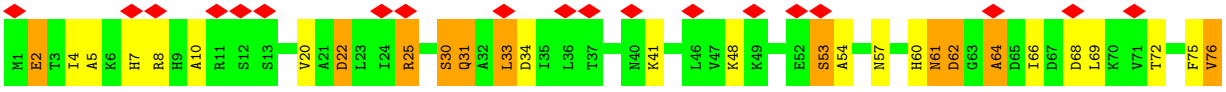
Chain BR:

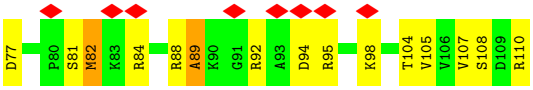




• Molecule 52: 50S RIBOSOMAL PROTEIN L22

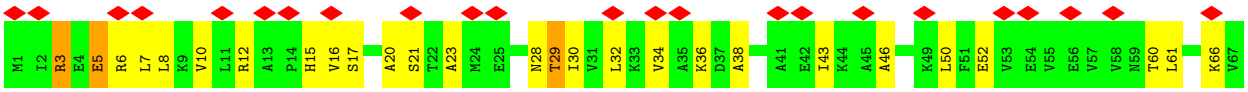
Chain BS:

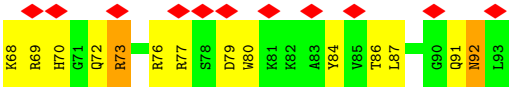




• Molecule 53: 50S RIBOSOMAL PROTEIN L23

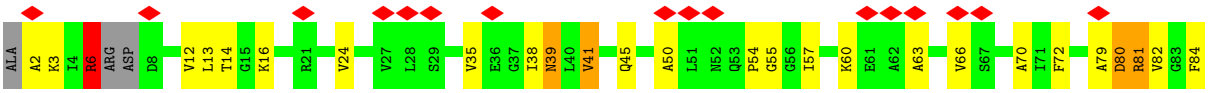
Chain BT:

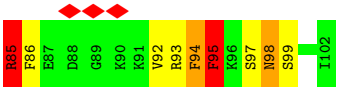




• Molecule 54: 50S RIBOSOMAL PROTEIN L24

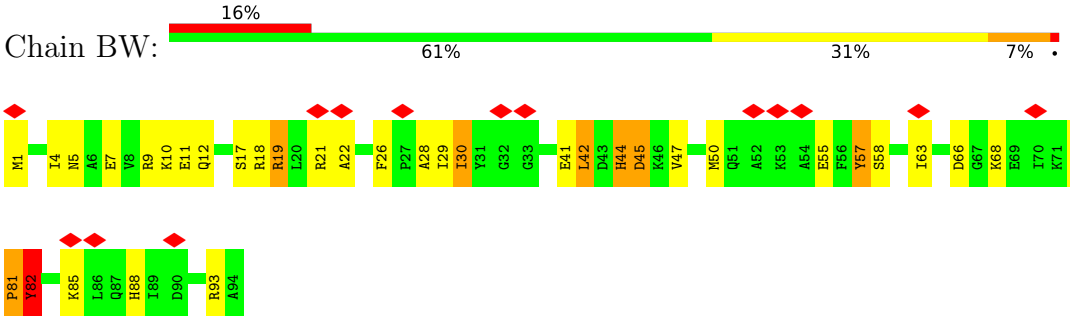
Chain BU:





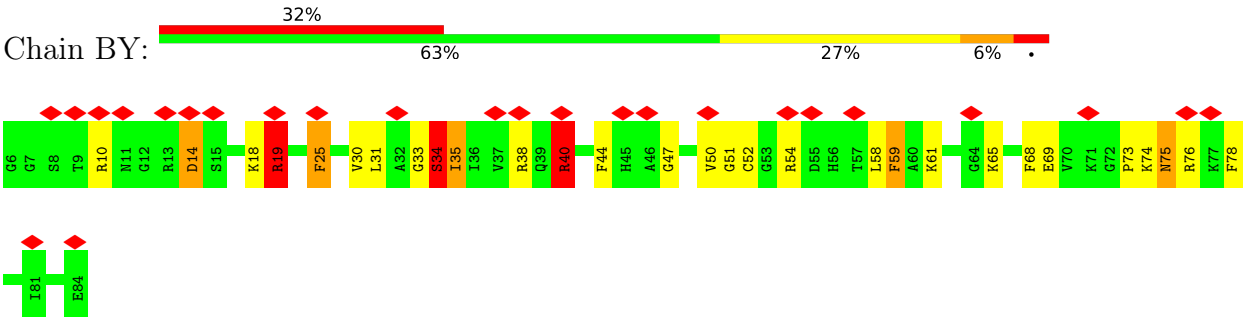
• Molecule 55: 50S RIBOSOMAL PROTEIN L25

Chain BW:



• Molecule 56: 50S RIBOSOMAL PROTEIN L27

Chain BY:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	263000	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	38900	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.760	Depositor
Minimum map value	-0.510	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	361.62, 363.82498, 361.62	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.2375, 1.23	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU

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	3.37	4837/36762 (13.2%)	3.72	8282/57350 (14.4%)
2	AB	1.71	14/1735 (0.8%)	2.05	53/2338 (2.3%)
3	AC	1.73	20/1651 (1.2%)	2.05	55/2225 (2.5%)
4	AD	1.80	24/1665 (1.4%)	2.05	48/2227 (2.2%)
5	AE	1.73	17/1118 (1.5%)	1.97	27/1504 (1.8%)
6	AF	1.77	7/835 (0.8%)	1.96	17/1128 (1.5%)
7	AG	1.82	18/1187 (1.5%)	2.01	40/1591 (2.5%)
8	AH	1.79	10/989 (1.0%)	2.07	29/1326 (2.2%)
9	AI	1.97	21/1034 (2.0%)	2.09	33/1375 (2.4%)
10	AJ	1.78	11/796 (1.4%)	1.89	15/1077 (1.4%)
11	AK	1.75	7/893 (0.8%)	1.96	18/1205 (1.5%)
12	AL	1.85	13/969 (1.3%)	1.98	28/1300 (2.2%)
13	AM	1.73	12/884 (1.4%)	2.02	28/1181 (2.4%)
14	AN	1.80	6/785 (0.8%)	1.92	19/1043 (1.8%)
15	AO	1.77	11/724 (1.5%)	1.90	24/966 (2.5%)
16	AP	1.84	9/648 (1.4%)	2.16	26/870 (3.0%)
17	AQ	1.73	4/657 (0.6%)	1.93	18/881 (2.0%)
18	AR	1.74	6/462 (1.3%)	2.28	16/621 (2.6%)
19	AS	1.78	8/652 (1.2%)	2.15	26/877 (3.0%)
20	AT	1.66	4/671 (0.6%)	1.93	17/888 (1.9%)
21	AU	1.82	6/430 (1.4%)	2.16	13/570 (2.3%)
22	AV	2.38	76/1820 (4.2%)	2.84	256/2836 (9.0%)
23	AX	1.81	4/264 (1.5%)	2.14	19/407 (4.7%)
24	AZ	1.97	1/99 (1.0%)	1.94	5/137 (3.6%)
25	B0	1.75	7/635 (1.1%)	2.27	19/848 (2.2%)
26	B1	1.72	5/510 (1.0%)	1.94	14/677 (2.1%)
27	B2	1.75	4/453 (0.9%)	1.86	10/605 (1.7%)
28	B3	1.82	6/450 (1.3%)	2.19	16/599 (2.7%)
29	B4	1.63	4/416 (1.0%)	2.02	13/554 (2.3%)
30	B5	1.56	11/1748 (0.6%)	1.95	40/2355 (1.7%)
31	B6	1.85	4/380 (1.1%)	2.31	17/498 (3.4%)
32	B7	1.68	4/513 (0.8%)	2.03	12/676 (1.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	B8	1.83	4/303 (1.3%)	2.01	7/397 (1.8%)
34	BA	3.34	356/2753 (12.9%)	3.78	615/4288 (14.3%)
35	BB	3.39	9308/69800 (13.3%)	3.73	15832/108892 (14.5%)
36	BC	1.81	24/2121 (1.1%)	2.05	60/2852 (2.1%)
37	BD	1.77	16/1586 (1.0%)	2.01	31/2134 (1.5%)
38	BE	1.69	8/1571 (0.5%)	1.97	41/2113 (1.9%)
39	BF	1.73	14/1444 (1.0%)	2.17	40/1937 (2.1%)
40	BG	1.76	13/1335 (1.0%)	2.04	28/1803 (1.6%)
41	BH	1.74	11/1122 (1.0%)	2.05	35/1515 (2.3%)
42	BI	0.62	2/1046 (0.2%)	0.56	1/1410 (0.1%)
43	BJ	1.77	12/1152 (1.0%)	2.04	30/1551 (1.9%)
44	BK	1.76	13/939 (1.4%)	1.99	23/1257 (1.8%)
45	BL	1.78	10/1054 (0.9%)	1.94	28/1403 (2.0%)
46	BM	1.83	9/1093 (0.8%)	2.07	30/1460 (2.1%)
47	BN	1.76	12/973 (1.2%)	2.22	32/1301 (2.5%)
48	BO	1.79	15/902 (1.7%)	2.02	24/1209 (2.0%)
49	BP	1.68	5/929 (0.5%)	2.03	20/1242 (1.6%)
50	BQ	1.89	15/960 (1.6%)	2.11	29/1278 (2.3%)
51	BR	1.80	11/829 (1.3%)	2.03	23/1107 (2.1%)
52	BS	1.71	7/864 (0.8%)	2.16	34/1156 (2.9%)
53	BT	1.69	5/744 (0.7%)	1.99	18/994 (1.8%)
54	BU	1.73	3/761 (0.4%)	2.02	25/1013 (2.5%)
55	BW	1.79	13/766 (1.7%)	2.05	18/1025 (1.8%)
56	BY	1.73	3/603 (0.5%)	2.11	23/797 (2.9%)
All	All	2.98	15080/158485 (9.5%)	3.34	26300/236869 (11.1%)

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	740
2	AB	0	5
3	AC	0	7
4	AD	0	11
5	AE	0	5
6	AF	0	3
7	AG	0	3
8	AH	0	3
9	AI	0	7
10	AJ	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	3
12	AL	0	5
13	AM	0	9
14	AN	0	3
15	AO	0	6
16	AP	0	4
17	AQ	0	1
18	AR	0	5
19	AS	0	4
20	AT	0	3
22	AV	0	13
23	AX	0	4
25	B0	0	4
26	B1	0	1
28	B3	0	2
29	B4	0	3
30	B5	0	6
31	B6	0	3
32	B7	0	1
34	BA	0	50
35	BB	0	1343
36	BC	0	8
37	BD	0	6
38	BE	0	5
39	BF	0	10
40	BG	0	3
41	BH	0	1
43	BJ	0	4
44	BK	0	5
45	BL	0	1
46	BM	0	3
47	BN	0	5
48	BO	0	2
49	BP	0	5
50	BQ	0	5
51	BR	0	3
52	BS	0	1
53	BT	0	1
54	BU	0	2
55	BW	0	4
56	BY	0	5
All	All	0	2342

The worst 5 of 15080 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BB	1403	A	N9-C4	21.34	1.50	1.37
35	BB	1301	A	N7-C5	-20.38	1.27	1.39
1	AA	930	C	N1-C6	19.80	1.49	1.37
1	AA	816	A	N7-C5	-19.29	1.27	1.39
35	BB	1821	A	N9-C4	19.18	1.49	1.37

The worst 5 of 26300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	753	A	N1-C6-N6	30.52	136.91	118.60
35	BB	666	A	N1-C6-N6	26.10	134.26	118.60
35	BB	533	G	N1-C6-O6	25.90	135.44	119.90
1	AA	242	G	C5-C6-O6	-25.60	113.24	128.60
35	BB	1014	A	N1-C6-N6	25.57	133.94	118.60

There are no chirality outliers.

5 of 2342 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	11	G	Sidechain
1	AA	12	U	Sidechain
1	AA	5	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	A	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	32831	0	16502	183	0
2	AB	1704	0	1732	3	0
3	AC	1624	0	1699	12	0
4	AD	1643	0	1710	5	0
5	AE	1105	0	1148	6	0
6	AF	817	0	808	7	0
7	AG	1174	0	1230	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	979	0	1034	1	0
9	AI	1022	0	1070	9	0
10	AJ	786	0	828	3	0
11	AK	877	0	887	9	0
12	AL	955	0	1019	2	0
13	AM	876	0	937	7	0
14	AN	774	0	827	2	0
15	AO	716	0	742	3	0
16	AP	638	0	656	0	0
17	AQ	648	0	691	4	0
18	AR	455	0	478	1	0
19	AS	637	0	665	5	0
20	AT	665	0	714	4	0
21	AU	425	0	449	2	0
22	AV	1649	0	832	21	0
23	AX	236	0	121	10	0
24	AZ	100	0	99	0	0
25	B0	625	0	655	1	0
26	B1	509	0	543	1	0
27	B2	449	0	491	1	0
28	B3	444	0	461	3	0
29	B4	409	0	440	0	0
30	B5	1733	0	1824	4	0
31	B6	377	0	418	3	0
32	B7	504	0	574	5	0
33	B8	302	0	343	0	0
34	BA	2464	0	1246	8	0
35	BB	62321	0	31294	336	0
36	BC	2082	0	2157	14	0
37	BD	1565	0	1616	8	0
38	BE	1552	0	1619	9	0
39	BF	1420	0	1460	9	0
40	BG	1316	0	1364	4	0
41	BH	1111	0	1148	1	0
42	BI	1032	0	1088	118	0
43	BJ	1129	0	1162	8	0
44	BK	930	0	1003	6	0
45	BL	1045	0	1117	6	0
46	BM	1074	0	1157	4	0
47	BN	960	0	1000	2	0
48	BO	892	0	923	2	0
49	BP	917	0	965	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BQ	947	0	1022	8	0
51	BR	816	0	839	8	0
52	BS	857	0	922	3	0
53	BT	738	0	807	5	0
54	BU	755	0	807	10	0
55	BW	753	0	780	5	0
56	BY	596	0	610	1	0
All	All	145960	0	98733	840	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 3.

The worst 5 of 840 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)
22:AV:35:G:N2	23:AX:18:C:C2	2.08	1.22
42:BI:11:GLN:HG2	42:BI:55:PRO:HB3	1.51	0.91
42:BI:140:GLU:O	42:BI:141:ASP:OXT	1.91	0.89
42:BI:27:LEU:HD23	42:BI:27:LEU:H	1.43	0.82
42:BI:121:ILE:HD13	42:BI:121:ILE:H	1.44	0.82

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	AB	216/218 (99%)	159 (74%)	41 (19%)	16 (7%)	1 13
3	AC	204/206 (99%)	158 (78%)	31 (15%)	15 (7%)	1 13
4	AD	203/205 (99%)	160 (79%)	34 (17%)	9 (4%)	2 22
5	AE	148/150 (99%)	110 (74%)	27 (18%)	11 (7%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	98/100 (98%)	73 (74%)	18 (18%)	7 (7%)	1	14
7	AG	148/150 (99%)	109 (74%)	33 (22%)	6 (4%)	3	22
8	AH	127/129 (98%)	94 (74%)	27 (21%)	6 (5%)	2	21
9	AI	125/127 (98%)	99 (79%)	21 (17%)	5 (4%)	3	23
10	AJ	96/98 (98%)	71 (74%)	14 (15%)	11 (12%)	0	6
11	AK	115/117 (98%)	96 (84%)	14 (12%)	5 (4%)	2	22
12	AL	121/123 (98%)	100 (83%)	12 (10%)	9 (7%)	1	13
13	AM	111/113 (98%)	80 (72%)	19 (17%)	12 (11%)	0	7
14	AN	92/96 (96%)	57 (62%)	22 (24%)	13 (14%)	0	4
15	AO	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	6	33
16	AP	78/80 (98%)	62 (80%)	10 (13%)	6 (8%)	1	12
17	AQ	78/80 (98%)	65 (83%)	7 (9%)	6 (8%)	1	12
18	AR	53/55 (96%)	42 (79%)	8 (15%)	3 (6%)	1	17
19	AS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	3	23
20	AT	83/85 (98%)	68 (82%)	13 (16%)	2 (2%)	6	33
21	AU	49/51 (96%)	41 (84%)	5 (10%)	3 (6%)	1	16
24	AZ	18/20 (90%)	16 (89%)	1 (6%)	1 (6%)	2	18
25	B0	75/77 (97%)	52 (69%)	20 (27%)	3 (4%)	3	23
26	B1	61/63 (97%)	45 (74%)	14 (23%)	2 (3%)	4	26
27	B2	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
28	B3	54/56 (96%)	42 (78%)	9 (17%)	3 (6%)	2	18
29	B4	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	3	22
30	B5	232/234 (99%)	190 (82%)	37 (16%)	5 (2%)	6	35
31	B6	44/46 (96%)	29 (66%)	11 (25%)	4 (9%)	1	10
32	B7	62/64 (97%)	52 (84%)	5 (8%)	5 (8%)	1	12
33	B8	36/38 (95%)	30 (83%)	4 (11%)	2 (6%)	2	18
36	BC	269/271 (99%)	209 (78%)	47 (18%)	13 (5%)	2	20
37	BD	207/209 (99%)	149 (72%)	37 (18%)	21 (10%)	0	9
38	BE	199/201 (99%)	161 (81%)	23 (12%)	15 (8%)	1	13
39	BF	176/178 (99%)	131 (74%)	26 (15%)	19 (11%)	0	7
40	BG	171/176 (97%)	134 (78%)	28 (16%)	9 (5%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	BH	147/149 (99%)	111 (76%)	31 (21%)	5 (3%)	3 26
42	BI	139/141 (99%)	113 (81%)	21 (15%)	5 (4%)	3 25
43	BJ	140/142 (99%)	106 (76%)	24 (17%)	10 (7%)	1 14
44	BK	119/121 (98%)	95 (80%)	14 (12%)	10 (8%)	1 11
45	BL	141/143 (99%)	115 (82%)	16 (11%)	10 (7%)	1 14
46	BM	134/136 (98%)	105 (78%)	21 (16%)	8 (6%)	1 16
47	BN	118/120 (98%)	96 (81%)	16 (14%)	6 (5%)	2 19
48	BO	114/116 (98%)	98 (86%)	14 (12%)	2 (2%)	8 40
49	BP	112/114 (98%)	85 (76%)	19 (17%)	8 (7%)	1 14
50	BQ	115/117 (98%)	84 (73%)	21 (18%)	10 (9%)	1 11
51	BR	101/103 (98%)	80 (79%)	13 (13%)	8 (8%)	1 12
52	BS	108/110 (98%)	76 (70%)	21 (19%)	11 (10%)	0 8
53	BT	91/93 (98%)	60 (66%)	25 (28%)	6 (7%)	1 15
54	BU	94/102 (92%)	71 (76%)	16 (17%)	7 (7%)	1 13
55	BW	92/94 (98%)	76 (83%)	10 (11%)	6 (6%)	1 15
56	BY	77/79 (98%)	46 (60%)	18 (23%)	13 (17%)	0 3
All	All	5858/5971 (98%)	4523 (77%)	956 (16%)	379 (6%)	2 15

5 of 379 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	17	TRP
3	AC	116	ALA
5	AE	11	GLN
5	AE	17	VAL
9	AI	58	GLU

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	AB	180/180 (100%)	171 (95%)	9 (5%)	24 49
3	AC	170/170 (100%)	158 (93%)	12 (7%)	14 39
4	AD	172/172 (100%)	165 (96%)	7 (4%)	30 55
5	AE	113/113 (100%)	103 (91%)	10 (9%)	10 31
6	AF	87/87 (100%)	85 (98%)	2 (2%)	50 70
7	AG	123/123 (100%)	120 (98%)	3 (2%)	49 69
8	AH	104/104 (100%)	99 (95%)	5 (5%)	25 51
9	AI	105/105 (100%)	100 (95%)	5 (5%)	25 51
10	AJ	86/86 (100%)	81 (94%)	5 (6%)	20 45
11	AK	90/90 (100%)	86 (96%)	4 (4%)	28 53
12	AL	103/103 (100%)	98 (95%)	5 (5%)	25 50
13	AM	91/91 (100%)	89 (98%)	2 (2%)	52 71
14	AN	79/79 (100%)	76 (96%)	3 (4%)	33 57
15	AO	76/76 (100%)	69 (91%)	7 (9%)	9 29
16	AP	65/65 (100%)	62 (95%)	3 (5%)	27 52
17	AQ	74/74 (100%)	68 (92%)	6 (8%)	11 35
18	AR	48/48 (100%)	44 (92%)	4 (8%)	11 34
19	AS	70/70 (100%)	64 (91%)	6 (9%)	10 32
20	AT	65/65 (100%)	64 (98%)	1 (2%)	65 80
21	AU	44/44 (100%)	38 (86%)	6 (14%)	3 17
25	B0	67/67 (100%)	65 (97%)	2 (3%)	41 63
26	B1	55/55 (100%)	50 (91%)	5 (9%)	9 30
27	B2	48/48 (100%)	47 (98%)	1 (2%)	53 72
28	B3	47/47 (100%)	46 (98%)	1 (2%)	53 72
29	B4	45/45 (100%)	42 (93%)	3 (7%)	16 40
30	B5	181/181 (100%)	175 (97%)	6 (3%)	38 61
31	B6	38/38 (100%)	33 (87%)	5 (13%)	4 18
32	B7	51/51 (100%)	48 (94%)	3 (6%)	19 45
33	B8	34/34 (100%)	34 (100%)	0	100 100
36	BC	216/216 (100%)	204 (94%)	12 (6%)	21 46
37	BD	164/164 (100%)	146 (89%)	18 (11%)	6 22
38	BE	165/165 (100%)	157 (95%)	8 (5%)	25 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	BF	149/149 (100%)	143 (96%)	6 (4%)	31 55
40	BG	136/137 (99%)	125 (92%)	11 (8%)	11 35
41	BH	114/114 (100%)	110 (96%)	4 (4%)	36 59
42	BI	109/109 (100%)	104 (95%)	5 (5%)	27 52
43	BJ	116/116 (100%)	112 (97%)	4 (3%)	37 60
44	BK	102/102 (100%)	92 (90%)	10 (10%)	8 26
45	BL	102/102 (100%)	98 (96%)	4 (4%)	32 56
46	BM	109/109 (100%)	104 (95%)	5 (5%)	27 52
47	BN	100/100 (100%)	96 (96%)	4 (4%)	31 55
48	BO	86/86 (100%)	84 (98%)	2 (2%)	50 70
49	BP	99/99 (100%)	96 (97%)	3 (3%)	41 63
50	BQ	89/89 (100%)	83 (93%)	6 (7%)	16 40
51	BR	84/84 (100%)	76 (90%)	8 (10%)	8 28
52	BS	93/93 (100%)	87 (94%)	6 (6%)	17 42
53	BT	80/80 (100%)	68 (85%)	12 (15%)	3 15
54	BU	81/83 (98%)	76 (94%)	5 (6%)	18 43
55	BW	78/78 (100%)	73 (94%)	5 (6%)	17 42
56	BY	59/59 (100%)	54 (92%)	5 (8%)	10 33
All	All	4842/4845 (100%)	4568 (94%)	274 (6%)	24 45

5 of 274 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	BQ	40	LYS
51	BR	78	ARG
54	BU	14	THR
19	AS	60	PHE
19	AS	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
43	BJ	40	HIS
51	BR	91	GLN
43	BJ	80	HIS

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Mol	Chain	Res	Type
49	BP	76	HIS
54	BU	39	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1530 (99%)	269 (17%)	34 (2%)
22	AV	76/77 (98%)	15 (19%)	0
23	AX	10/11 (90%)	8 (80%)	0
34	BA	112/117 (95%)	16 (14%)	2 (1%)
35	BB	2902/2903 (99%)	471 (16%)	56 (1%)
All	All	4629/4638 (99%)	779 (16%)	92 (1%)

5 of 779 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	15	G
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BB	1332	G
35	BB	2131	U
35	BB	1459	G
35	BB	1808	A
35	BB	2145	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	5MU	AV	54	22	18,21,23	0.64	0	26,30,35	0.71	1 (3%)

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
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	54	5MU	O4'-C1'-N1	2.42	113.90	108.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
54	BU	1
14	AN	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BU	4:ILE	C	6:ARG	N	4.65
1	AN	35:ALA	C	40:ARG	N	4.56

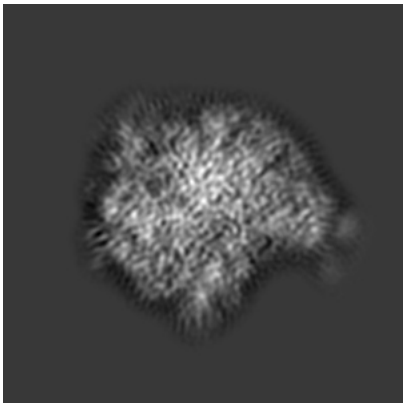
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1657. These allow visual inspection of the internal detail of the map and identification of artifacts.

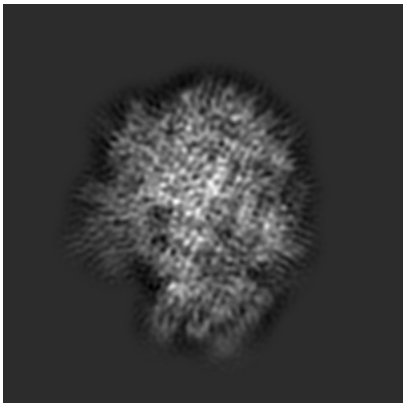
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

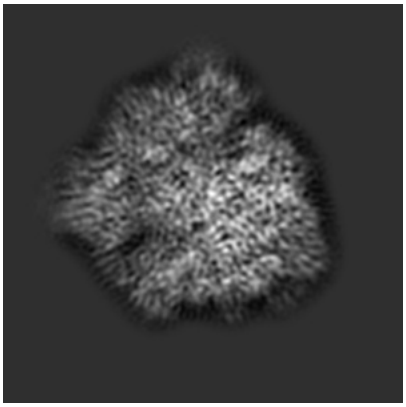
6.1.1 Primary map



X



Y

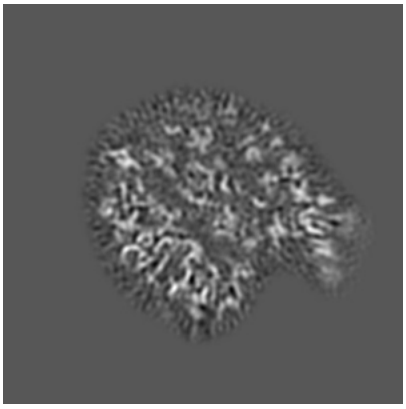


Z

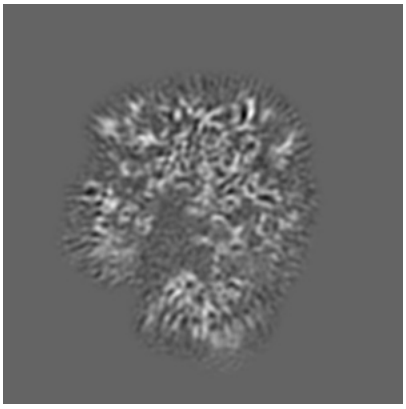
The images above show the map projected in three orthogonal directions.

6.2 Central slices

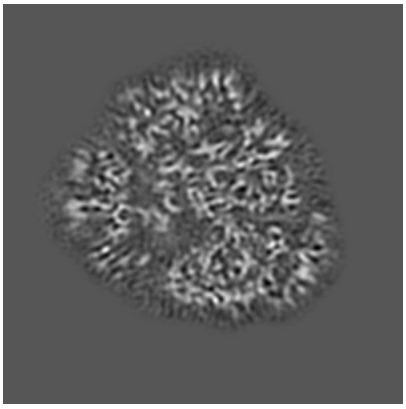
6.2.1 Primary map



X Index: 147



Y Index: 147

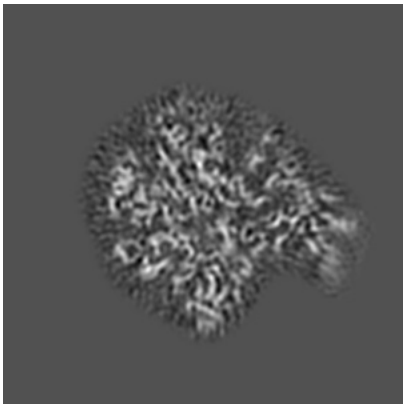


Z Index: 147

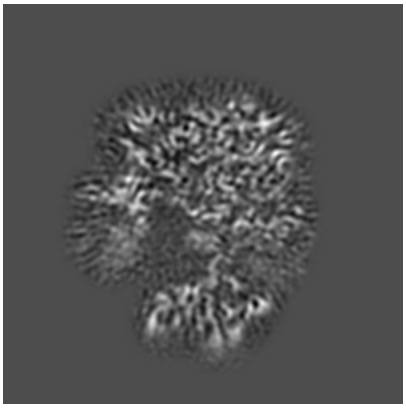
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

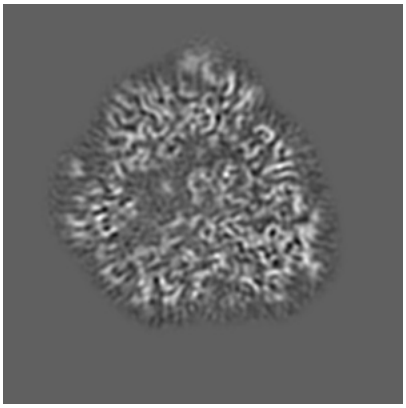
6.3.1 Primary map



X Index: 152



Y Index: 155



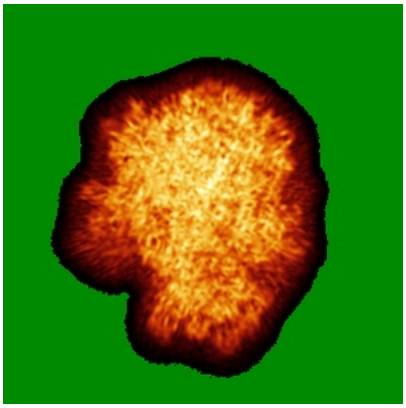
Z Index: 136

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

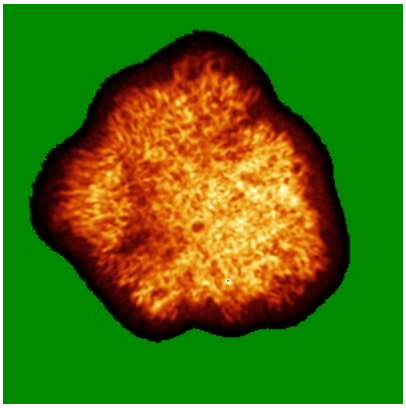
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

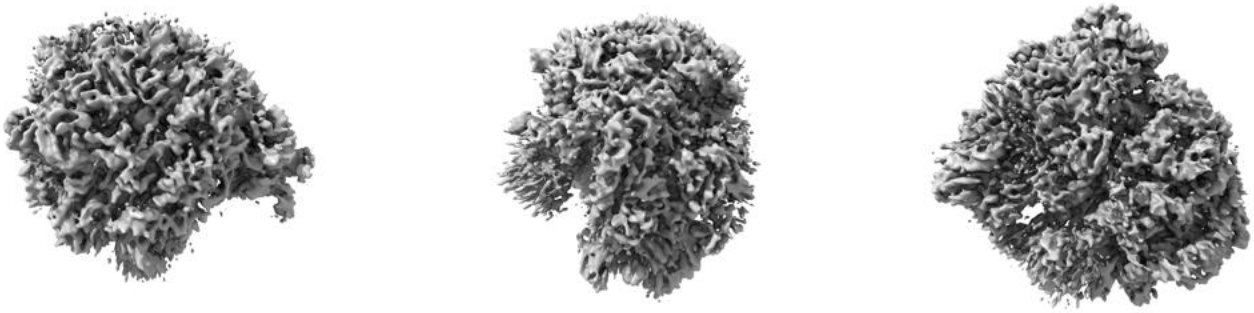


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

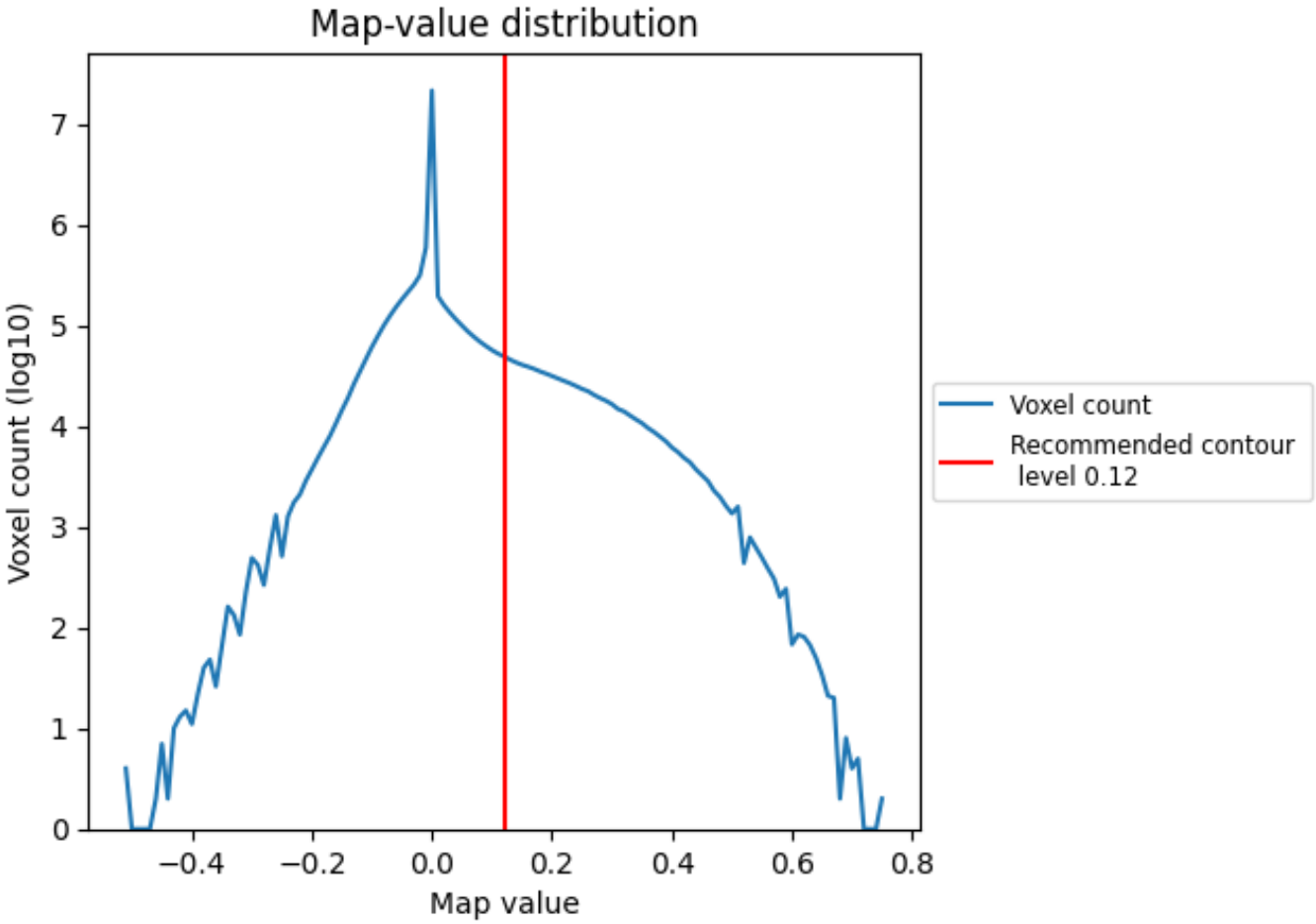
6.6 Mask visualisation (i)

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

7 Map analysis

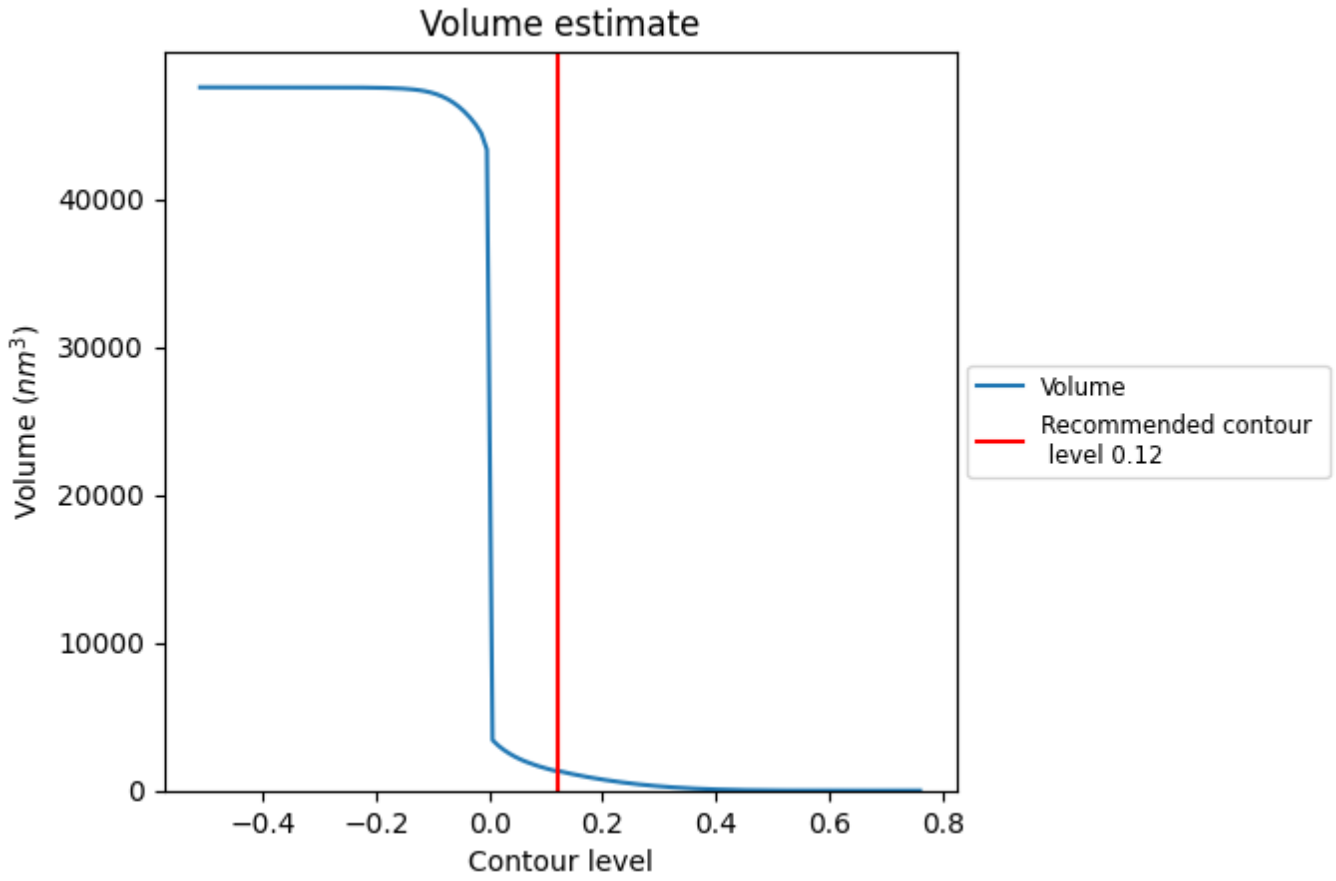
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

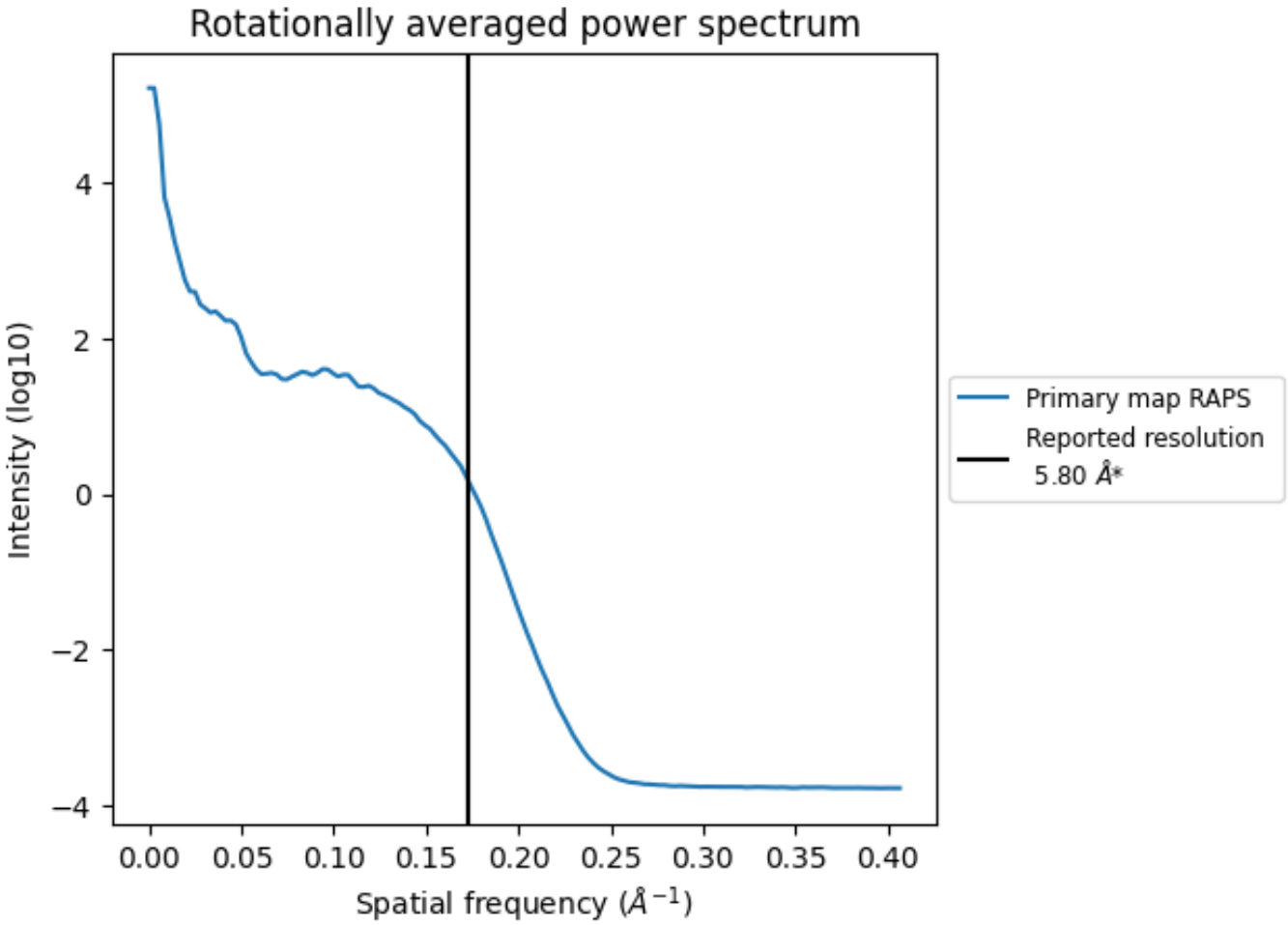
7.2 Volume estimate (i)



The volume at the recommended contour level is 1327 nm^3; this corresponds to an approximate mass of 1198 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 0.172 Å^{-1}

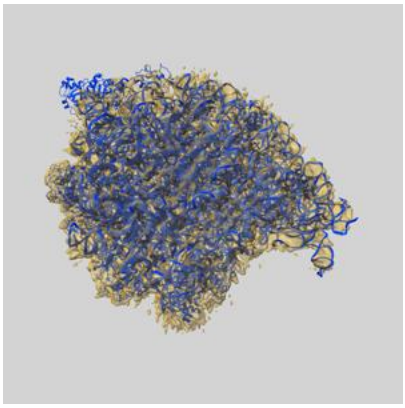
8 Fourier-Shell correlation (i)

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

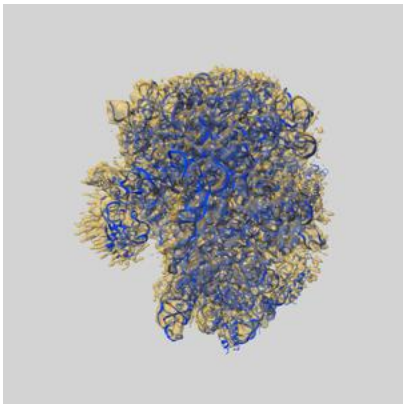
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1657 and PDB model 4V5H. Per-residue inclusion information can be found in section 3 on page 14.

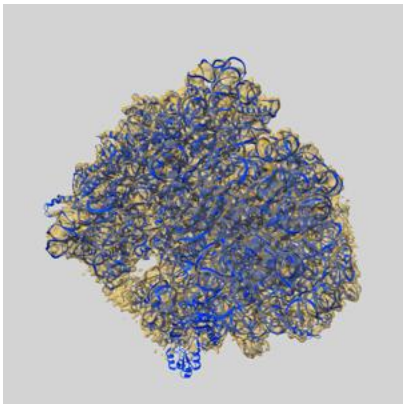
9.1 Map-model overlay



X



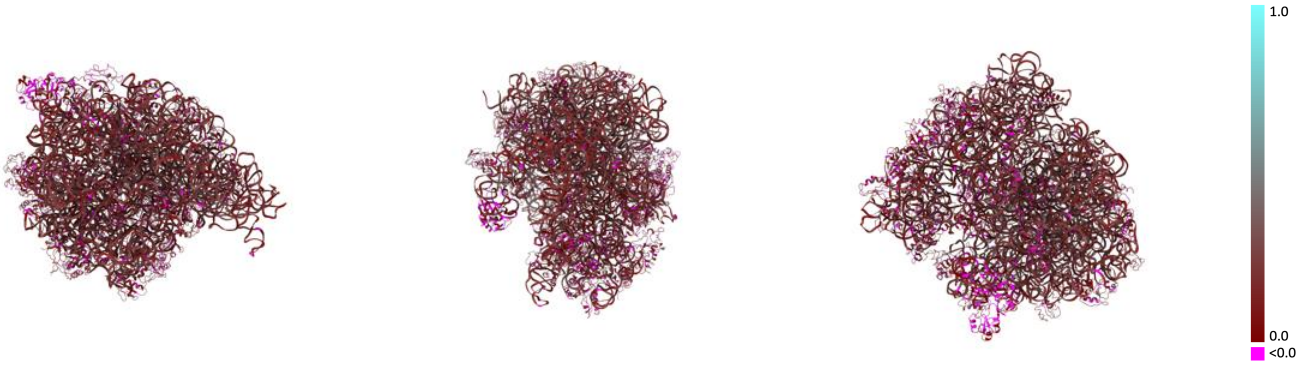
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

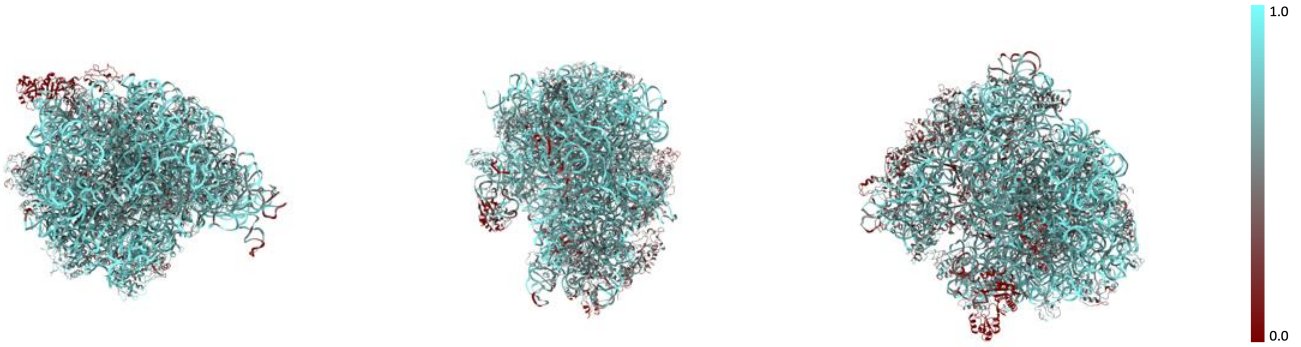
9.2 Q-score mapped to coordinate model



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.

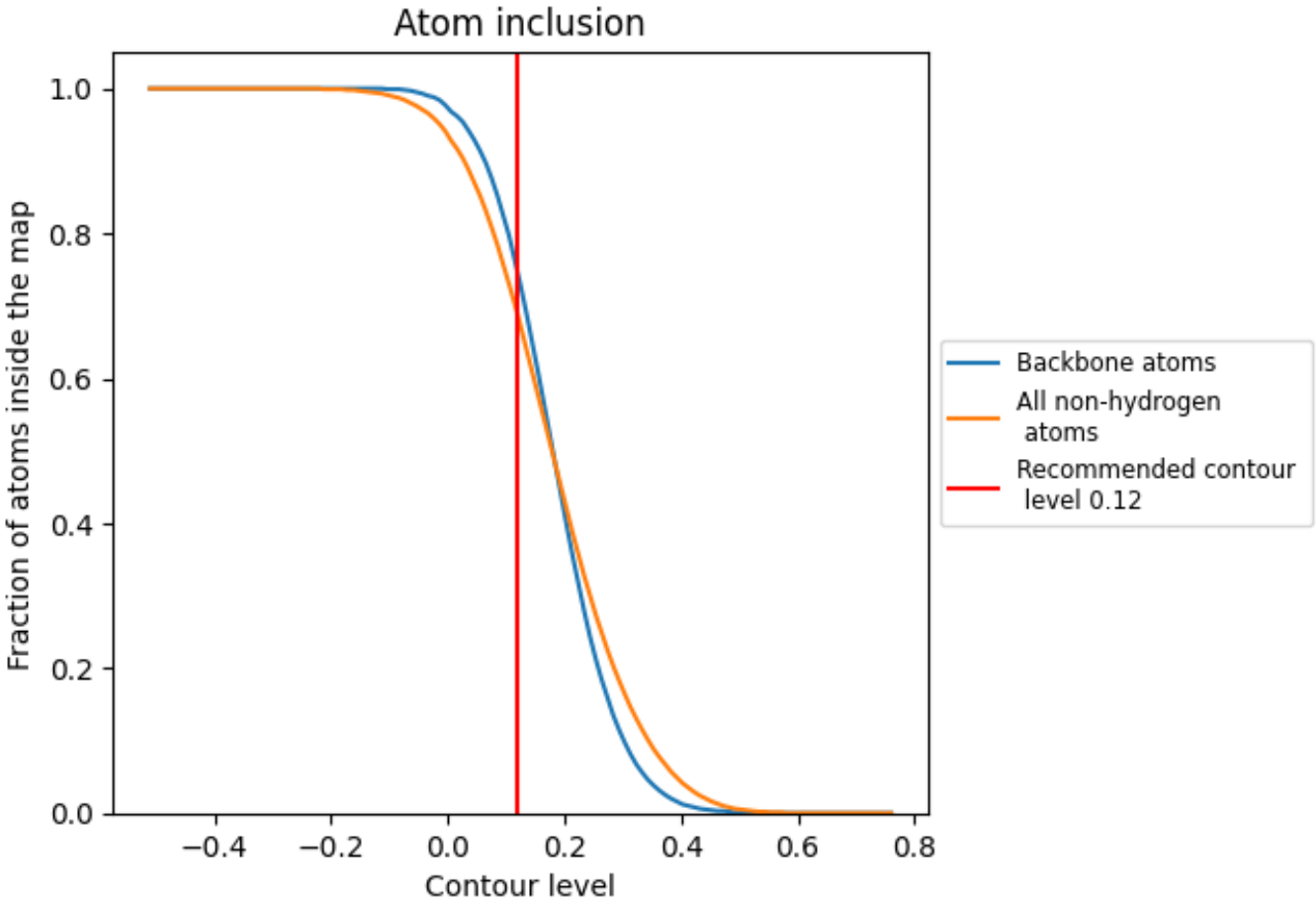
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.1890
AA	0.7560	0.2050
AB	0.3910	0.1500
AC	0.4960	0.1420
AD	0.4610	0.1350
AE	0.5320	0.1500
AF	0.6060	0.1760
AG	0.4700	0.1610
AH	0.5290	0.1450
AI	0.4710	0.1220
AJ	0.3250	0.1070
AK	0.5430	0.1610
AL	0.5160	0.1630
AM	0.5490	0.1550
AN	0.5610	0.1400
AO	0.5640	0.1650
AP	0.5310	0.1390
AQ	0.5680	0.1720
AR	0.5870	0.1720
AS	0.5860	0.1570
AT	0.5280	0.1460
AU	0.3500	0.1570
AV	0.5620	0.1430
AX	0.2630	0.1480
AZ	0.4900	0.3070
B0	0.5410	0.1620
B1	0.5510	0.1390
B2	0.5810	0.1740
B3	0.5650	0.1600
B4	0.5760	0.1680
B5	0.0180	-0.0010
B6	0.4650	0.1340
B7	0.5580	0.1530
B8	0.5620	0.1810
BA	0.8170	0.2140

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Chain	Atom inclusion	Q-score
BB	0.7850	0.2140
BC	0.5570	0.1700
BD	0.5980	0.1590
BE	0.4930	0.1400
BF	0.5940	0.1600
BG	0.6720	0.1850
BH	0.2460	0.1340
BI	0.2170	0.0320
BJ	0.6080	0.1750
BK	0.5070	0.1660
BL	0.5340	0.1610
BM	0.5540	0.1740
BN	0.5570	0.1360
BO	0.6230	0.1600
BP	0.5640	0.1720
BQ	0.5560	0.1160
BR	0.6200	0.1840
BS	0.5420	0.1360
BT	0.5230	0.1380
BU	0.5570	0.1560
BW	0.6440	0.1700
BY	0.5190	0.1080