



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2025 – 09:58 AM EDT

PDB ID : 4V68
EMDB ID : EMD-5030
Title : T. thermophilus 70S ribosome in complex with mRNA, tRNAs and EF-Tu.GDP.kirromycin ternary complex, fitted to a 6.4 Å Cryo-EM map.
Authors : Schuette, J.-C.; Spahn, C.M.T.
Deposited on : 2008-12-11
Resolution : 6.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

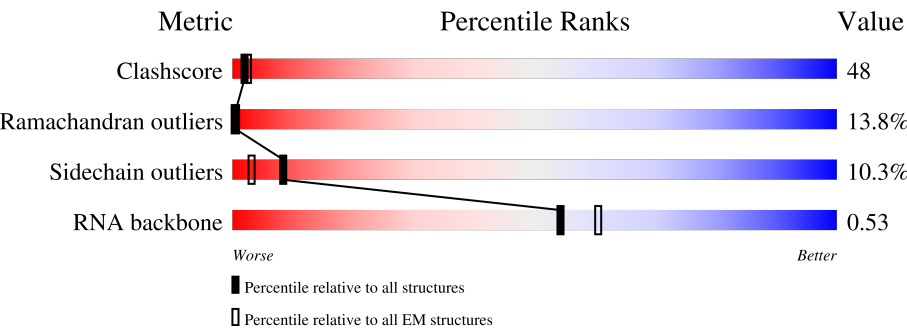
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

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 6.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1504	
2	AB	235	
3	AD	208	
4	AE	151	
5	AF	101	
6	AH	138	
7	AK	119	

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Mol	Chain	Length	Quality of chain
8	AL	125	
9	AO	88	
10	AP	84	
11	AQ	100	
12	AR	70	
13	AT	99	
14	AC	207	
15	AG	155	
16	AI	127	
17	AJ	99	
18	AM	125	
19	AN	60	
20	AS	79	
21	AU	25	
22	AV	77	
23	AX	6	
24	AW	76	
25	AY	72	
26	A0	3	
27	AZ	405	
28	B0	85	
29	B1	89	
30	B2	51	
31	B3	60	
32	B4	50	



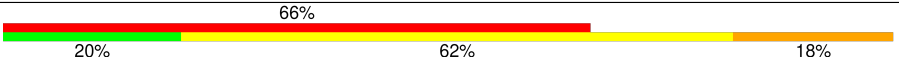
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Mol	Chain	Length	Quality of chain
33	B5	59	
34	B6	45	
35	B7	49	
36	B8	64	
37	B9	35	
38	BA	2852	
39	BB	119	
40	BC	191	
41	BD	272	
42	BE	205	
43	BF	208	
44	BG	181	
45	BH	160	
46	BI	146	
47	BL	138	
48	BN	139	
49	BO	122	
50	BP	146	
51	BQ	136	
52	BR	117	
53	BS	99	
54	BT	138	
55	BU	117	
56	BV	101	
57	BW	113	

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Mol	Chain	Length	Quality of chain
58	BX	93	
59	BY	101	
60	BZ	177	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	M2G	AY	26	-	-	X	-
25	OMG	AY	34	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 152000 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0
			32329	14390	5992	10444	1503		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	235	Total	C	N	O	S	0	1
			1901	1213	342	341	5		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AD	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	151	Total	C	N	O	S	0	1
			1147	724	218	201	4		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 6 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AH	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 7 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AK	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AL	125	Total	C	N	O	S	0	1
			971	611	196	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AO	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AP	84	Total	C	N	O	S	0	1
			701	443	140	117	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AQ	100	Total	C	N	O	S	0	1
			824	528	152	142	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AR	70	Total	C	N	O	0	0
			574	367	112	95		

- Molecule 13 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AT	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AC	207	Total	C	N	O	S	0	1
			1613	1016	315	281	1		

- Molecule 15 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AG	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AI	127	Total	C	N	O	S	0	0
			1011	639	198	174			

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AJ	99	Total	C	N	O	S	0	1
			795	499	157	138	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AM	125	Total	C	N	O	S	0	1
			988	611	206	169	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AN	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AS	79	Total	C	N	O	S	0	1
			630	403	115	110	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	AU	25	Total	C	N	O	0	1
			209	128	51	30		

- 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
			1645	733	297	538	77		

- Molecule 23 is a RNA chain called SYNTHETIC MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AX	6	Total	C	N	O	P	0	0
			132	59	27	40	6		

- Molecule 24 is a RNA chain called E-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AW	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 25 is a RNA chain called AT-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	72	Total	C	N	O	P	0	0
			1546	698	275	501	72		

- Molecule 26 is a RNA chain called MRNA CODON.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A0	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A0	100	U	A	conflict	UNP Q5SHN6
A0	101	U	K	conflict	UNP Q5SHN6
A0	102	U	G	conflict	UNP Q5SHN6

- Molecule 27 is a protein called Elongation factor Tu-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AZ	378	Total	C	N	O	S	8	0
			2962	1879	513	557	13		

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B0	85	Total	C	N	O	S	0	0
			650	401	137	111	1		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B1	89	Total	C	N	O	S	0	1
			693	435	140	118			

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B2	51	Total	C	N	O	S	0	1
			421	263	85	72	1		

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B3	60	Total	C	N	O	S	0	1
			468	298	91	78	1		

- Molecule 32 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B4	50	Total	C	N	O	S	0	1
			242	143	50	49			

- Molecule 33 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B5	59	Total	C	N	O	S	0	0
			459	288	90	76	5		

- Molecule 34 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B6	45	Total	C	N	O	S	0	1
			381	235	78	64	4		

- Molecule 35 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B7	49	Total	C	N	O	S	0	1
			419	257	105	55	2		

- Molecule 36 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B8	64	Total	C	N	O	S	0	1
			508	326	102	78	2		

- Molecule 37 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B9	35	Total	C	N	O	S	0	0
			294	181	66	44	3		

- Molecule 38 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BA	2852	Total	C	N	O	P	0	0
			61426	27338	11485	19752	2851		

- Molecule 39 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BB	119	Total	C	N	O	P	0	0
			2551	1136	471	826	118		

- Molecule 40 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BC	191	Total	C	N	O		0	1
			1142	691	221	230			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	?	-	LEU	deletion	UNP Q5SLP7
BC	?	-	VAL	deletion	UNP Q5SLP7
BC	?	-	LYS	deletion	UNP Q5SLP7
BC	?	-	GLU	deletion	UNP Q5SLP7
BC	?	-	LEU	deletion	UNP Q5SLP7
BC	?	-	ALA	deletion	UNP Q5SLP7
BC	?	-	ASP	deletion	UNP Q5SLP7
BC	?	-	ALA	deletion	UNP Q5SLP7
BC	?	-	VAL	deletion	UNP Q5SLP7
BC	?	-	VAL	deletion	UNP Q5SLP7
BC	?	-	ALA	deletion	UNP Q5SLP7
BC	?	-	THR	deletion	UNP Q5SLP7
BC	?	-	PRO	deletion	UNP Q5SLP7
BC	?	-	ASP	deletion	UNP Q5SLP7
BC	?	-	LEU	deletion	UNP Q5SLP7
BC	?	-	PRO	deletion	UNP Q5SLP7

- Molecule 41 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BD	272	Total	C	N	O	S	0	1
			2105	1329	417	356	3		

- Molecule 42 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BE	205	Total	C	N	O	S	0	1
			1564	988	300	270	6		

- Molecule 43 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BF	208	Total	C	N	O	S	0	1
			1624	1035	304	282	3		

- Molecule 44 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BG	181	Total	C	N	O	S	0	0
			1474	942	268	260	4		

- Molecule 45 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BH	160	Total	C	N	O	S	0	1
			1223	773	229	220	1		

- Molecule 46 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BI	146	Total	C	N	O	S	0	1
			1132	723	201	207	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	146	VAL	ALA	conflict	UNP Q5SLQ1

- Molecule 47 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BL	138	Total	C	N	O	S	0	0
			1025	654	181	185	5		

- Molecule 48 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	139	Total	C	N	O	S	0	1
			1105	712	207	182	4		

- Molecule 49 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BO	122	Total	C	N	O	S	0	0
			933	588	171	170	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BP	146	Total	C	N	O	S	0	0
			1114	692	227	193	2		

- Molecule 51 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	136	Total	C	N	O	S	0	0
			1080	688	204	183	5		

- Molecule 52 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BR	117	Total	C	N	O		0	0
			960	599	202	159			

- Molecule 53 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	99	Total	C	N	O		0	1
			771	486	155	130			

- Molecule 54 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BT	138	Total	C	N	O	S	0	1
			1142	710	235	196	1		

- Molecule 55 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BU	117	Total	C	N	O	S	0	0
			958	604	202	151	1		

- Molecule 56 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 57 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BW	113	Total	C	N	O	S	0	0
			896	563	176	155	2		

- Molecule 58 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	BX	93	Total	C	N	O	0	1
			726	471	132	123		

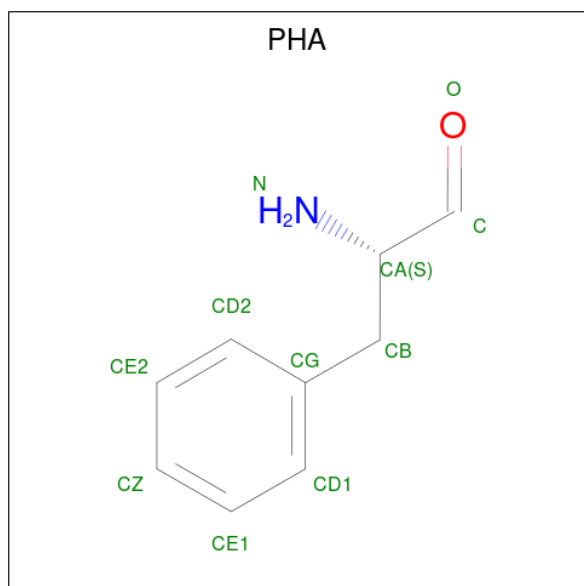
- Molecule 59 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	BY	101	Total	C	N	O	S	0
			776	500	149	123	4	1

- Molecule 60 is a protein called 50S ribosomal protein L25.

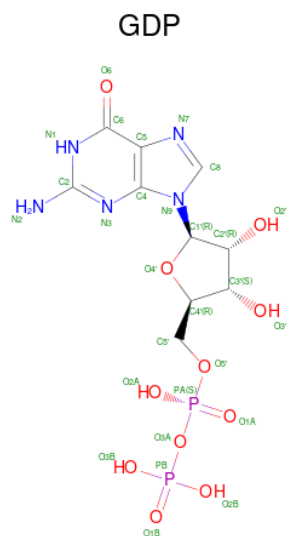
Mol	Chain	Residues	Atoms				AltConf	Trace
60	BZ	177	Total	C	N	O	S	0
			1404	897	253	252	2	1

- Molecule 61 is PHENYLALANINAL (three-letter code: PHA) (formula: $C_9H_{11}NO$).



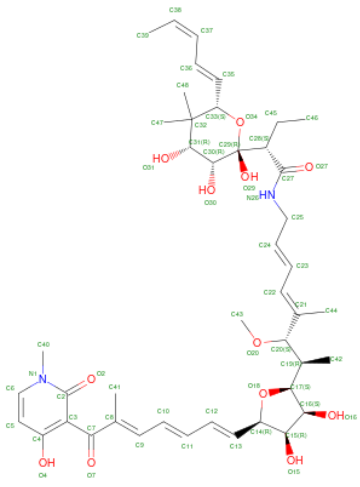
Mol	Chain	Residues	Atoms				AltConf
61	AY	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



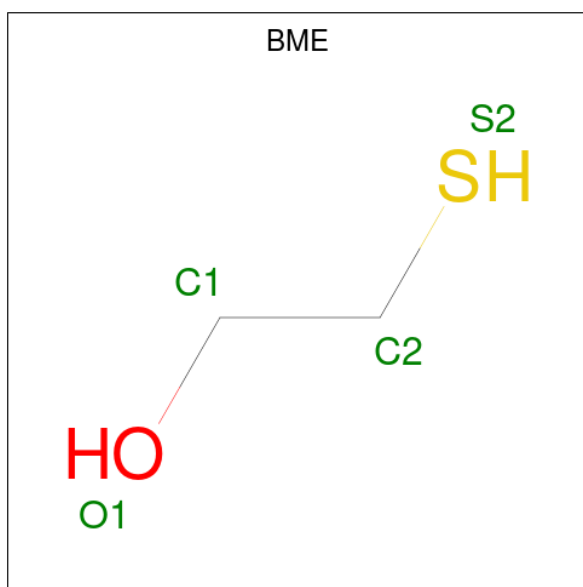
Mol	Chain	Residues	Atoms					AltConf
62	AZ	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 63 is N-METHYL KIRROMYCIN (three-letter code: MAU) (formula: $C_{44}H_{62}N_2O_{12}$).



Mol	Chain	Residues	Atoms				AltConf
63	AZ	1	Total	C	N	O	0
			58	44	2	12	

- Molecule 64 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).

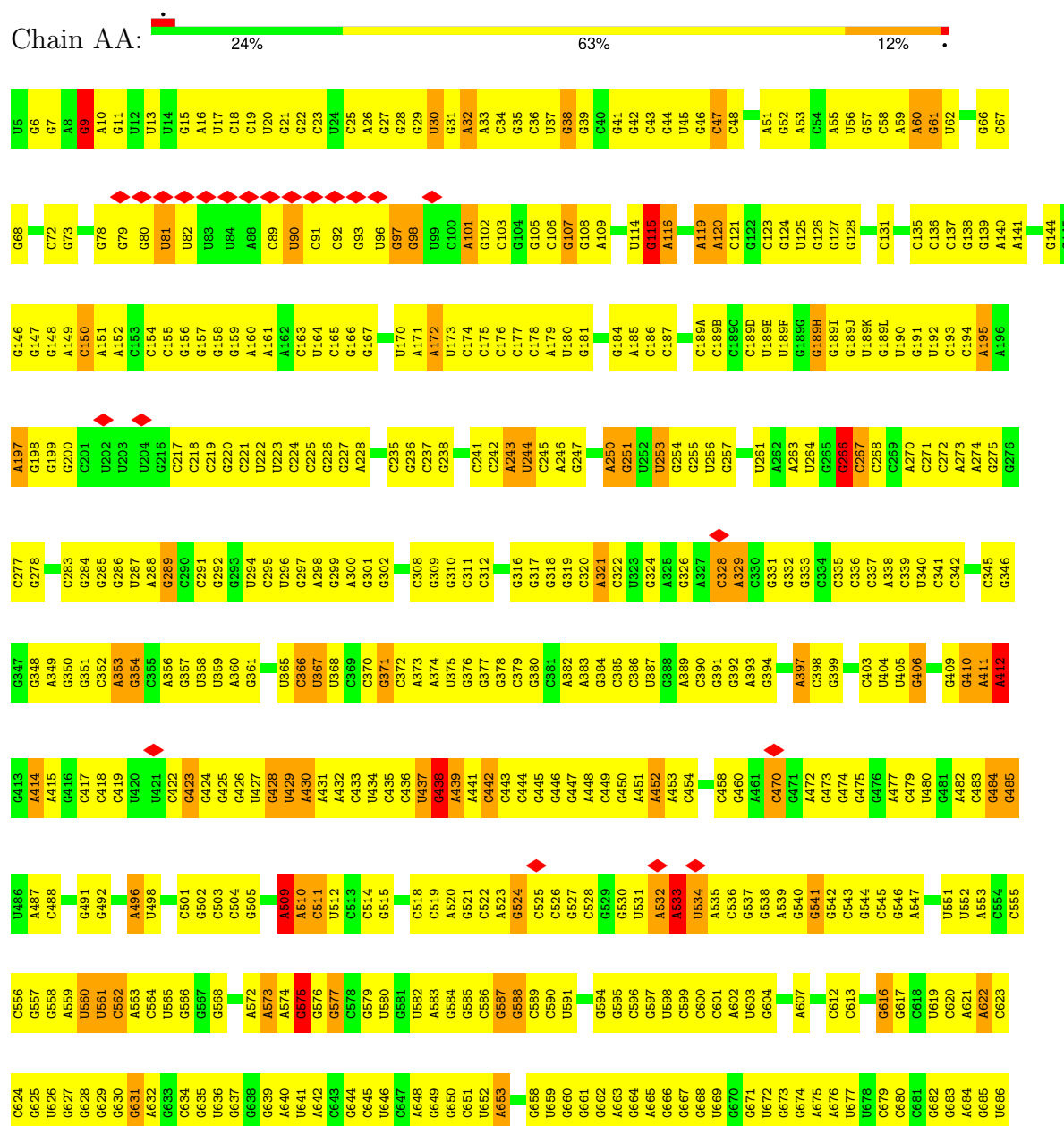


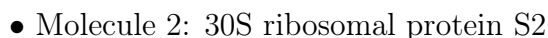
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
64	AZ	1	4	2	1	1	0

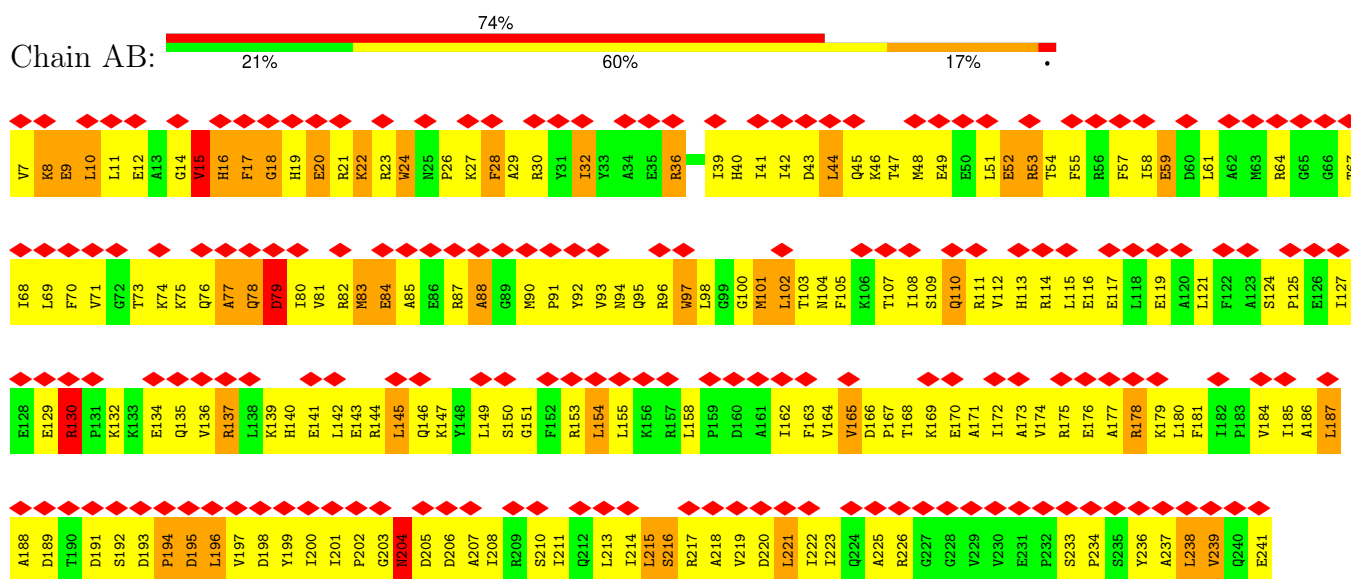
3 Residue-property plots

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.

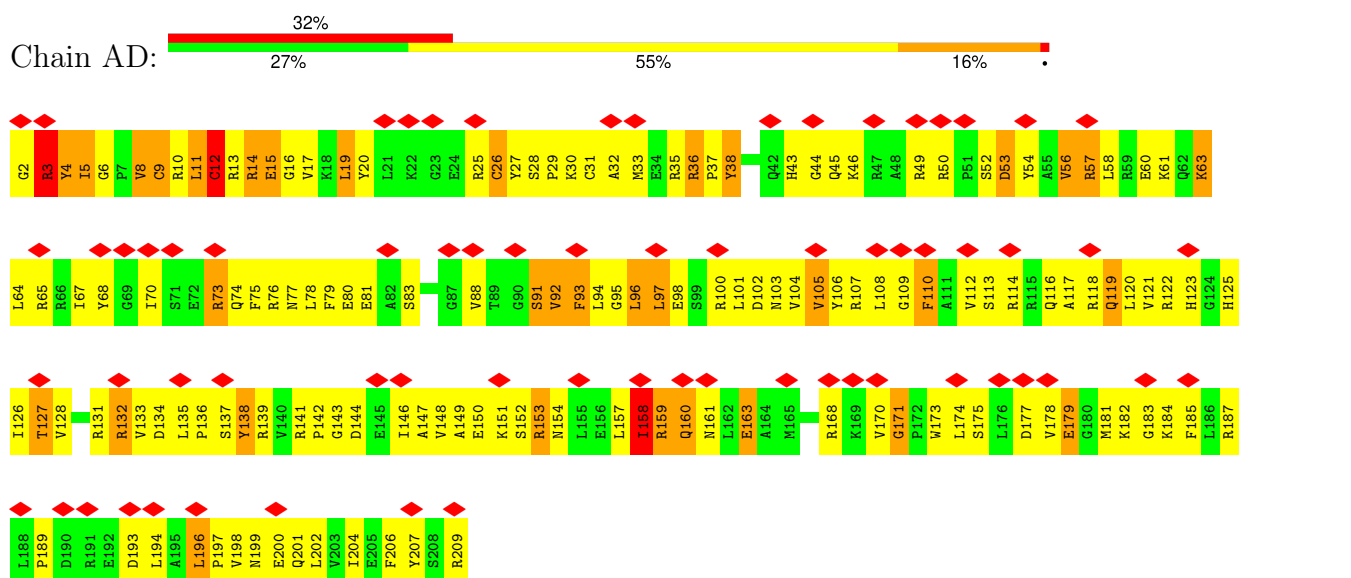
• Molecule 1: 16S rRNA





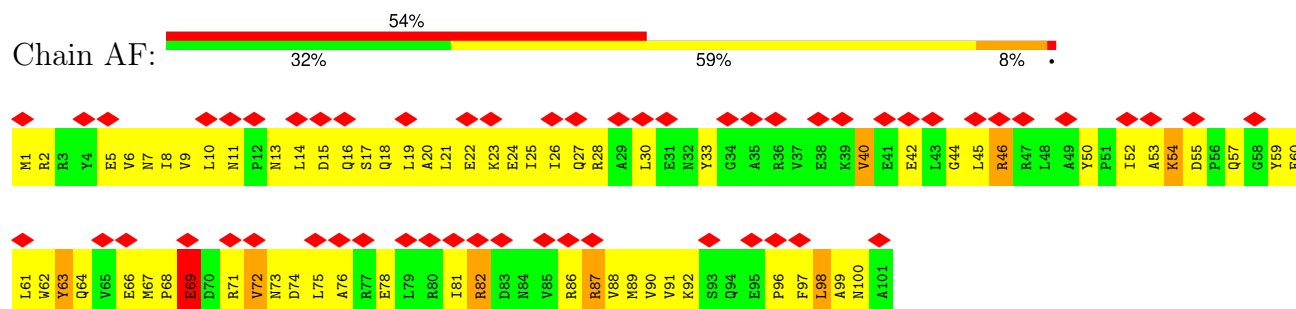


• Molecule 3: 30S ribosomal protein S4



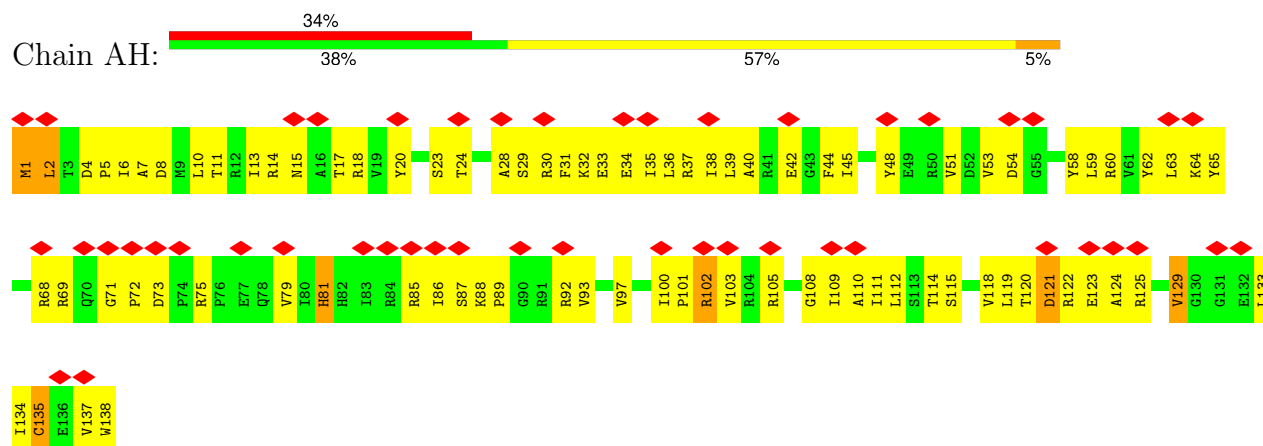
- Molecule 5: 30S ribosomal protein S6

Chain AF:



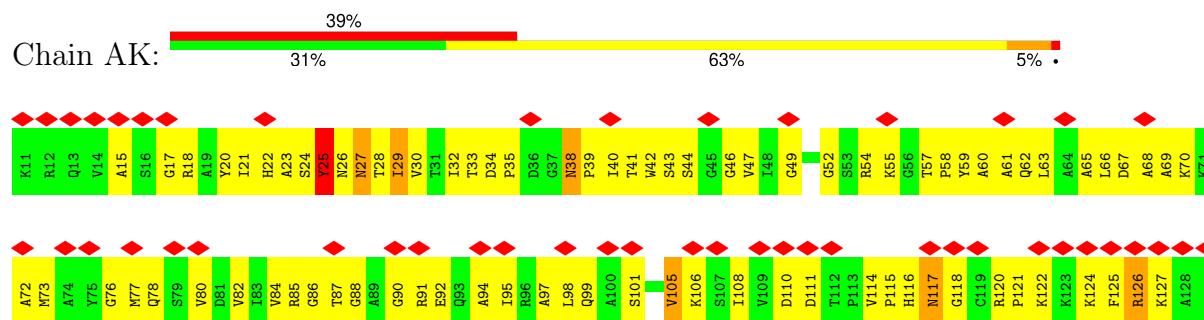
- Molecule 6: 30S ribosomal protein S8

Chain AH:



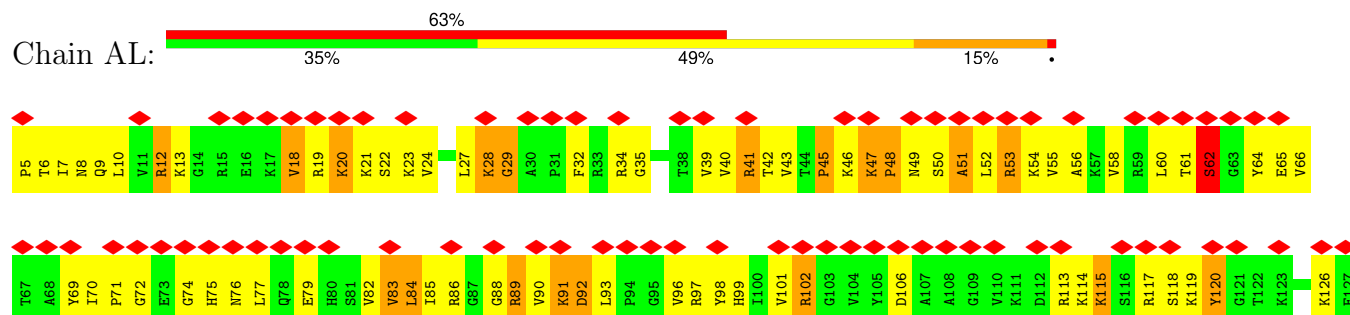
- Molecule 7: 30S ribosomal protein S11

Chain AK:



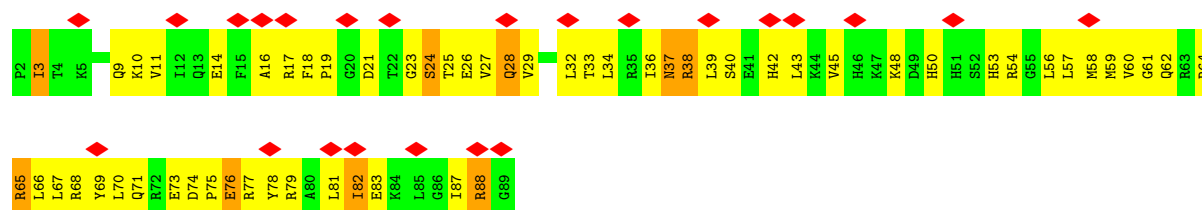
- Molecule 8: 30S ribosomal protein S12

Chain AL:

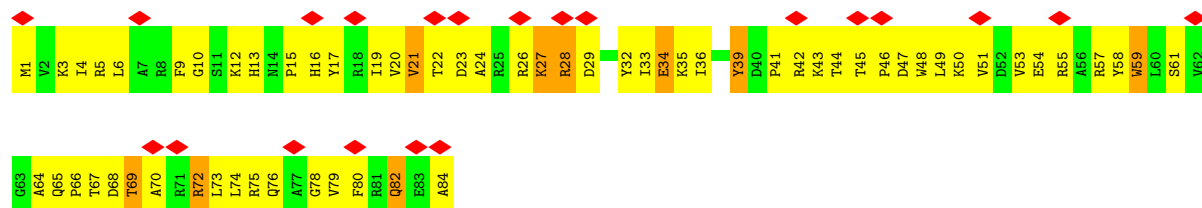




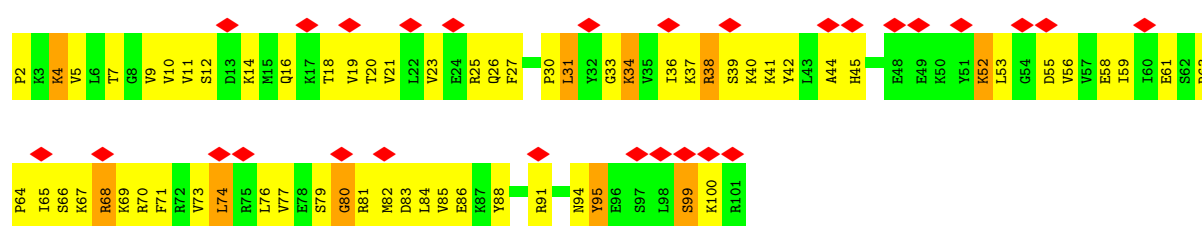
- Molecule 9: 30S ribosomal protein S15



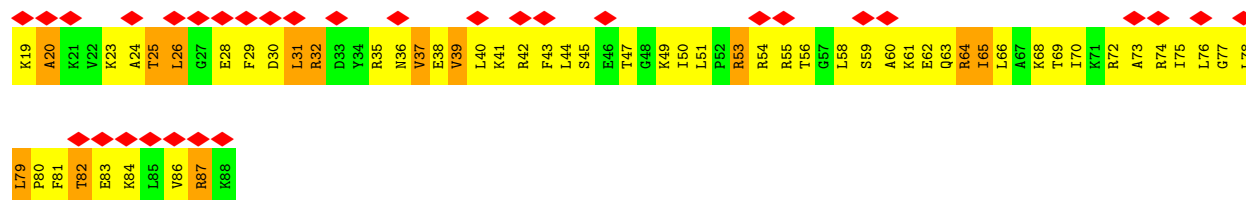
- Molecule 10: 30S ribosomal protein S16



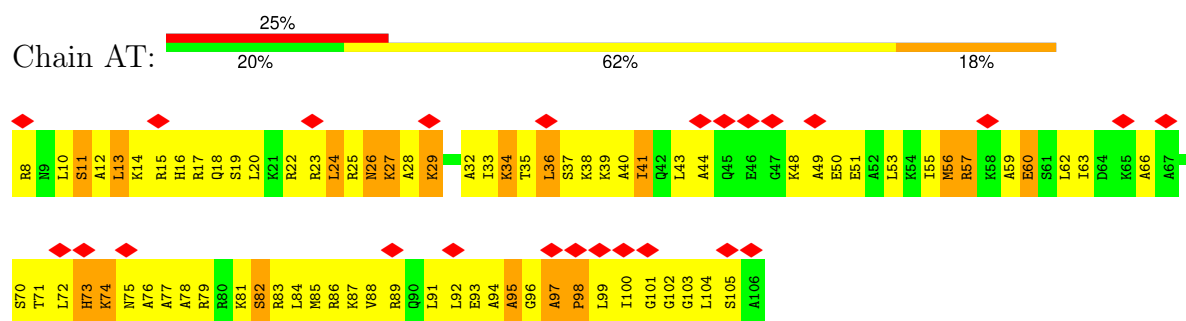
- Molecule 11: 30S ribosomal protein S17



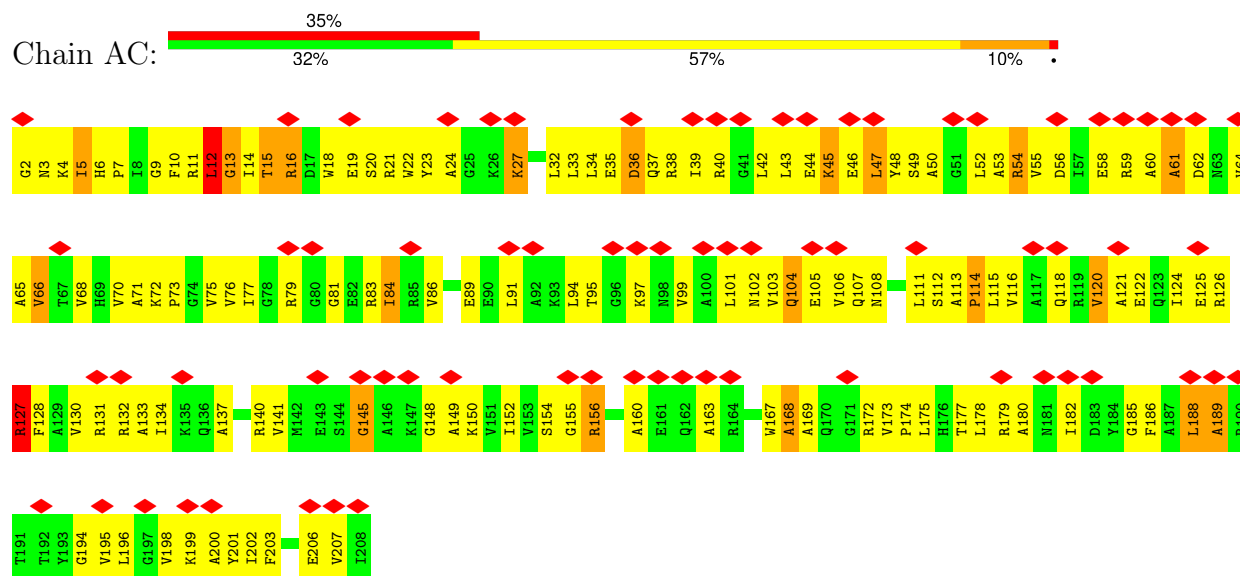
- Molecule 12: 30S ribosomal protein S18



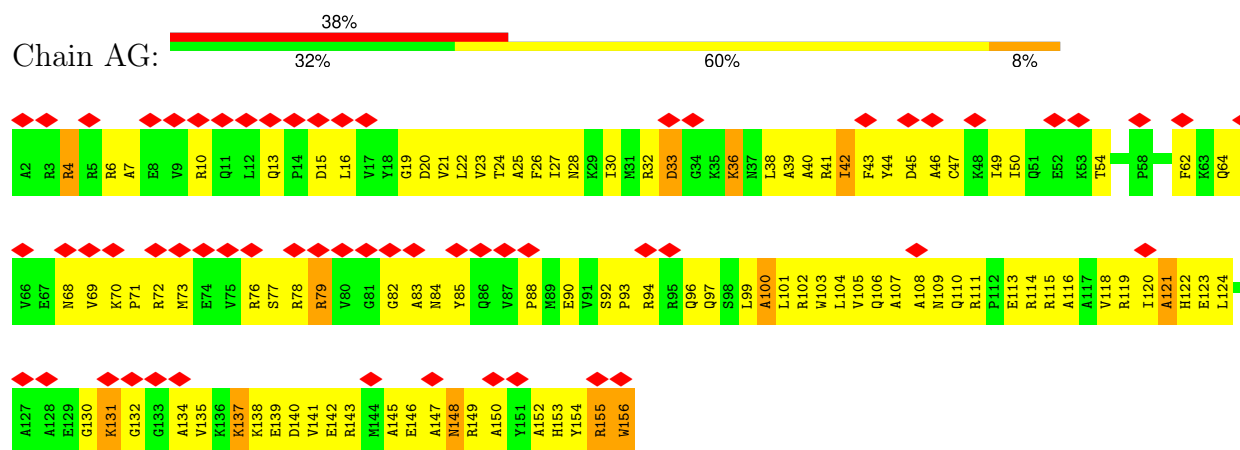
- Molecule 13: 30S ribosomal protein S20



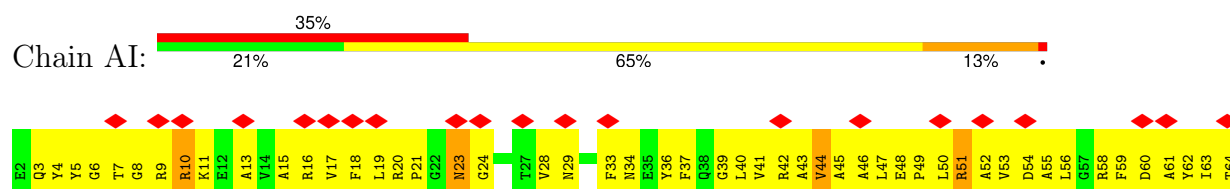
• Molecule 14: 30S ribosomal protein S3

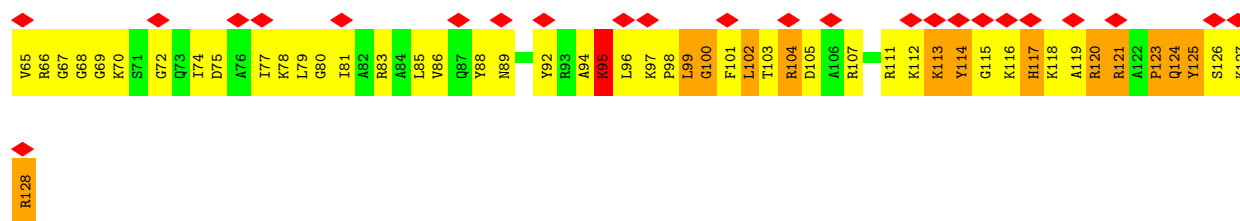


• Molecule 15: 30S ribosomal protein S7

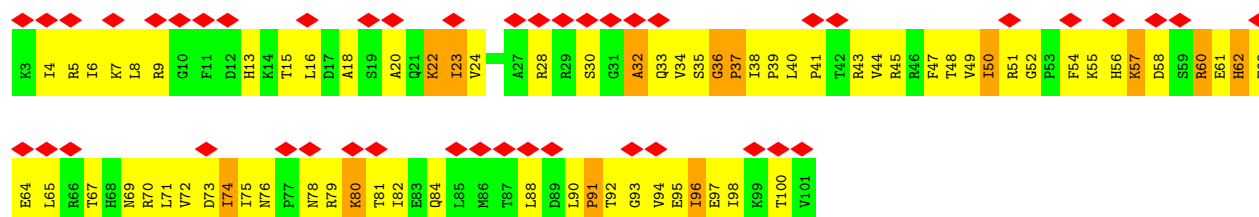


• Molecule 16: 30S ribosomal protein S9

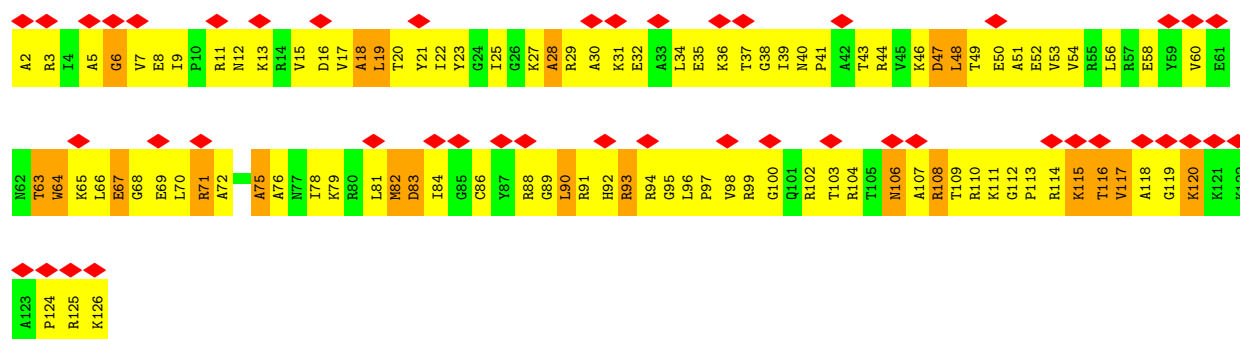




• Molecule 17: 30S ribosomal protein S10



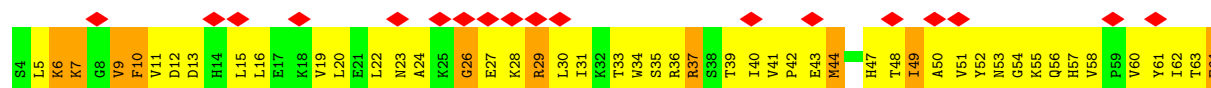
• Molecule 18: 30S ribosomal protein S13

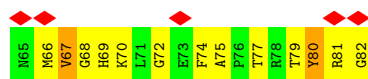


• Molecule 19: 30S ribosomal protein S14



• Molecule 20: 30S ribosomal protein S19

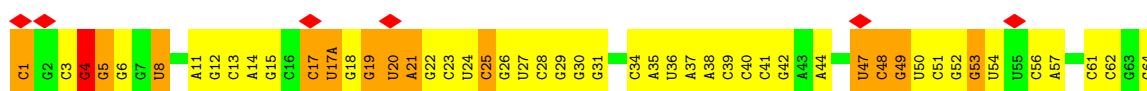




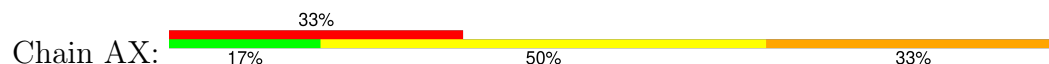
- Molecule 21: 30S ribosomal protein Thx



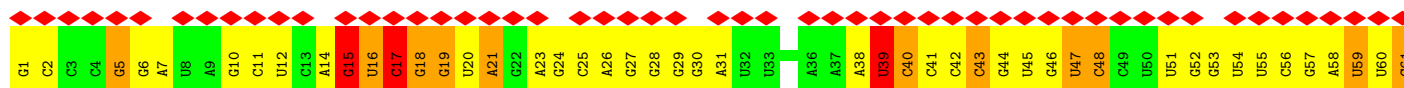
- Molecule 22: P-SITE TRNA



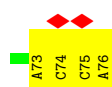
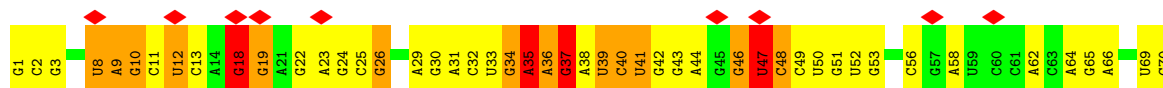
- Molecule 23: SYNTHETIC MRNA



- Molecule 24: E-SITE TRNA



- Molecule 25: AT-SITE TRNA




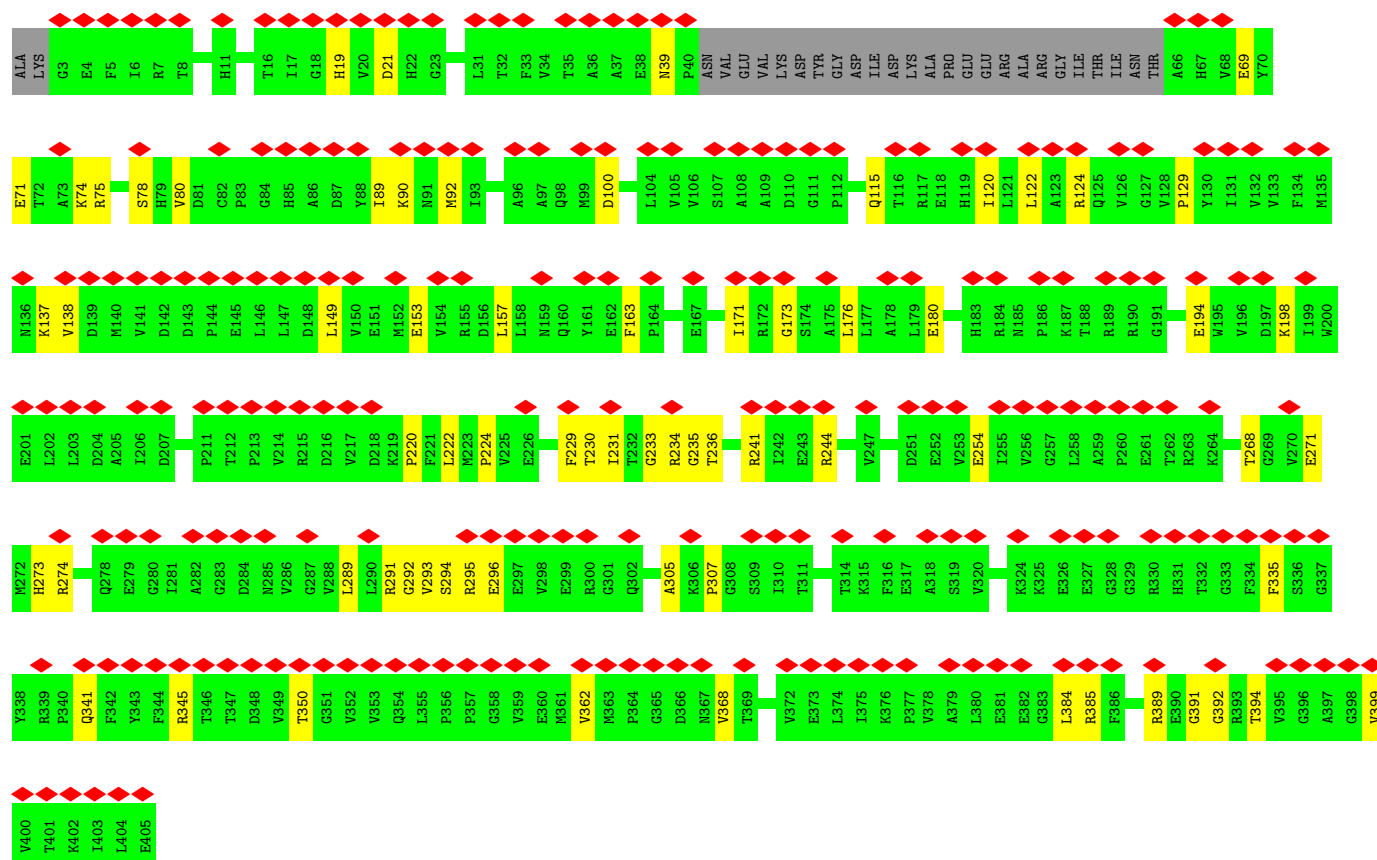
- Molecule 26: MRNA CODON

Chain A0: 

U100
U101
U102

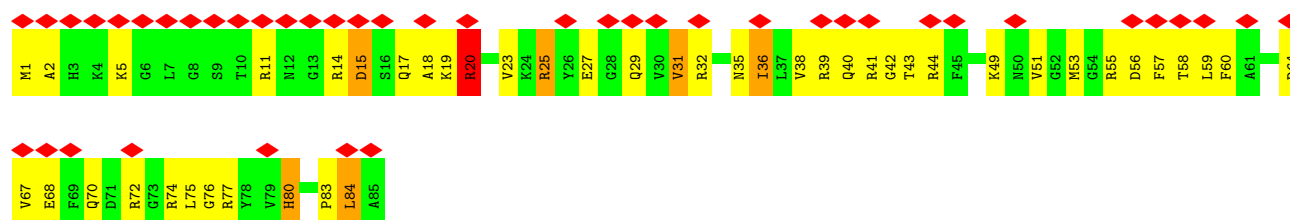
- Molecule 27: Elongation factor Tu-A

Chain AZ: 



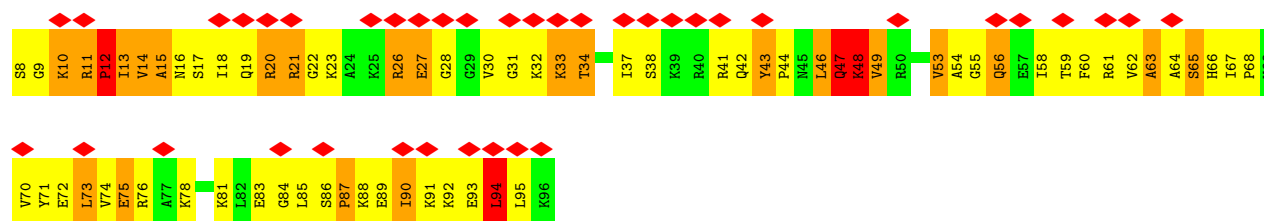
- Molecule 28: 50S ribosomal protein L27

Chain B0: 



- Molecule 29: 50S ribosomal protein L28

Chain B1: 



- Molecule 30: 50S ribosomal protein L29



- Molecule 31: 50S ribosomal protein L30



- Molecule 32: 50S ribosomal protein L31



- Molecule 33: 50S ribosomal protein L32

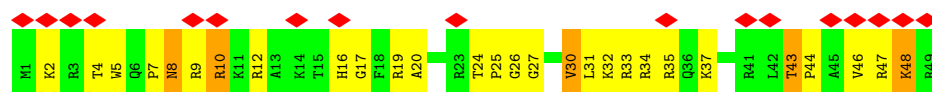


- Molecule 34: 50S ribosomal protein L33

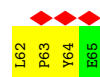


- Molecule 35: 50S ribosomal protein L34

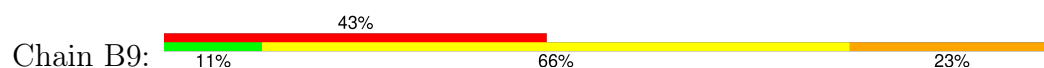




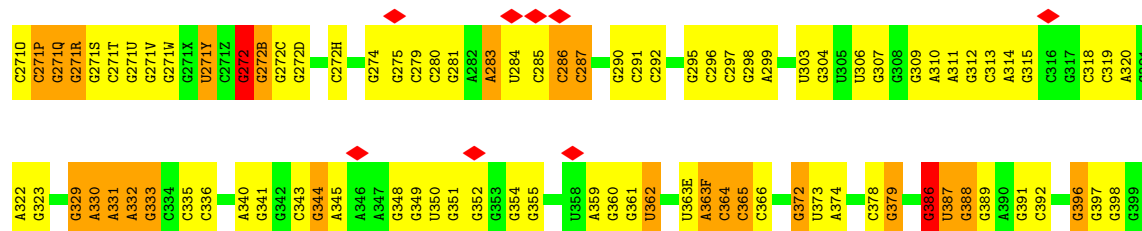
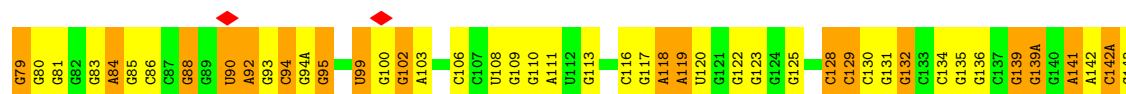
• Molecule 36: 50S ribosomal protein L35

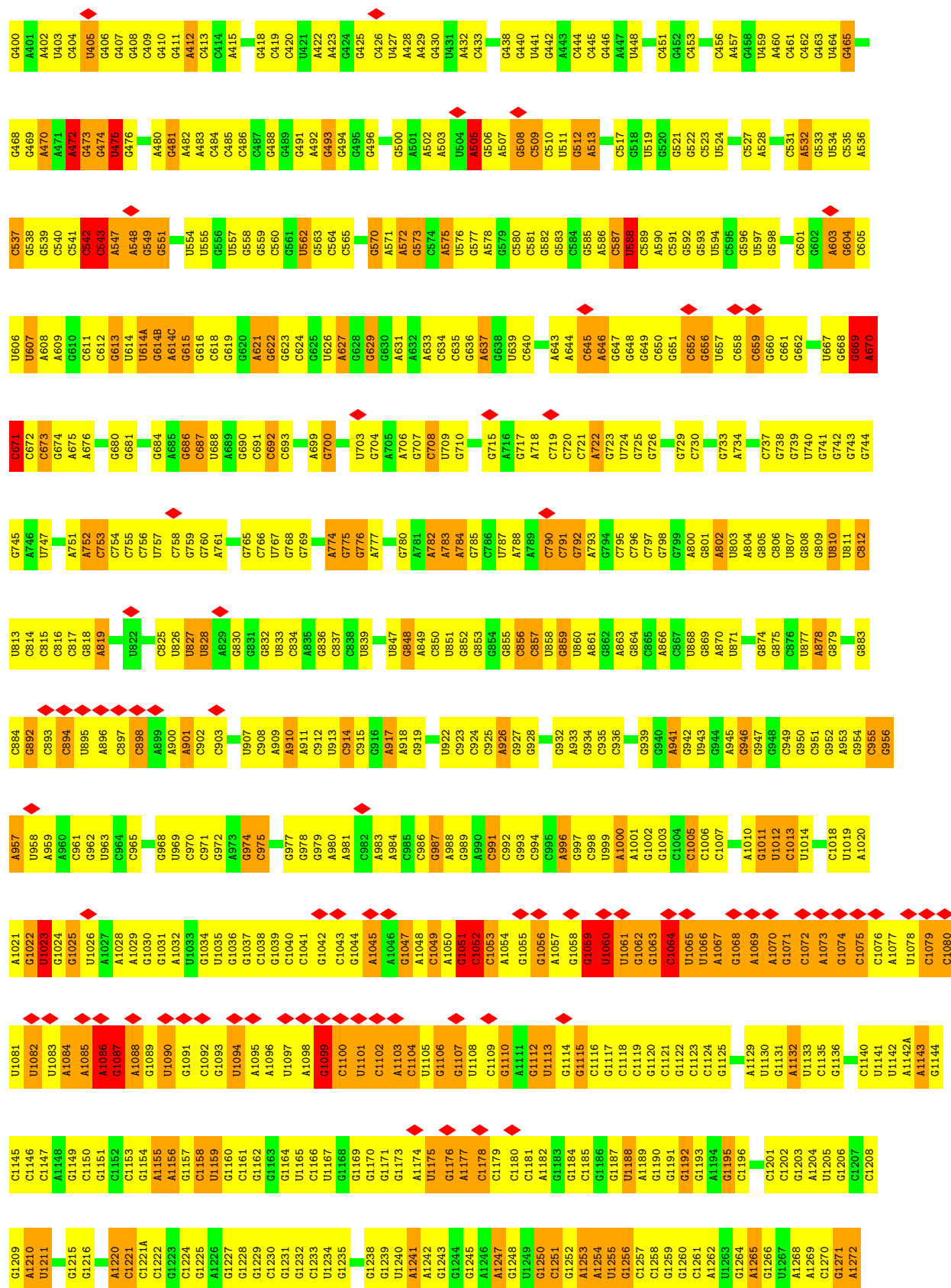


• Molecule 37: 50S ribosomal protein L36

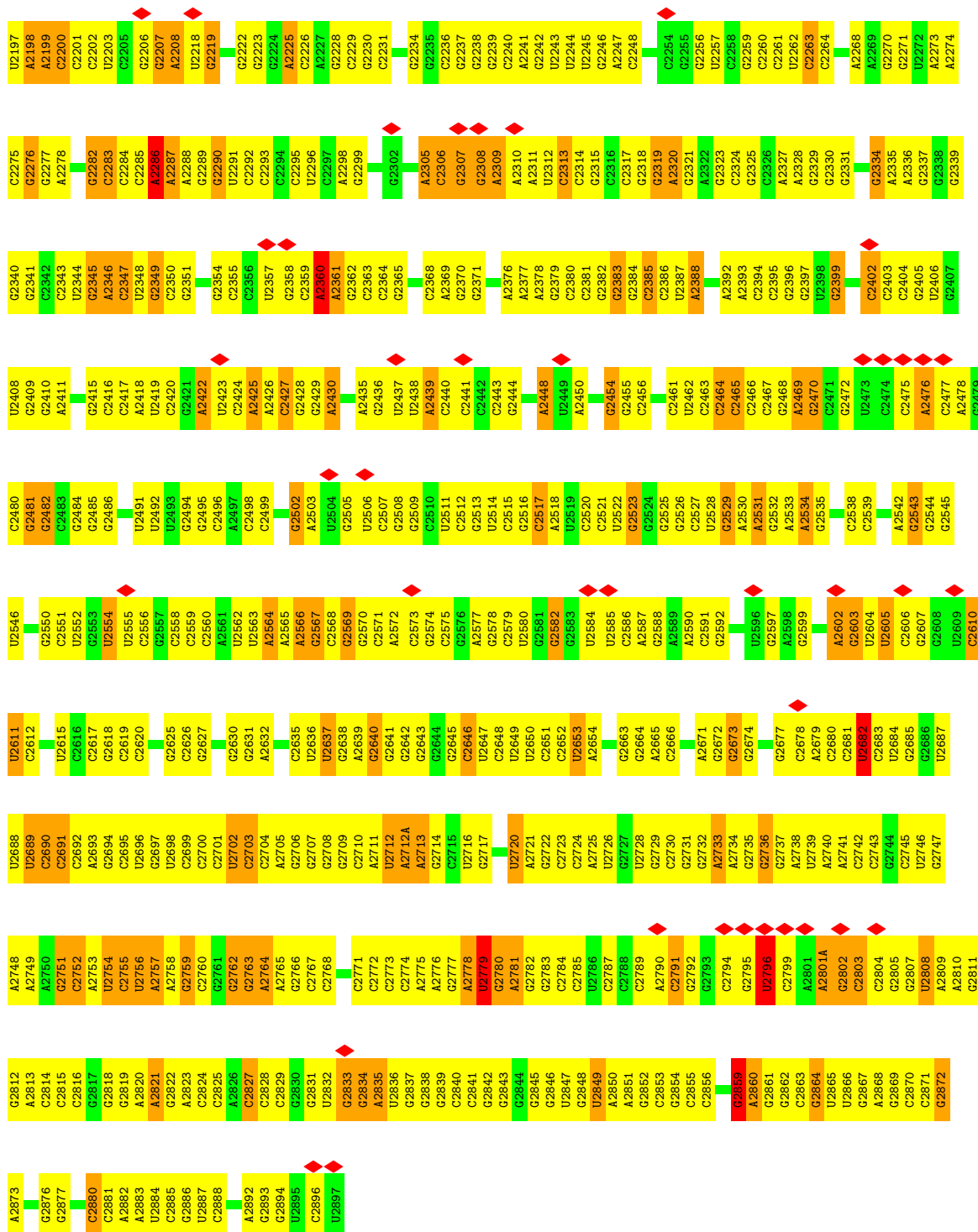


• Molecule 38: 23S rRNA



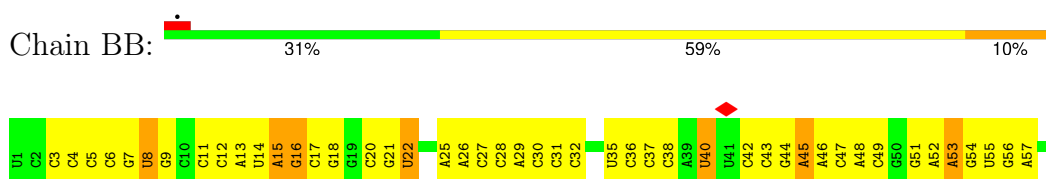


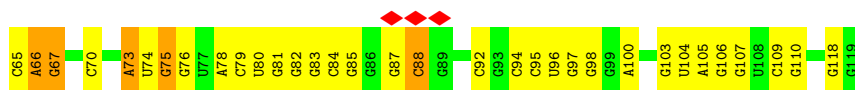




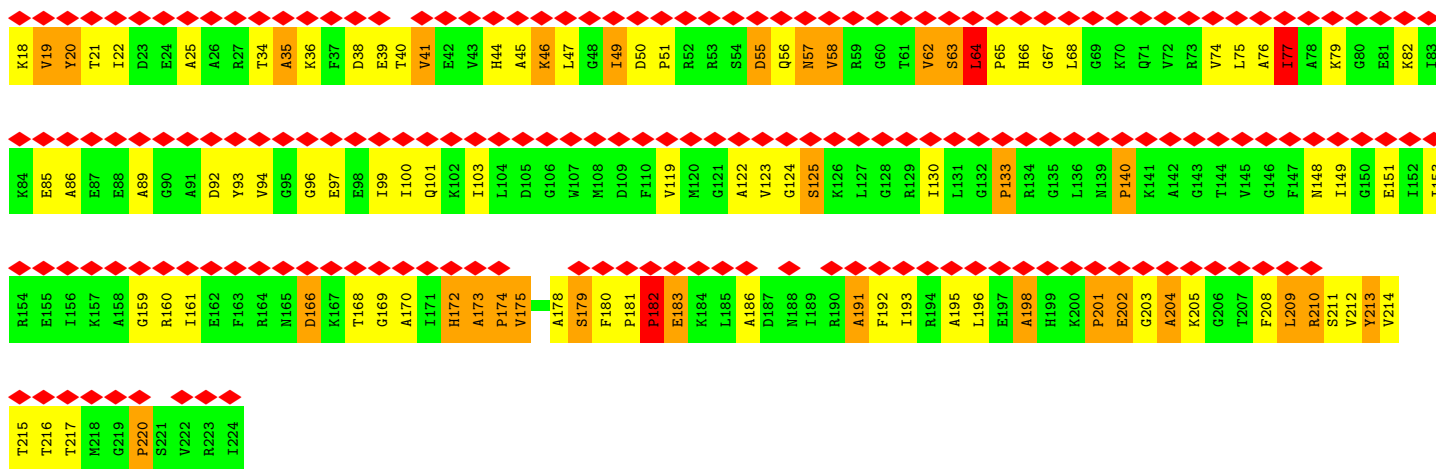
• Molecule 39: 5S rRNA

Chain BB:

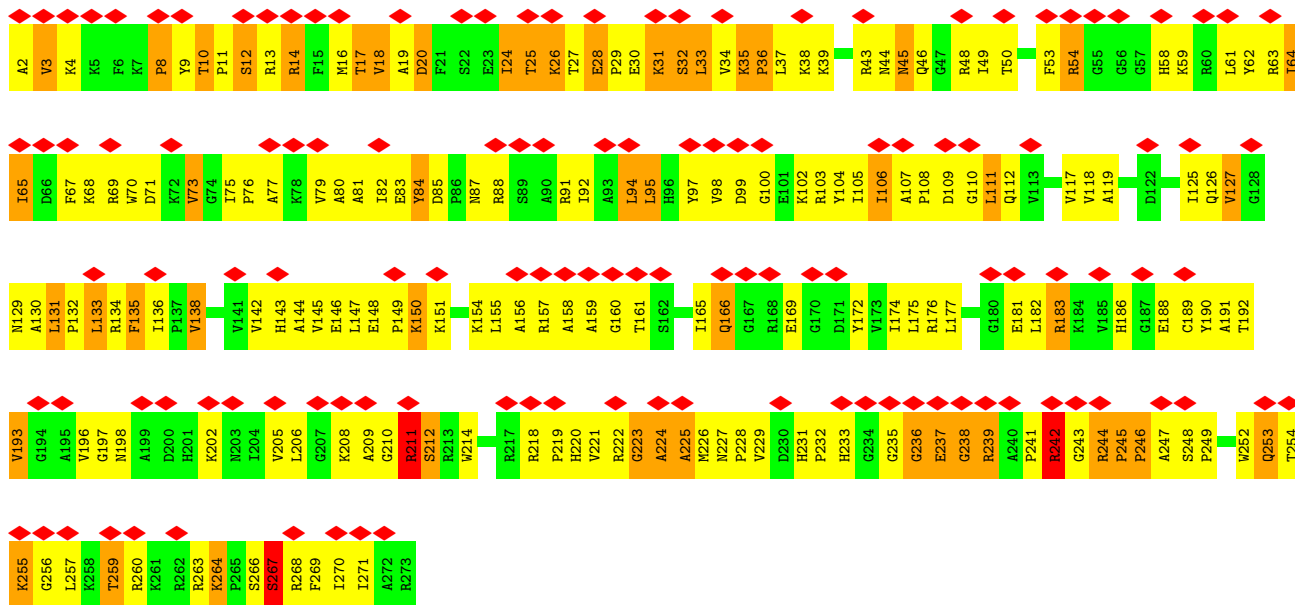




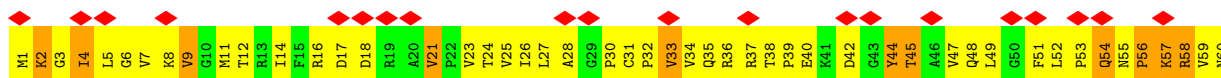
• Molecule 40: 50S ribosomal protein L1

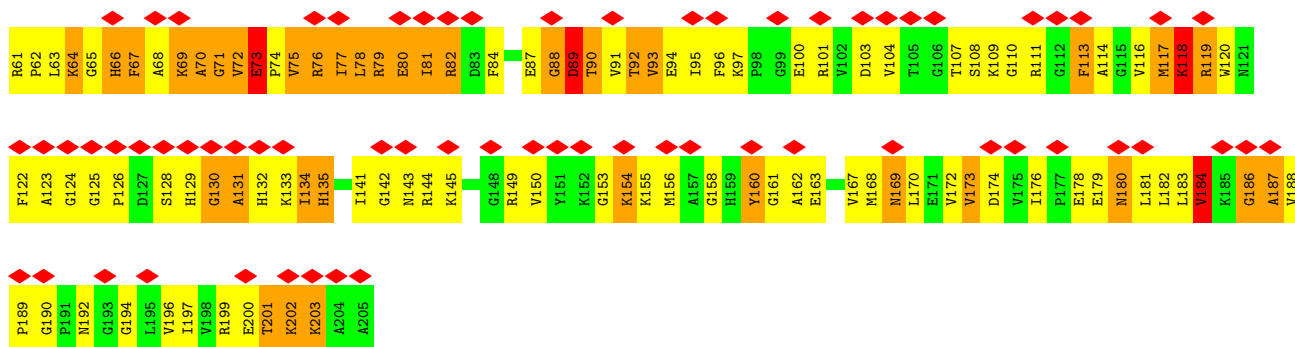


• Molecule 41: 50S ribosomal protein L2

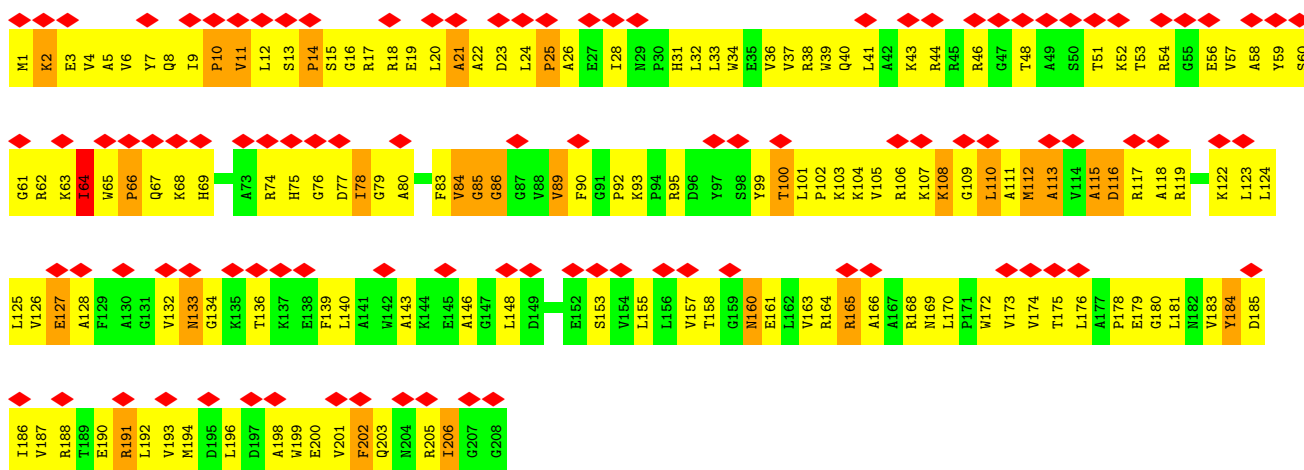


• Molecule 42: 50S ribosomal protein L3

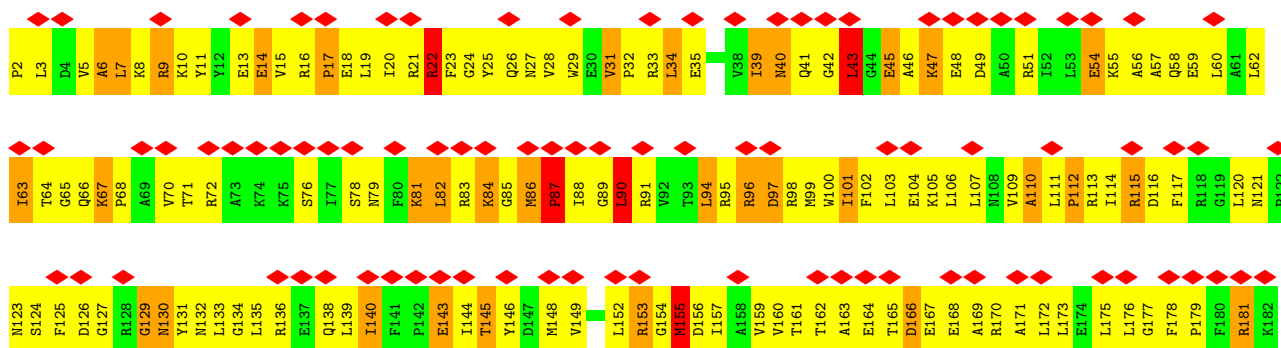




• Molecule 43: 50S ribosomal protein L4

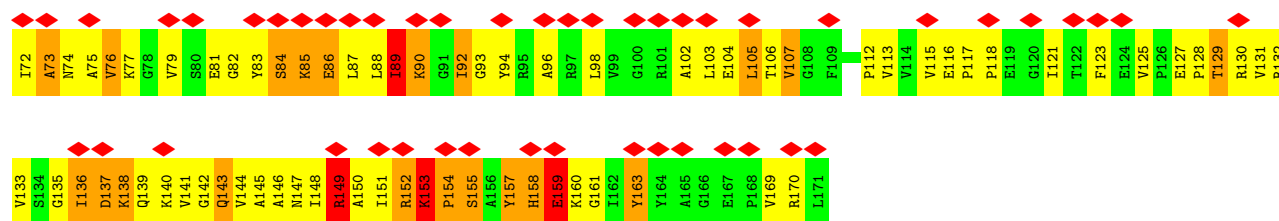


• Molecule 44: 50S ribosomal protein L5

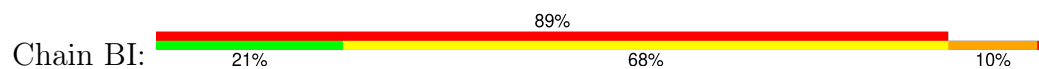


• Molecule 45: 50S ribosomal protein L6

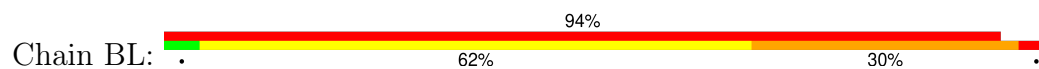




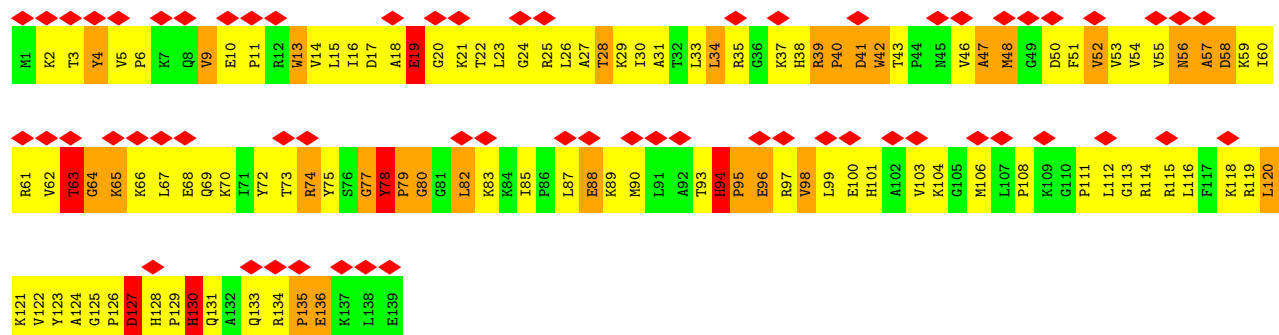
• Molecule 46: 50S ribosomal protein L9



• Molecule 47: 50S ribosomal protein L11

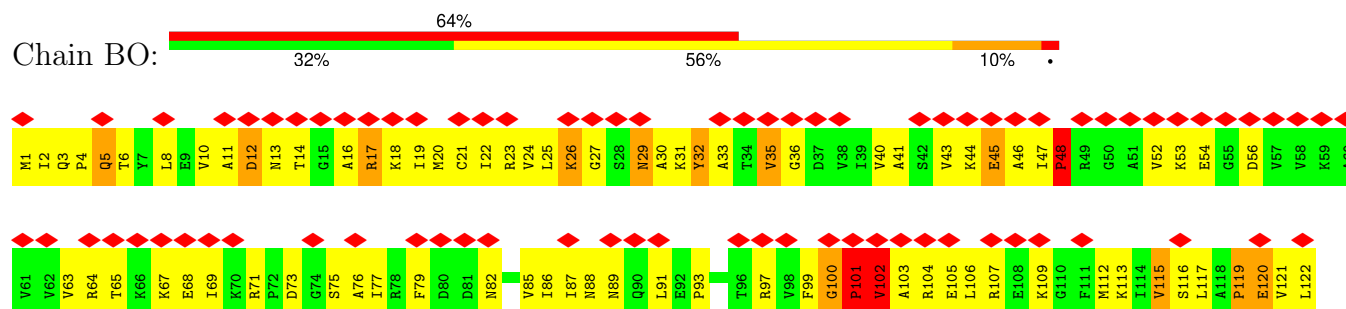


• Molecule 48: 50S ribosomal protein L13



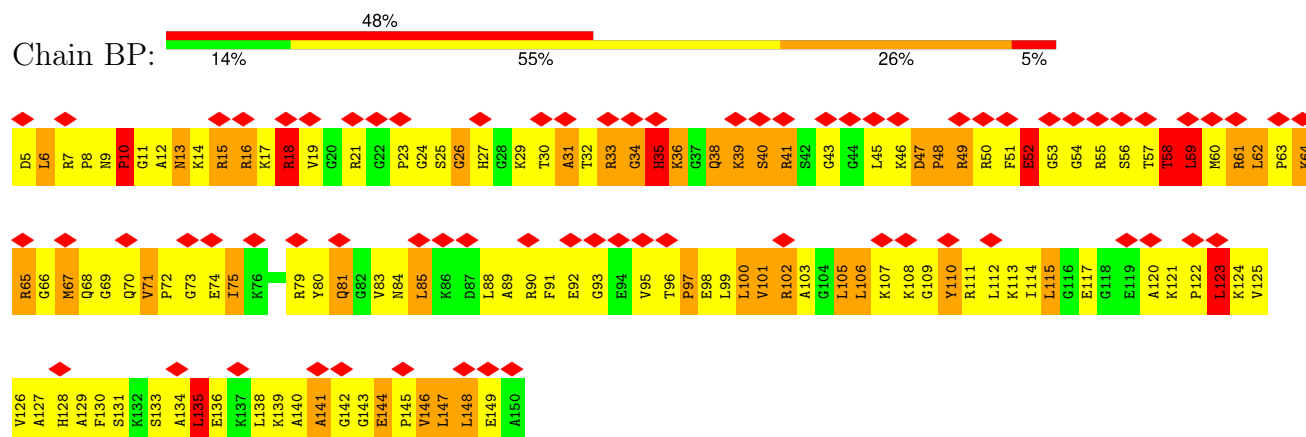
- Molecule 49: 50S ribosomal protein L14

Chain BO:



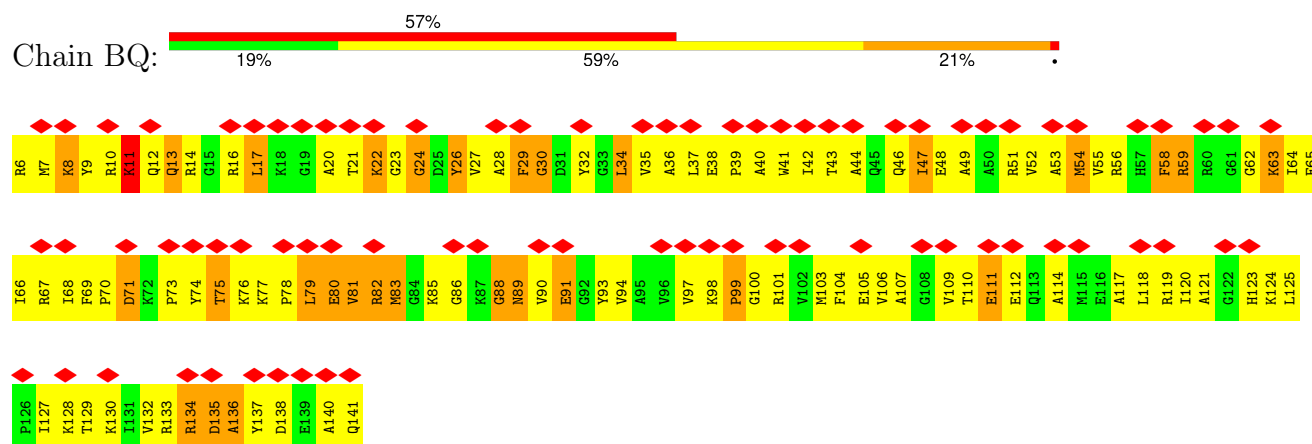
- Molecule 50: 50S ribosomal protein L15

Chain BP:



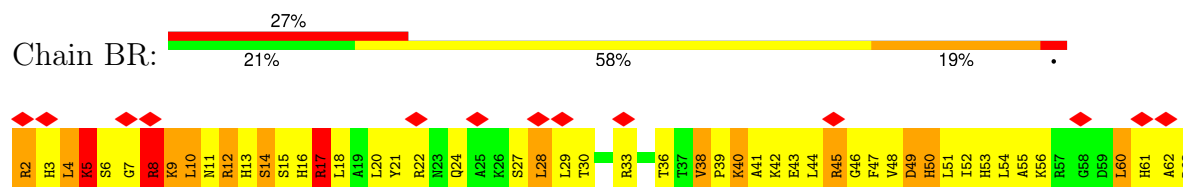
- Molecule 51: 50S ribosomal protein L16

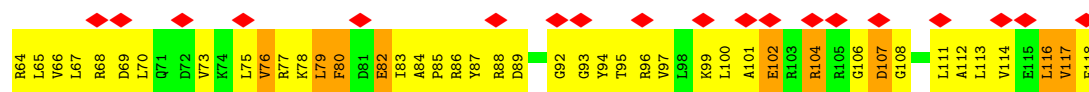
Chain BQ:



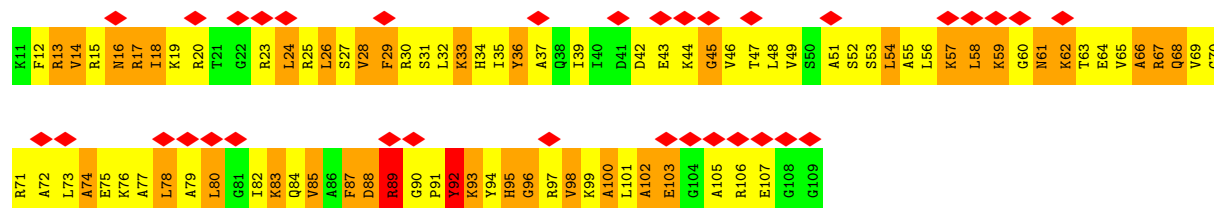
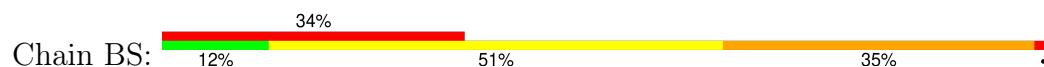
- Molecule 52: 50S ribosomal protein L17

Chain BR:

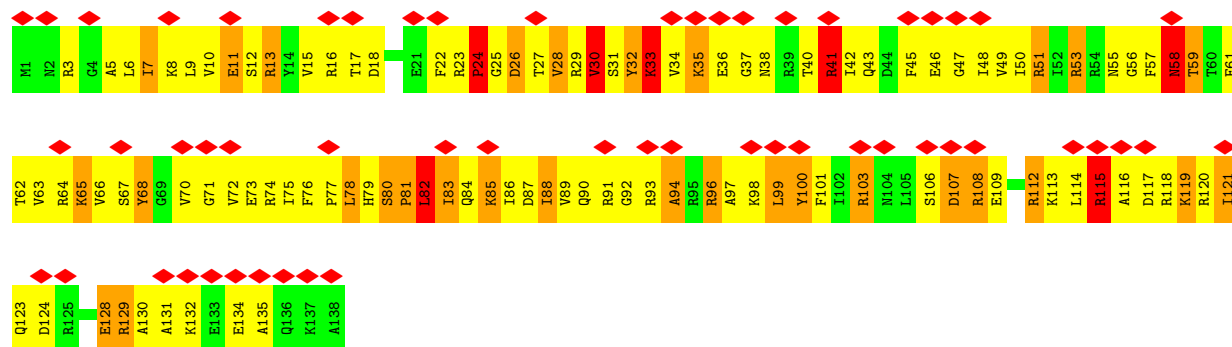




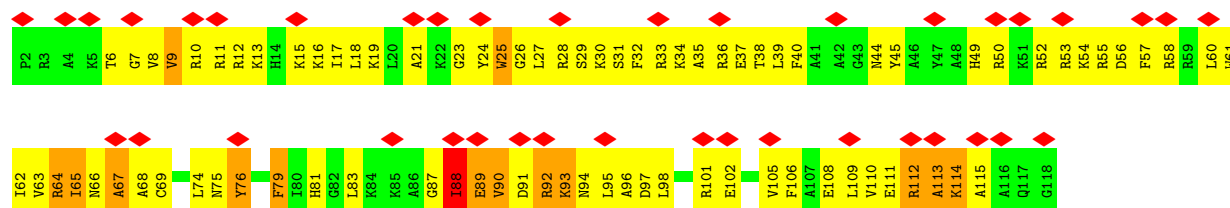
• Molecule 53: 50S ribosomal protein L18



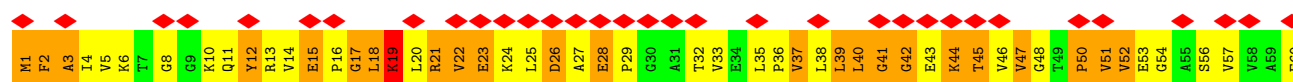
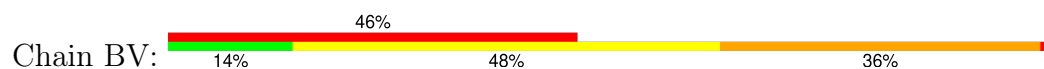
• Molecule 54: 50S ribosomal protein L19

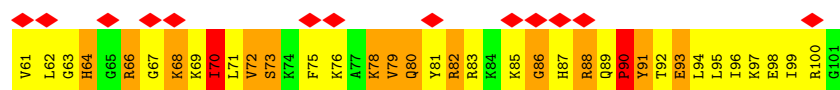


• Molecule 55: 50S ribosomal protein L20

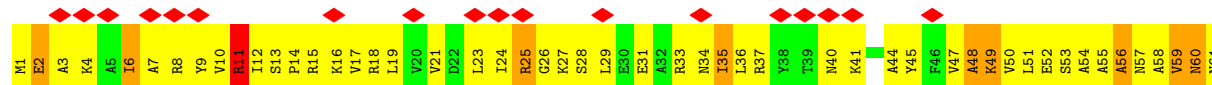


• Molecule 56: 50S ribosomal protein L21

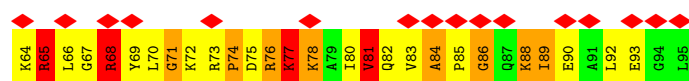
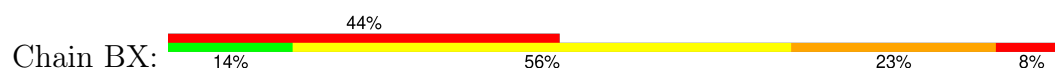




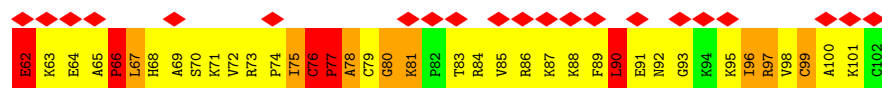
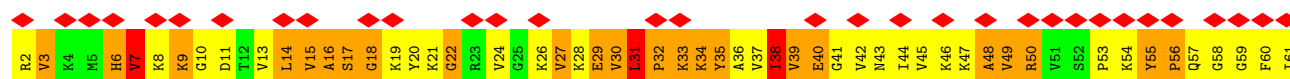
• Molecule 57: 50S ribosomal protein L22



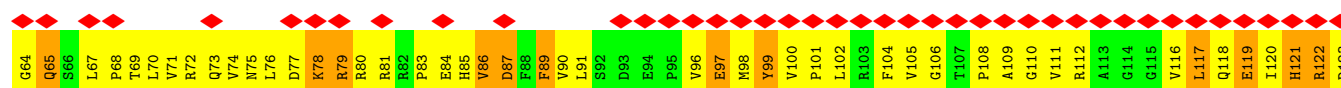
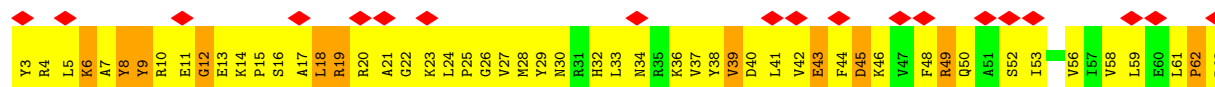
• Molecule 58: 50S ribosomal protein L23



• Molecule 59: 50S ribosomal protein L24



• Molecule 60: 50S ribosomal protein L25



I124	L125	V126	K127	V128	S129	P130	R131	N132	I133	P134	E135	F136	I137	E138	V139	D140	V141	S142	G143	L144	E145	I146	G147	D148	S149	L150	H151	A152	S153	D154	L155	K156	L157	P158	P159	G160	V161	E162	L163	A164	V165	S166	P167	E168	E169	T170	I171	A172	A173	V174	V175	P176	P177	E178	D179
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	323688	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF correction of each defocus group volume prior to back projection.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	23	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	17.496	Depositor
Minimum map value	-4.419	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.958	Depositor
Recommended contour level	3.5	Depositor
Map size (\AA)	378.0, 378.0, 378.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.26, 1.26, 1.26	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 2MG, YG, 5MU, OMG, 5MC, PHA, OMC, GDP, 7MG, 1MA, BME, MAU, M2G

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	0.51	0/36190	0.73	27/56486 (0.0%)
2	AB	0.33	0/1936	0.59	0/2611
3	AD	0.42	0/1733	0.67	0/2318
4	AE	0.42	0/1163	0.66	0/1566
5	AF	0.37	0/856	0.64	0/1154
6	AH	0.36	0/1136	0.62	0/1527
7	AK	0.38	0/900	0.64	0/1213
8	AL	0.42	0/987	0.72	0/1322
9	AO	0.38	0/745	0.63	0/992
10	AP	0.43	0/717	0.70	0/965
11	AQ	0.42	0/837	0.67	0/1119
12	AR	0.40	0/579	0.71	0/768
13	AT	0.34	0/765	0.59	0/1007
14	AC	0.35	0/1637	0.58	0/2207
15	AG	0.34	0/1276	0.55	0/1709
16	AI	0.32	0/1027	0.56	0/1372
17	AJ	0.36	0/808	0.62	0/1087
18	AM	0.35	0/994	0.63	0/1322
19	AN	0.39	0/501	0.66	0/664
20	AS	0.37	0/643	0.61	0/867
21	AU	0.46	0/213	0.56	0/279
22	AV	0.52	1/1814 (0.1%)	0.72	0/2825
23	AX	0.85	1/147 (0.7%)	0.83	0/223
24	AW	0.45	1/1813 (0.1%)	0.78	6/2823 (0.2%)
25	AY	1.12	4/1407 (0.3%)	2.35	13/2177 (0.6%)
26	A0	2.23	2/65 (3.1%)	1.08	0/98
27	AZ	0.30	0/3052	0.65	1/4141 (0.0%)
28	B0	0.39	0/658	0.65	0/878
29	B1	0.61	0/700	1.04	1/931 (0.1%)
30	B2	0.45	0/423	0.99	3/560 (0.5%)
31	B3	0.37	0/473	0.61	0/636
32	B4	0.47	0/241	0.88	4/334 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B5	0.43	0/473	0.74	0/639
34	B6	0.39	0/387	0.62	0/517
35	B7	0.51	0/427	0.73	0/563
36	B8	0.50	0/516	0.81	0/681
37	B9	0.55	0/297	0.61	0/392
38	BA	0.66	8/68796 (0.0%)	0.80	76/107396 (0.1%)
39	BB	0.39	0/2853	0.70	0/4451
40	BC	0.38	0/1145	0.68	7/1556 (0.4%)
41	BD	0.52	0/2155	0.87	3/2907 (0.1%)
42	BE	0.43	0/1597	0.76	0/2155
43	BF	0.44	0/1659	0.70	0/2246
44	BG	0.39	0/1498	0.72	1/2013 (0.0%)
45	BH	0.33	0/1246	0.69	0/1684
46	BI	0.35	0/1147	0.66	0/1553
47	BL	0.50	0/1044	0.92	1/1415 (0.1%)
48	BN	0.41	0/1132	0.78	0/1527
49	BO	0.48	0/943	0.74	0/1269
50	BP	0.42	0/1131	1.00	6/1504 (0.4%)
51	BQ	0.37	0/1100	0.72	1/1470 (0.1%)
52	BR	0.40	0/974	0.74	1/1302 (0.1%)
53	BS	0.40	0/779	0.73	0/1038
54	BT	0.43	0/1156	0.77	2/1544 (0.1%)
55	BU	0.38	0/975	0.68	0/1297
56	BV	0.38	0/789	0.73	0/1054
57	BW	0.43	0/907	0.72	0/1216
58	BX	0.53	0/740	0.89	3/995 (0.3%)
59	BY	0.41	0/789	0.78	0/1053
60	BZ	0.35	0/1436	0.64	0/1951
All	All	0.56	17/164527 (0.0%)	0.79	156/245569 (0.1%)

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	2	37
22	AV	0	2
24	AW	3	1
25	AY	0	5
29	B1	0	1
38	BA	29	93
All	All	34	139

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	BA	1051	G	O3'-P	37.08	2.05	1.61
38	BA	2190	G	O3'-P	-29.41	1.25	1.61
38	BA	2653	U	O3'-P	-27.37	1.28	1.61
25	AY	46	7MG	O3'-P	-19.71	1.37	1.61
25	AY	34	OMG	O3'-P	19.70	1.84	1.61

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	47	U	P-O3'-C3'	-79.00	24.90	119.70
38	BA	1051	G	P-O3'-C3'	-45.69	64.87	119.70
25	AY	35	A	P-O3'-C3'	41.14	169.07	119.70
38	BA	2190	G	P-O3'-C3'	27.80	153.06	119.70
25	AY	46	7MG	P-O3'-C3'	23.58	147.99	119.70

5 of 34 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	410	G	C3'
1	AA	412	A	C1'
24	AW	17	C	C1'
24	AW	47	U	C1'
24	AW	70	G	C3'

5 of 139 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	107	G	Sidechain
1	AA	253	U	Sidechain
1	AA	371	G	Sidechain
1	AA	38	G	Sidechain
1	AA	9	G	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	32329	0	16318	1554	0
2	AB	1901	0	1951	280	0
3	AD	1703	0	1767	184	0
4	AE	1147	0	1207	167	0
5	AF	843	0	857	94	0
6	AH	1116	0	1177	129	0
7	AK	885	0	904	116	0
8	AL	971	0	1057	122	0
9	AO	734	0	771	76	0
10	AP	701	0	720	82	0
11	AQ	824	0	891	86	0
12	AR	574	0	644	97	0
13	AT	763	0	861	104	0
14	AC	1613	0	1677	212	0
15	AG	1257	0	1296	129	0
16	AI	1011	0	1041	140	0
17	AJ	795	0	840	145	0
18	AM	988	0	1055	179	0
19	AN	492	0	533	62	0
20	AS	630	0	652	104	0
21	AU	209	0	221	22	0
22	AV	1645	0	836	146	0
23	AX	132	0	67	15	0
24	AW	1623	0	821	97	0
25	AY	1546	0	801	196	0
26	A0	60	0	30	22	0
27	AZ	2962	0	2975	133	0
28	B0	650	0	654	82	0
29	B1	693	0	764	179	0
30	B2	421	0	461	124	0
31	B3	468	0	523	52	0
32	B4	242	0	103	20	0
33	B5	459	0	480	75	0
34	B6	381	0	390	55	0
35	B7	419	0	467	35	0
36	B8	508	0	576	111	0
37	B9	294	0	316	182	0
38	BA	61426	0	30956	3131	0
39	BB	2551	0	1295	107	0
40	BC	1142	0	865	99	0
41	BD	2105	0	2182	360	0
42	BE	1564	0	1629	326	0
43	BF	1624	0	1677	233	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BG	1474	0	1534	270	0
45	BH	1223	0	1282	205	0
46	BI	1132	0	1218	203	0
47	BL	1025	0	1074	426	0
48	BN	1105	0	1180	213	0
49	BO	933	0	996	136	0
50	BP	1114	0	1187	325	0
51	BQ	1080	0	1127	225	0
52	BR	960	0	1021	176	0
53	BS	771	0	832	185	0
54	BT	1142	0	1202	238	0
55	BU	958	0	1015	188	0
56	BV	779	0	851	216	0
57	BW	896	0	953	112	0
58	BX	726	0	778	205	0
59	BY	776	0	870	220	0
60	BZ	1404	0	1429	241	0
61	AY	11	0	10	5	0
62	AZ	28	0	12	1	0
63	AZ	58	0	60	0	0
64	AZ	4	0	5	3	0
All	All	152000	0	103944	12176	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 48.

The worst 5 of 12176 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)
37:B9:33:LYS:CD	38:BA:2527:C:H4'	1.25	1.66
25:AY:65:G:C5'	27:AZ:391:GLY:HA2	1.20	1.60
37:B9:4:ARG:CZ	38:BA:2465:C:C4'	1.78	1.56
37:B9:33:LYS:HD3	38:BA:2527:C:C4'	1.34	1.54
25:AY:65:G:H5'	27:AZ:391:GLY:CA	1.08	1.53

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	233/235 (99%)	148 (64%)	53 (23%)	32 (14%)	0	4
3	AD	206/208 (99%)	130 (63%)	51 (25%)	25 (12%)	0	4
4	AE	149/151 (99%)	108 (72%)	28 (19%)	13 (9%)	0	9
5	AF	99/101 (98%)	72 (73%)	21 (21%)	6 (6%)	1	13
6	AH	136/138 (99%)	103 (76%)	27 (20%)	6 (4%)	2	17
7	AK	117/119 (98%)	87 (74%)	25 (21%)	5 (4%)	2	17
8	AL	123/125 (98%)	83 (68%)	22 (18%)	18 (15%)	0	3
9	AO	86/88 (98%)	48 (56%)	34 (40%)	4 (5%)	2	16
10	AP	82/84 (98%)	53 (65%)	24 (29%)	5 (6%)	1	13
11	AQ	98/100 (98%)	74 (76%)	15 (15%)	9 (9%)	0	8
12	AR	68/70 (97%)	38 (56%)	21 (31%)	9 (13%)	0	4
13	AT	97/99 (98%)	54 (56%)	29 (30%)	14 (14%)	0	3
14	AC	205/207 (99%)	130 (63%)	55 (27%)	20 (10%)	0	7
15	AG	153/155 (99%)	99 (65%)	42 (28%)	12 (8%)	1	9
16	AI	121/127 (95%)	80 (66%)	30 (25%)	11 (9%)	0	8
17	AJ	97/99 (98%)	70 (72%)	18 (19%)	9 (9%)	0	8
18	AM	113/125 (90%)	68 (60%)	26 (23%)	19 (17%)	0	2
19	AN	58/60 (97%)	35 (60%)	17 (29%)	6 (10%)	0	6
20	AS	77/79 (98%)	52 (68%)	15 (20%)	10 (13%)	0	4
21	AU	23/25 (92%)	18 (78%)	4 (17%)	1 (4%)	2	17
27	AZ	382/405 (94%)	373 (98%)	8 (2%)	1 (0%)	37	72
28	B0	83/85 (98%)	62 (75%)	16 (19%)	5 (6%)	1	13
29	B1	87/89 (98%)	43 (49%)	25 (29%)	19 (22%)	0	1
30	B2	49/51 (96%)	16 (33%)	16 (33%)	17 (35%)	0	0
31	B3	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B4	48/50 (96%)	14 (29%)	11 (23%)	23 (48%)	0	0
33	B5	57/59 (97%)	37 (65%)	13 (23%)	7 (12%)	0	4
34	B6	41/45 (91%)	18 (44%)	16 (39%)	7 (17%)	0	2
35	B7	47/49 (96%)	36 (77%)	10 (21%)	1 (2%)	5	30
36	B8	62/64 (97%)	38 (61%)	13 (21%)	11 (18%)	0	2
37	B9	33/35 (94%)	22 (67%)	5 (15%)	6 (18%)	0	2
40	BC	183/191 (96%)	87 (48%)	53 (29%)	43 (24%)	0	1
41	BD	270/272 (99%)	193 (72%)	51 (19%)	26 (10%)	0	7
42	BE	203/205 (99%)	116 (57%)	49 (24%)	38 (19%)	0	2
43	BF	206/208 (99%)	142 (69%)	40 (19%)	24 (12%)	0	4
44	BG	177/181 (98%)	93 (52%)	56 (32%)	28 (16%)	0	2
45	BH	158/160 (99%)	100 (63%)	31 (20%)	27 (17%)	0	2
46	BI	144/146 (99%)	98 (68%)	36 (25%)	10 (7%)	1	11
47	BL	136/138 (99%)	66 (48%)	32 (24%)	38 (28%)	0	0
48	BN	137/139 (99%)	75 (55%)	35 (26%)	27 (20%)	0	2
49	BO	120/122 (98%)	92 (77%)	17 (14%)	11 (9%)	0	8
50	BP	144/146 (99%)	72 (50%)	37 (26%)	35 (24%)	0	1
51	BQ	134/136 (98%)	82 (61%)	33 (25%)	19 (14%)	0	3
52	BR	115/117 (98%)	74 (64%)	20 (17%)	21 (18%)	0	2
53	BS	97/99 (98%)	49 (50%)	19 (20%)	29 (30%)	0	0
54	BT	136/138 (99%)	77 (57%)	34 (25%)	25 (18%)	0	2
55	BU	115/117 (98%)	61 (53%)	42 (36%)	12 (10%)	0	6
56	BV	97/101 (96%)	47 (48%)	23 (24%)	27 (28%)	0	0
57	BW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	4
58	BX	91/93 (98%)	45 (50%)	23 (25%)	23 (25%)	0	1
59	BY	99/101 (98%)	41 (41%)	24 (24%)	34 (34%)	0	0
60	BZ	175/177 (99%)	99 (57%)	48 (27%)	28 (16%)	0	2
All	All	6336/6487 (98%)	4034 (64%)	1428 (22%)	874 (14%)	0	4

5 of 874 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL

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Mol	Chain	Res	Type
2	AB	52	GLU
2	AB	77	ALA
2	AB	84	GLU
2	AB	154	LEU

5.3.2 Protein sidechains ⓘ

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	202/203 (100%)	182 (90%)	20 (10%)	6	21
3	AD	180/180 (100%)	159 (88%)	21 (12%)	4	16
4	AE	115/116 (99%)	102 (89%)	13 (11%)	4	17
5	AF	90/90 (100%)	84 (93%)	6 (7%)	13	34
6	AH	119/119 (100%)	114 (96%)	5 (4%)	25	46
7	AK	90/90 (100%)	85 (94%)	5 (6%)	17	38
8	AL	104/104 (100%)	95 (91%)	9 (9%)	8	25
9	AO	79/79 (100%)	74 (94%)	5 (6%)	15	35
10	AP	72/72 (100%)	65 (90%)	7 (10%)	6	22
11	AQ	94/95 (99%)	92 (98%)	2 (2%)	48	66
12	AR	61/61 (100%)	55 (90%)	6 (10%)	6	21
13	AT	76/76 (100%)	65 (86%)	11 (14%)	2	12
14	AC	160/161 (99%)	151 (94%)	9 (6%)	17	38
15	AG	126/126 (100%)	122 (97%)	4 (3%)	34	53
16	AI	98/98 (100%)	88 (90%)	10 (10%)	6	20
17	AJ	88/89 (99%)	82 (93%)	6 (7%)	13	33
18	AM	99/100 (99%)	93 (94%)	6 (6%)	15	36
19	AN	49/49 (100%)	47 (96%)	2 (4%)	26	47
20	AS	69/69 (100%)	62 (90%)	7 (10%)	6	20
21	AU	19/20 (95%)	17 (90%)	2 (10%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	AZ	325/339 (96%)	323 (99%)	2 (1%)	84	88
28	B0	61/67 (91%)	54 (88%)	7 (12%)	4	16
29	B1	73/74 (99%)	62 (85%)	11 (15%)	2	11
30	B2	46/47 (98%)	35 (76%)	11 (24%)	0	4
31	B3	51/52 (98%)	49 (96%)	2 (4%)	27	48
33	B5	51/51 (100%)	41 (80%)	10 (20%)	1	7
34	B6	43/44 (98%)	35 (81%)	8 (19%)	1	7
35	B7	41/42 (98%)	37 (90%)	4 (10%)	6	21
36	B8	53/54 (98%)	45 (85%)	8 (15%)	2	11
37	B9	33/33 (100%)	30 (91%)	3 (9%)	7	24
40	BC	61/148 (41%)	54 (88%)	7 (12%)	4	16
41	BD	213/214 (100%)	180 (84%)	33 (16%)	2	10
42	BE	165/165 (100%)	145 (88%)	20 (12%)	4	15
43	BF	165/165 (100%)	153 (93%)	12 (7%)	11	31
44	BG	155/155 (100%)	135 (87%)	20 (13%)	3	14
45	BH	132/133 (99%)	117 (89%)	15 (11%)	4	16
46	BI	122/123 (99%)	113 (93%)	9 (7%)	11	31
47	BL	105/105 (100%)	85 (81%)	20 (19%)	1	7
48	BN	117/118 (99%)	98 (84%)	19 (16%)	2	10
49	BO	100/100 (100%)	92 (92%)	8 (8%)	10	28
50	BP	112/112 (100%)	92 (82%)	20 (18%)	1	8
51	BQ	106/106 (100%)	93 (88%)	13 (12%)	4	15
52	BR	100/100 (100%)	91 (91%)	9 (9%)	8	24
53	BS	77/77 (100%)	65 (84%)	12 (16%)	2	10
54	BT	120/120 (100%)	99 (82%)	21 (18%)	1	8
55	BU	92/93 (99%)	85 (92%)	7 (8%)	11	30
56	BV	82/82 (100%)	64 (78%)	18 (22%)	1	5
57	BW	91/92 (99%)	85 (93%)	6 (7%)	14	34
58	BX	74/75 (99%)	59 (80%)	15 (20%)	1	6
59	BY	84/85 (99%)	67 (80%)	17 (20%)	1	6
60	BZ	155/156 (99%)	144 (93%)	11 (7%)	12	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5195/5324 (98%)	4661 (90%)	534 (10%)	8 20

5 of 534 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	BU	88	ILE
56	BV	66	ARG
55	BU	79	PHE
59	BY	77	PRO
33	B5	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
51	BQ	141	GLN
60	BZ	73	GLN
52	BR	61	HIS
55	BU	49	HIS
17	AJ	78	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	200 (13%)	36 (2%)
22	AV	76/77 (98%)	18 (23%)	0
23	AX	4/6 (66%)	2 (50%)	0
24	AW	75/76 (98%)	15 (20%)	3 (4%)
25	AY	65/72 (90%)	11 (16%)	3 (4%)
26	A0	2/3 (66%)	0	0
38	BA	2849/2852 (99%)	589 (20%)	78 (2%)
39	BB	118/119 (99%)	14 (11%)	1 (0%)
All	All	4692/4709 (99%)	849 (18%)	121 (2%)

5 of 849 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

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Mol	Chain	Res	Type
1	AA	47	C

5 of 121 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	BA	512	G
38	BA	2422	A
38	BA	1176	G
38	BA	2290	G
38	BA	2859	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	5MU	AV	54	22	19,22,23	0.26	0	27,32,35	0.37	0
25	5MC	AY	49	25	19,22,23	0.73	0	26,32,35	0.76	1 (3%)
25	5MC	AY	40	25	19,22,23	0.68	1 (5%)	26,32,35	0.70	1 (3%)
25	OMG	AY	34	26	19,26,27	1.06	2 (10%)	21,38,41	0.87	1 (4%)
25	M2G	AY	26	25	20,27,28	1.28	2 (10%)	19,40,43	0.74	0
25	OMC	AY	32	25	19,22,23	0.46	0	25,31,34	0.60	0
25	2MG	AY	10	25	18,26,27	1.24	3 (16%)	16,38,41	0.90	1 (6%)
25	YG	AY	37	25	30,42,43	0.96	1 (3%)	32,62,65	2.74	10 (31%)
25	PSU	AY	55	25	18,21,22	0.73	0	21,30,33	0.92	0
25	1MA	AY	58	25	17,25,26	2.88	5 (29%)	17,37,40	2.20	4 (23%)
25	7MG	AY	46	25	23,26,27	2.62	3 (13%)	27,39,42	1.58	2 (7%)
25	PSU	AY	39	25	18,21,22	0.70	1 (5%)	21,30,33	0.70	0
25	5MU	AY	54	25	19,22,23	0.48	0	27,32,35	0.65	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2
25	5MC	AY	49	25	-	0/7/25/26	0/2/2/2
25	5MC	AY	40	25	-	1/7/25/26	0/2/2/2
25	OMG	AY	34	26	-	1/5/27/28	0/3/3/3
25	M2G	AY	26	25	-	0/7/29/30	0/3/3/3
25	OMC	AY	32	25	-	0/9/27/28	0/2/2/2
25	2MG	AY	10	25	-	0/5/27/28	0/3/3/3
25	YG	AY	37	25	-	8/20/42/43	0/3/4/4
25	PSU	AY	55	25	-	0/7/25/26	0/2/2/2
25	1MA	AY	58	25	-	0/3/25/26	0/3/3/3
25	7MG	AY	46	25	-	0/7/37/38	0/3/3/3
25	PSU	AY	39	25	-	0/7/25/26	0/2/2/2
25	5MU	AY	54	25	-	0/7/25/26	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AY	46	7MG	C8-N9	-12.04	1.38	1.45
25	AY	58	1MA	C6-N6	7.91	1.48	1.27
25	AY	58	1MA	C2-N3	7.12	1.37	1.28
25	AY	58	1MA	C6-N1	3.39	1.45	1.41
25	AY	26	M2G	C5-C6	-3.28	1.41	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	37	YG	C11-C12-N1	8.48	111.32	106.53
25	AY	37	YG	C24-O23-C21	6.39	123.03	115.63
25	AY	46	7MG	N9-C8-N7	6.30	112.28	103.37
25	AY	37	YG	C3-N3-C4	5.77	125.48	116.76
25	AY	58	1MA	CM1-N1-C6	-4.96	112.47	120.15

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	AY	37	YG	C12-C13-C14-C15
25	AY	37	YG	C15-C16-O18-C19
25	AY	37	YG	O17-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
25	AY	37	YG	C13-C14-C15-C16
25	AY	37	YG	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	2	0
25	AY	40	5MC	3	0
25	AY	34	OMG	12	0
25	AY	26	M2G	18	0
25	AY	32	OMC	1	0
25	AY	10	2MG	3	0
25	AY	37	YG	20	0
25	AY	46	7MG	8	0
25	AY	39	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
62	GDP	AZ	501	-	25,30,30	1.25	3 (12%)	30,47,47	1.01	1 (3%)
64	BME	AZ	503	-	3,3,3	0.36	0	2,2,2	0.27	0
61	PHA	AY	101	-	10,11,11	0.47	0	8,13,13	0.39	0
63	MAU	AZ	502	-	57,60,60	3.68	13 (22%)	62,86,86	1.49	11 (17%)

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
62	GDP	AZ	501	-	-	3/12/32/32	0/3/3/3
64	BME	AZ	503	-	-	0/1/1/1	-
61	PHA	AY	101	-	-	1/5/6/6	0/1/1/1
63	MAU	AZ	502	-	-	1/54/98/98	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	AZ	502	MAU	O18-C17	-16.16	1.20	1.44
63	AZ	502	MAU	O34-C33	-14.15	1.21	1.44
63	AZ	502	MAU	O30-C30	-13.62	1.15	1.42
63	AZ	502	MAU	C22-C21	3.81	1.37	1.33
63	AZ	502	MAU	C27-N26	3.75	1.42	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	AZ	502	MAU	C29-C30-C31	-4.49	104.76	110.80
62	AZ	501	GDP	O4'-C1'-N9	4.04	114.10	108.75
63	AZ	502	MAU	O18-C17-C16	3.78	111.24	104.21
63	AZ	502	MAU	C11-C10-C9	-2.96	117.46	123.52
63	AZ	502	MAU	C3-C2-N1	2.95	120.12	116.62

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	AZ	501	GDP	PA-O3A-PB-O2B
62	AZ	501	GDP	PA-O3A-PB-O3B
63	AZ	502	MAU	C36-C37-C38-C39
61	AY	101	PHA	C-CA-CB-CG
62	AZ	501	GDP	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 9 short contacts:

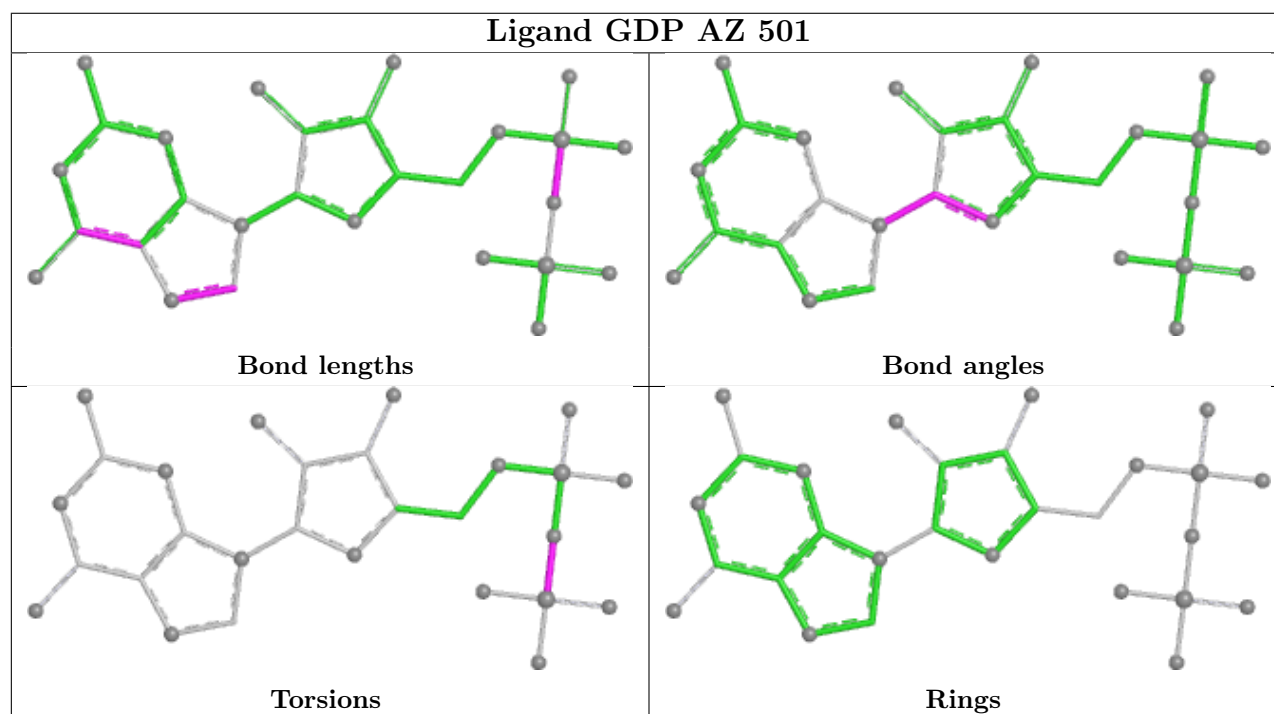
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	AZ	501	GDP	1	0

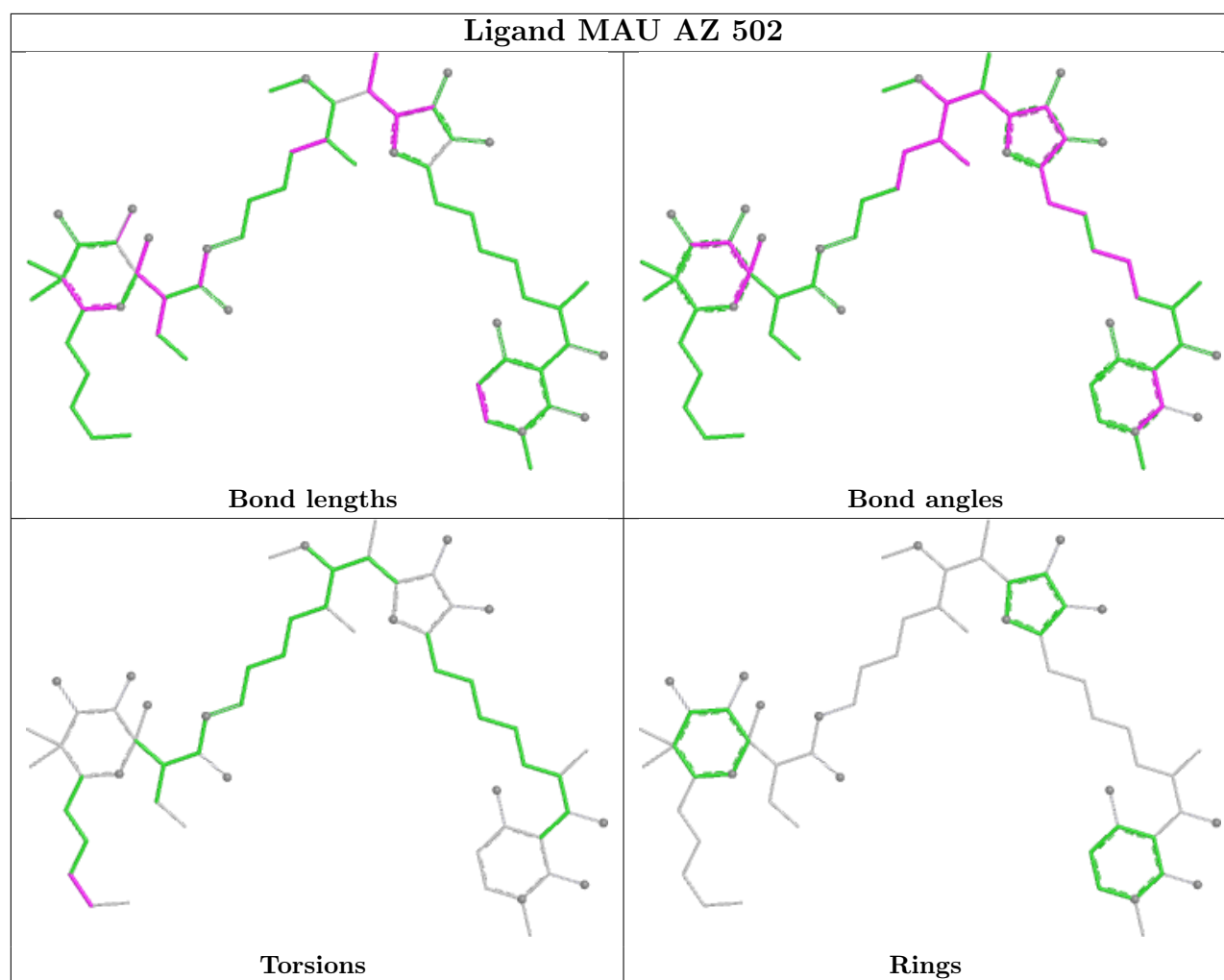
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	AZ	503	BME	3	0
61	AY	101	PHA	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	AY	10
38	BA	6
18	AM	5
40	BC	3
16	AI	2
23	AX	1
34	B6	1
44	BG	1

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Mol	Chain	Number of breaks
56	BV	1

The worst 5 of 30 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BC	110:PHE	C	119:VAL	N	11.81
1	AY	14:A	O3'	18:G	P	11.44
1	AX	14:A	O3'	16:A	P	8.56
1	AY	19:G	O3'	21:A	P	5.14
1	BC	27:ARG	C	34:THR	N	5.01

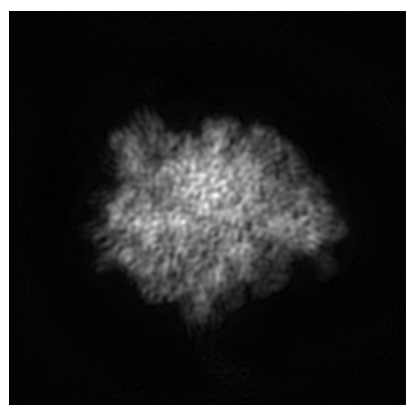
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5030. These allow visual inspection of the internal detail of the map and identification of artifacts.

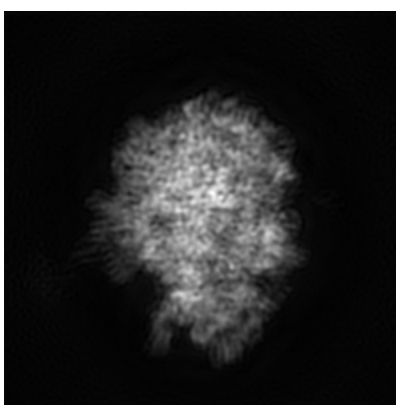
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

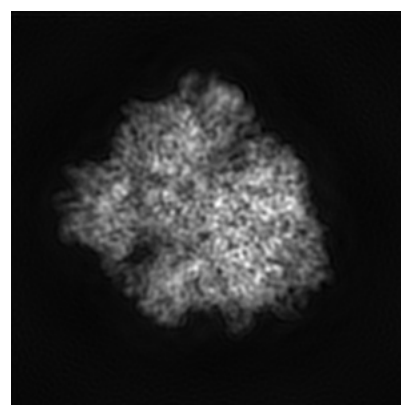
6.1.1 Primary map



X



Y

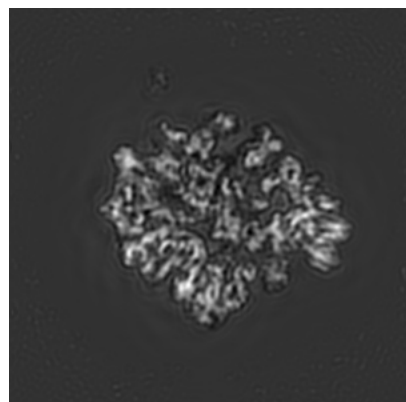


Z

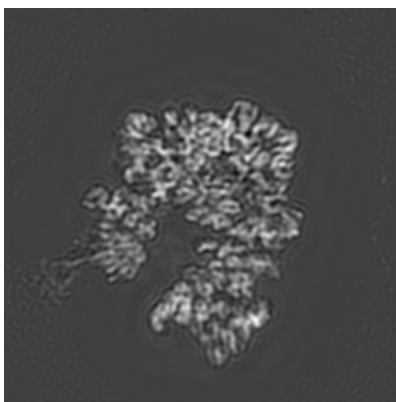
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

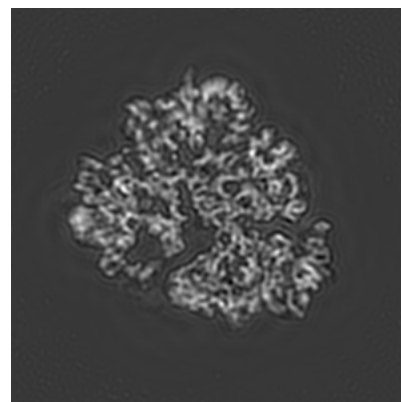
6.2.1 Primary map



X Index: 150



Y Index: 150

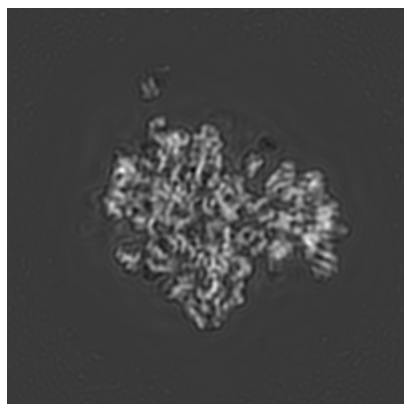


Z Index: 150

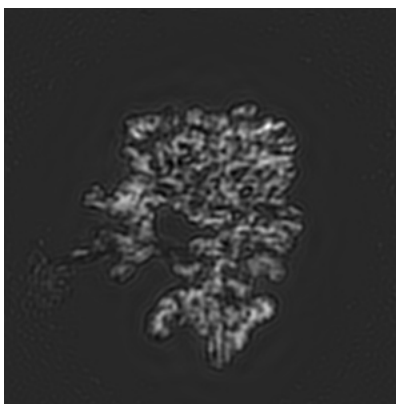
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

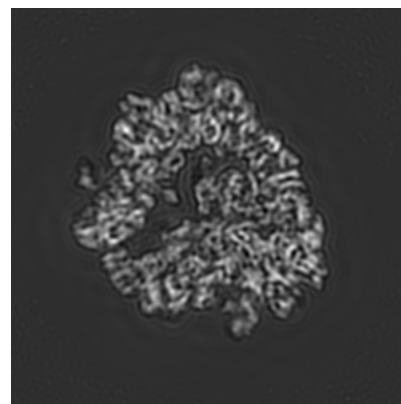
6.3.1 Primary map



X Index: 156



Y Index: 155

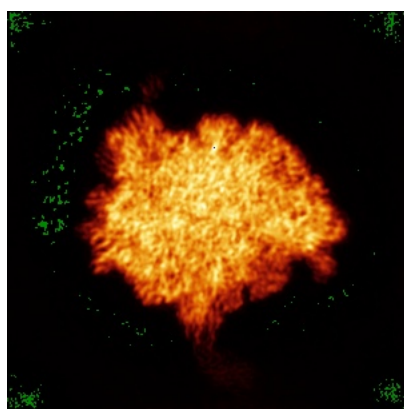


Z Index: 140

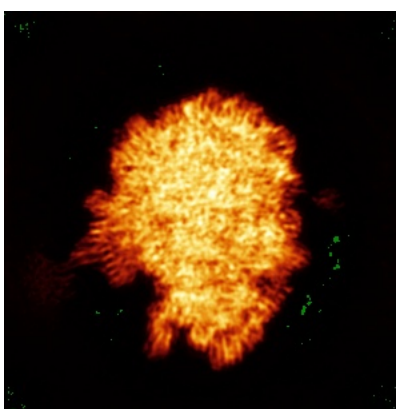
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

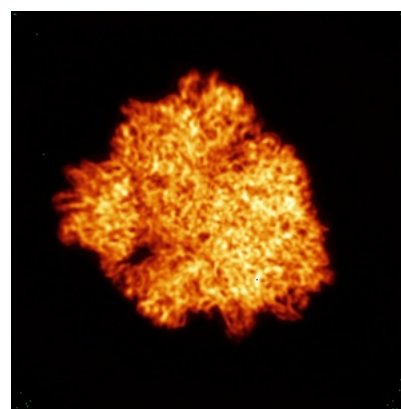
6.4.1 Primary map



X



Y

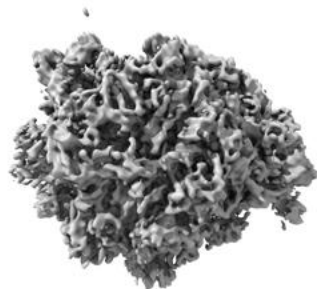


Z

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

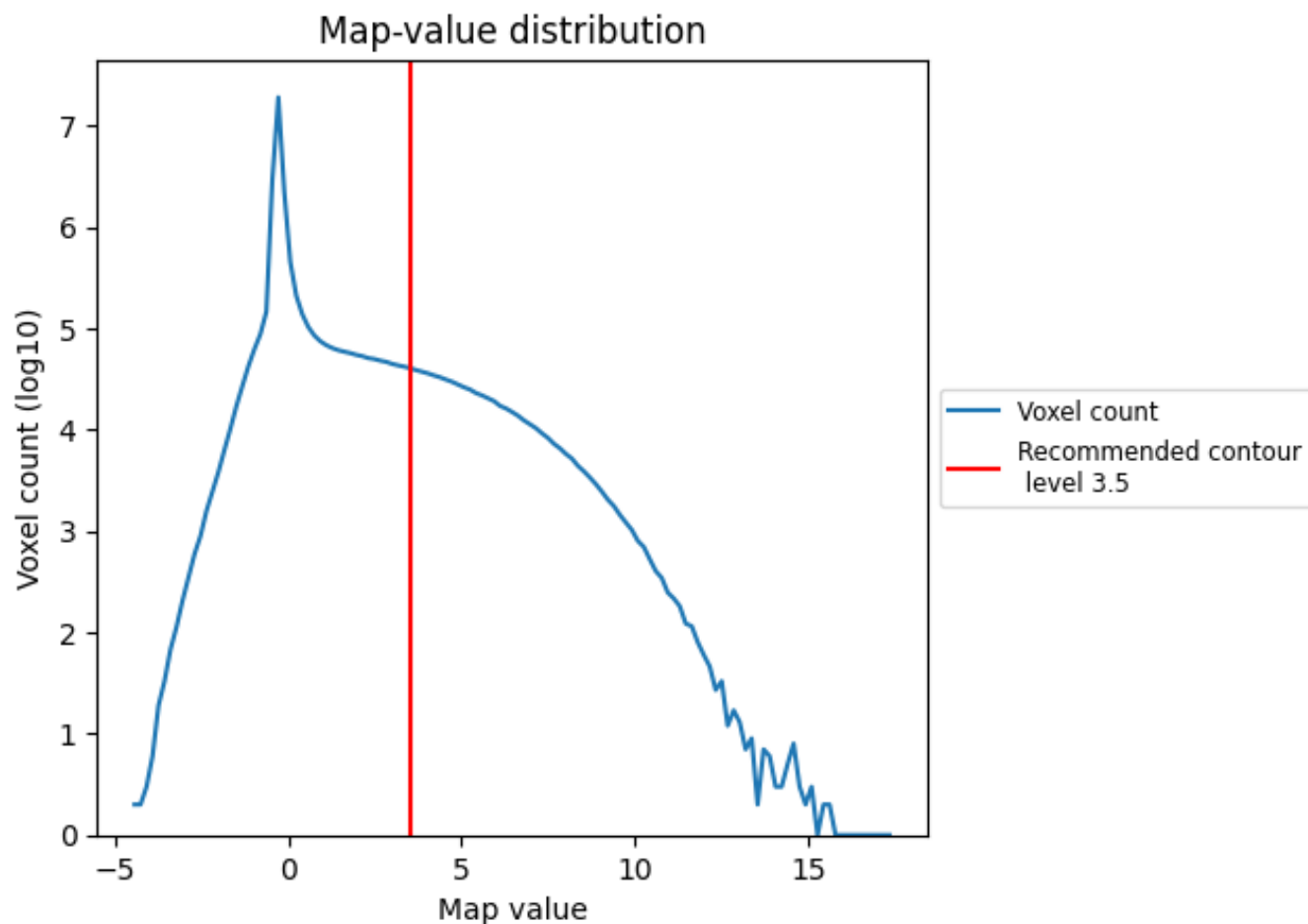
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

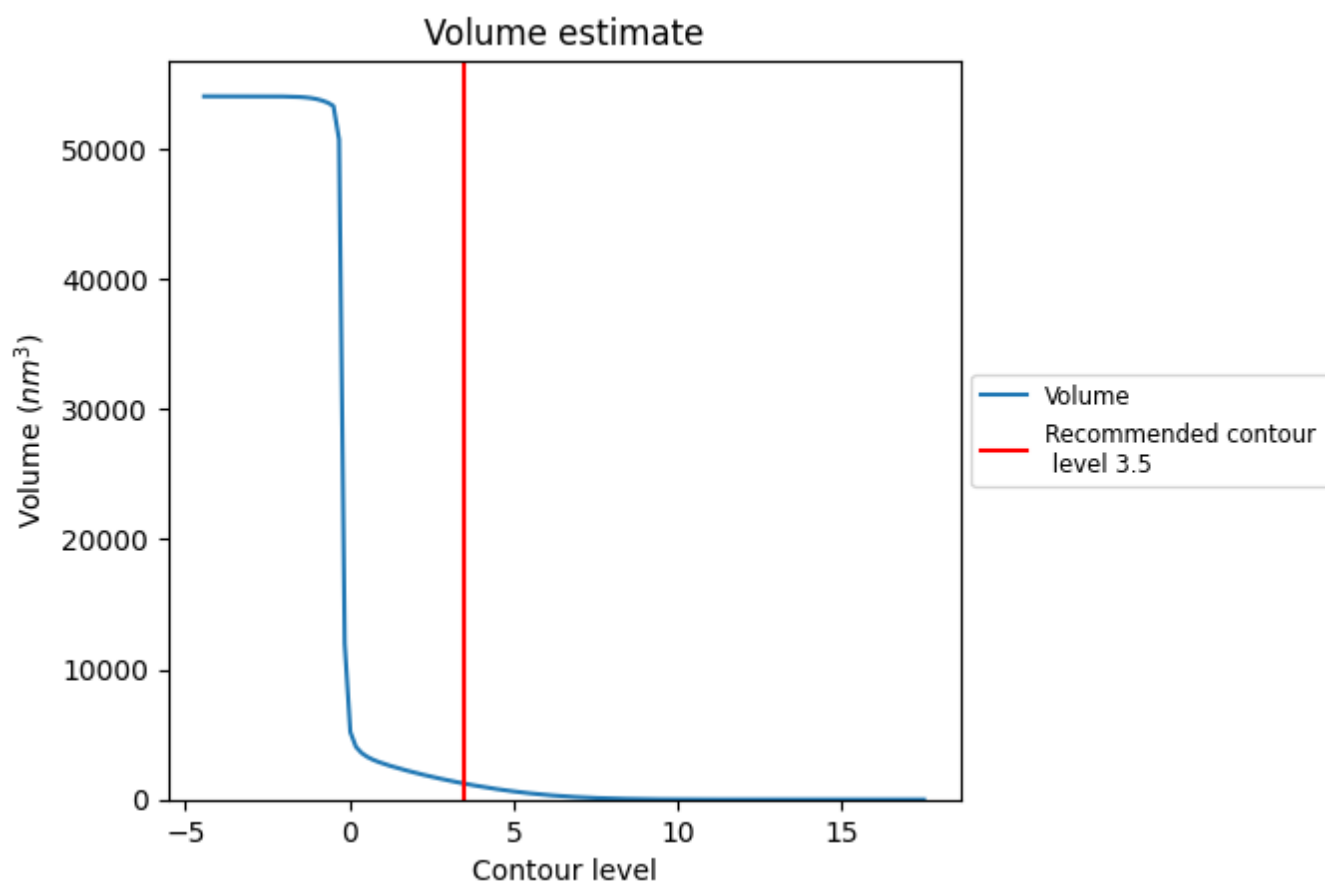
This section contains the results of statistical analysis of the map.

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.

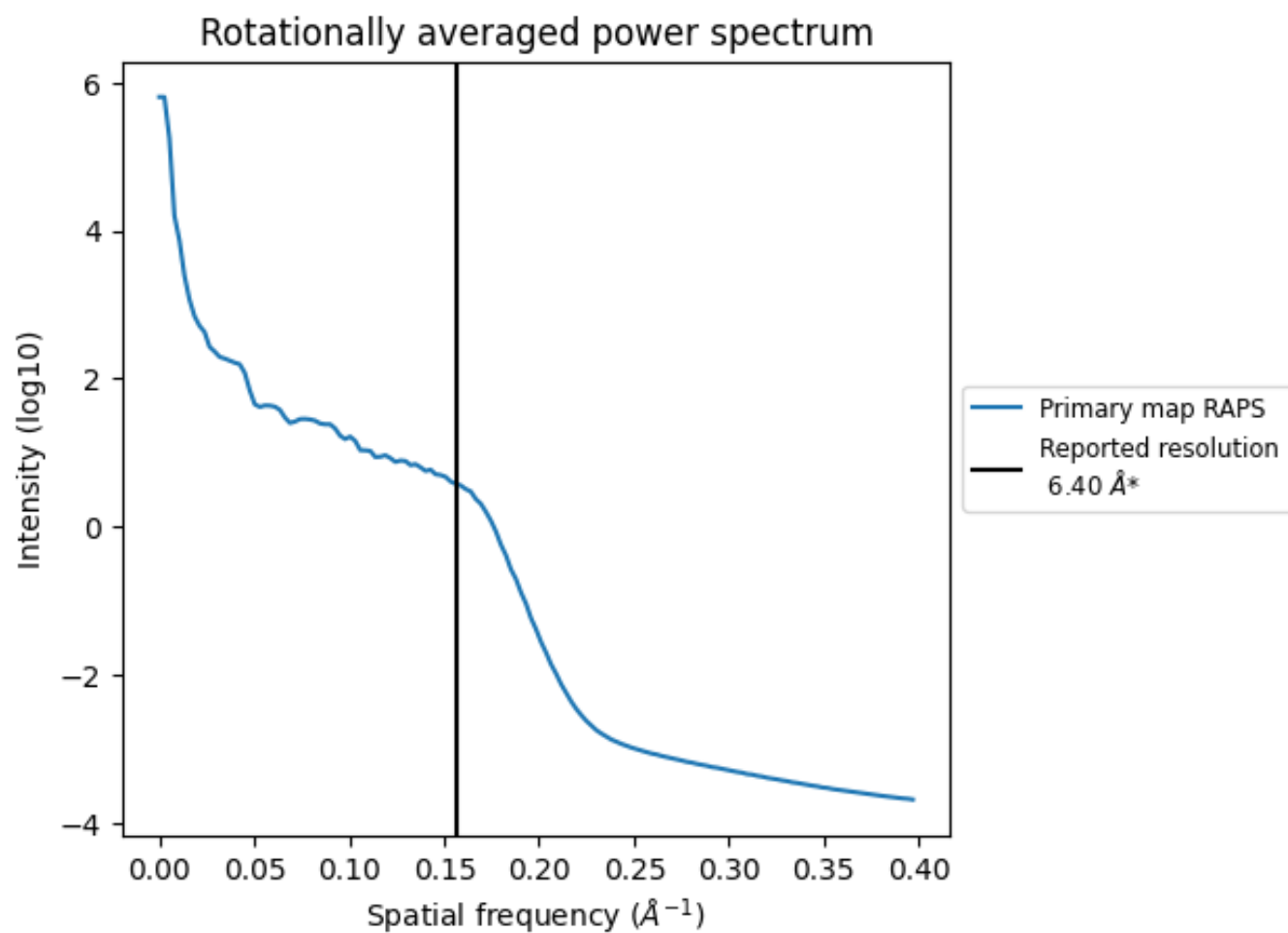
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1230 nm³; this corresponds to an approximate mass of 1111 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.156 \AA^{-1}

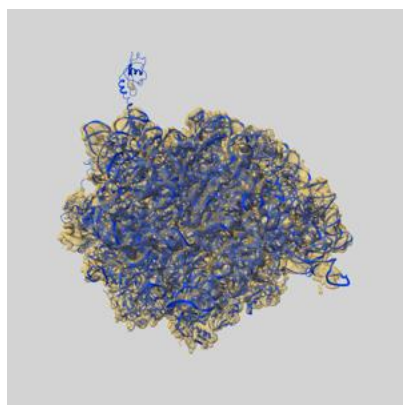
8 Fourier-Shell correlation

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

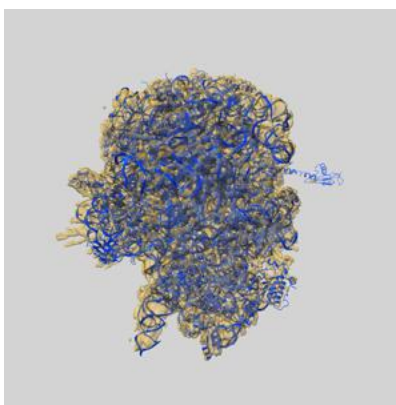
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5030 and PDB model 4V68. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

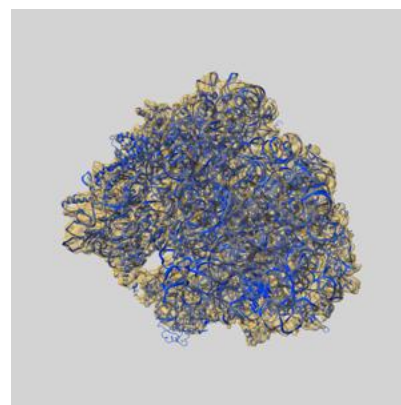
9.1 Map-model overlay [i](#)



X



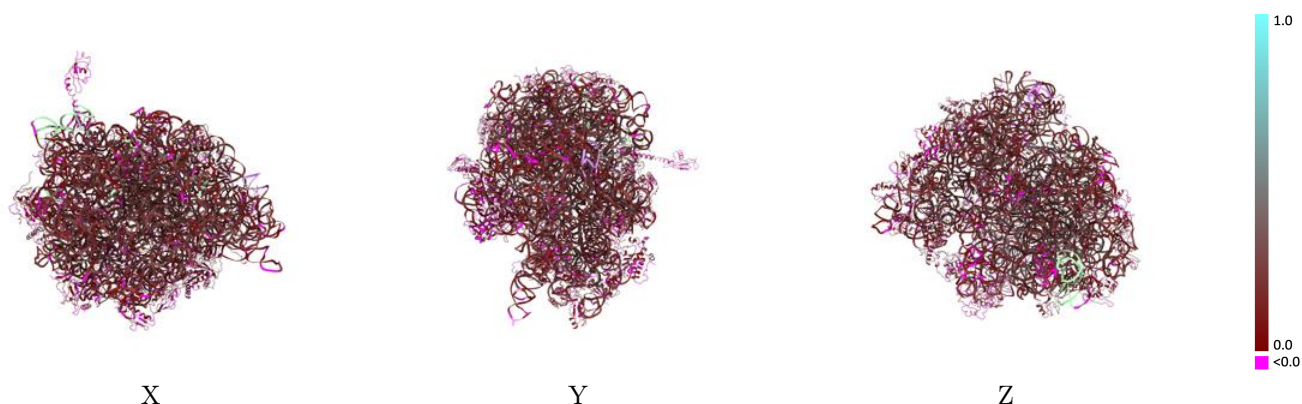
Y



Z

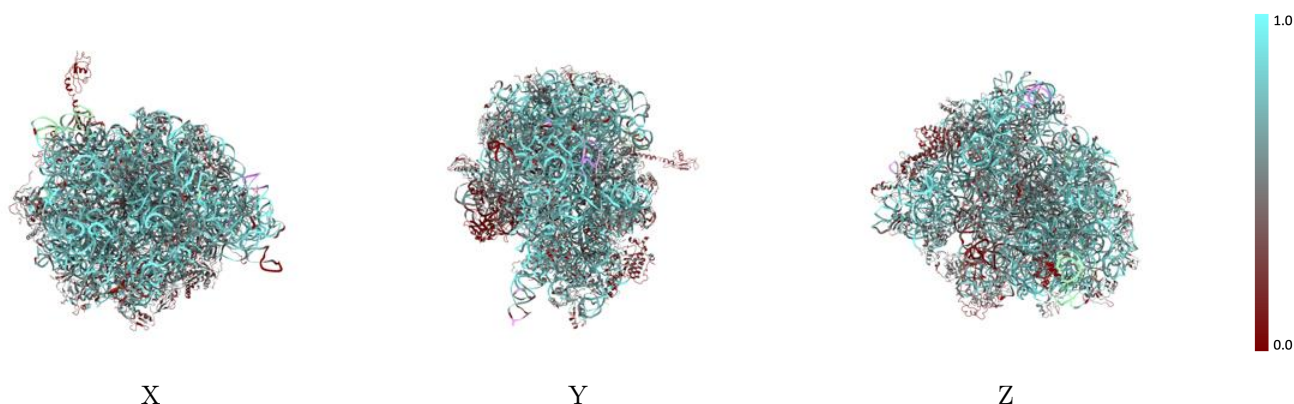
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



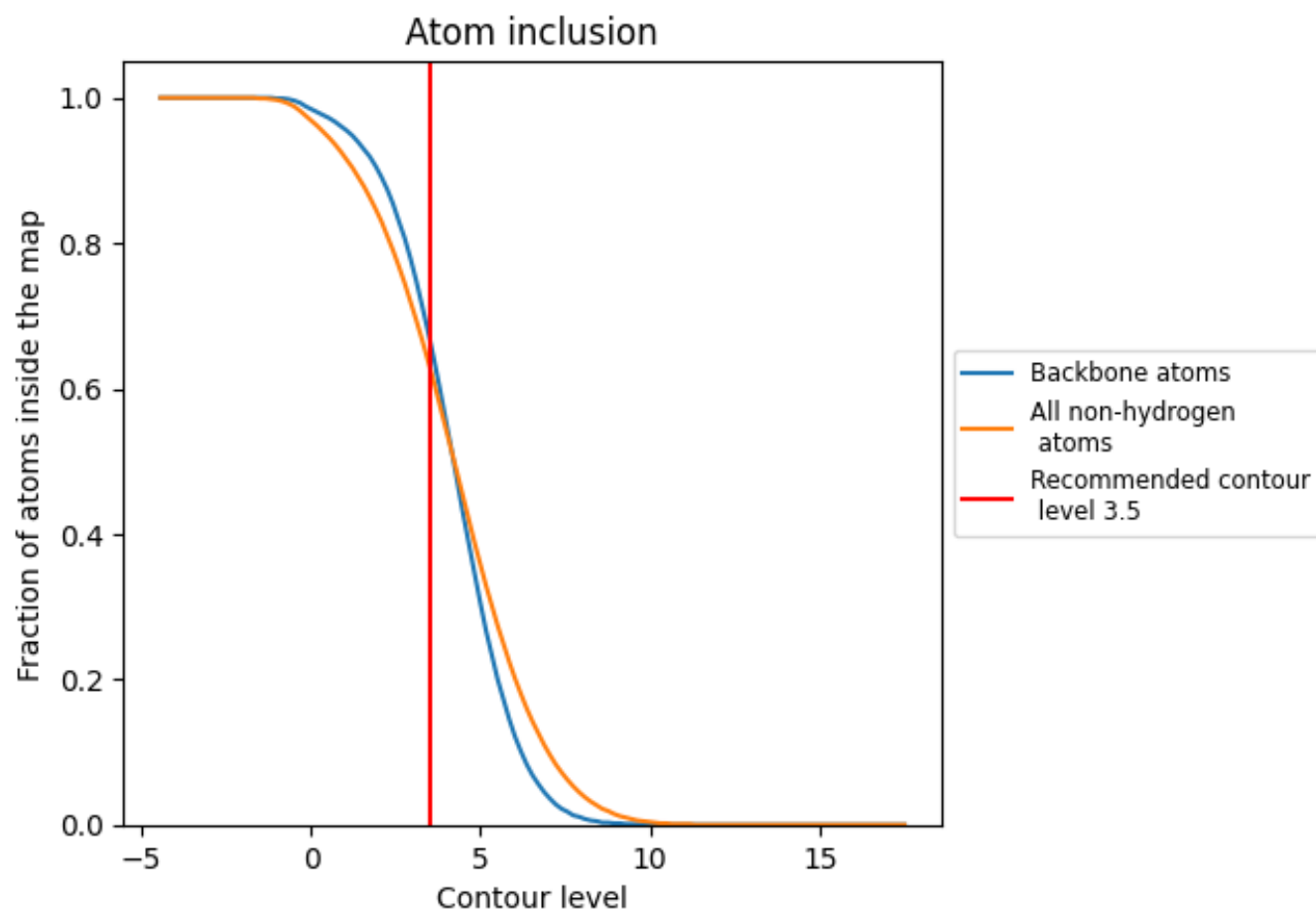
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 63% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6320	 0.1870
A0	 0.6000	 0.0570
AA	 0.7900	 0.2170
AB	 0.2440	 0.1130
AC	 0.4890	 0.1540
AD	 0.5050	 0.1550
AE	 0.4710	 0.1660
AF	 0.3850	 0.1220
AG	 0.4690	 0.1650
AH	 0.4880	 0.1610
AI	 0.4910	 0.1460
AJ	 0.4210	 0.1330
AK	 0.4790	 0.1730
AL	 0.3380	 0.1780
AM	 0.4900	 0.1470
AN	 0.5500	 0.1730
AO	 0.5230	 0.1560
AP	 0.5600	 0.1570
AQ	 0.4870	 0.1700
AR	 0.4190	 0.1660
AS	 0.5580	 0.1580
AT	 0.5530	 0.1380
AU	 0.6510	 0.1820
AV	 0.6330	 0.2120
AW	 0.1760	 0.1480
AX	 0.5910	 0.1740
AY	 0.6010	 0.1870
AZ	 0.3290	 0.1310
B0	 0.4280	 0.1290
B1	 0.4410	 0.1490
B2	 0.4320	 0.1310
B3	 0.4440	 0.1350
B4	 0.1320	 0.1370
B5	 0.4700	 0.1510
B6	 0.5160	 0.0910



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Chain	Atom inclusion	Q-score
B7	 0.4680	 0.1760
B8	 0.3970	 0.1610
B9	 0.4520	 0.1430
BA	 0.7350	 0.2130
BB	 0.7750	 0.1810
BC	 0.0730	 0.0470
BD	 0.4350	 0.1710
BE	 0.4560	 0.1690
BF	 0.4120	 0.1380
BG	 0.4290	 0.1190
BH	 0.3730	 0.1140
BI	 0.0970	 0.0270
BL	 0.0770	 0.0490
BN	 0.4350	 0.1340
BO	 0.3080	 0.1670
BP	 0.4210	 0.1630
BQ	 0.3640	 0.1340
BR	 0.5240	 0.1580
BS	 0.5280	 0.1470
BT	 0.4420	 0.1600
BU	 0.5050	 0.1460
BV	 0.4380	 0.1220
BW	 0.4970	 0.1520
BX	 0.4500	 0.1240
BY	 0.3650	 0.1060
BZ	 0.2780	 0.0840