



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 12:44 AM UTC

PDB ID : 4V8Y / pdb_00004v8y
EMDB ID : EMD-2421
Title : Cryo-EM reconstruction of the 80S-eIF5B-Met-itRNAMet Eukaryotic Translation Initiation Complex
Authors : Fernandez, I.S.; Bai, X.C.; Hussain, T.; Kelley, A.C.; Lorsch, J.R.; Ramakrishnan, V.; Scheres, S.H.W.
Deposited on : 2013-07-20
Resolution : 4.30 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:

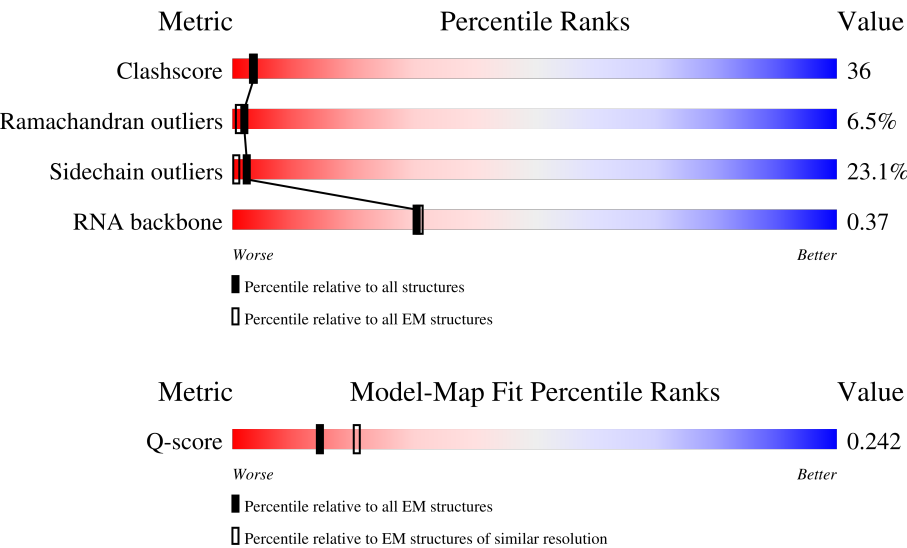
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	A0	119	68% 28% 34% 15% 5% 18%
2	A1	82	60% 52% 30% 15% ..
3	A2	67	85% 27% 43% 24% 6%

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Mol	Chain	Length	Quality of chain
4	A3	56	
5	A4	63	
6	A5	152	
7	A6	319	
8	A7	273	
9	AA	252	
10	AB	255	
11	AC	254	
12	AD	240	
13	AE	261	
14	AF	225	
15	AG	236	
16	AH	190	
17	AI	200	
18	AJ	197	
19	AK	105	
20	AL	156	
21	AM	143	
22	AN	151	
23	AO	137	
24	AP	142	
25	AQ	143	
26	AR	136	
27	AS	146	
28	AT	144	

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Mol	Chain	Length	Quality of chain
29	AU	121	
30	AV	87	
31	AW	130	
32	AX	145	
33	AY	135	
34	AZ	108	
35	BA	253	
36	BB	386	
37	BC	361	
38	BD	296	
39	BE	175	
40	BF	243	
41	BG	255	
42	BH	191	
43	BI	220	
44	BJ	173	
45	BK	174	
46	BL	198	
47	BM	137	
48	BN	203	
49	BO	218	
50	BP	183	
51	BQ	185	
52	BR	188	
53	BS	172	

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Mol	Chain	Length	Quality of chain
54	BT	159	
55	BU	120	
56	BV	136	
57	BW	155	
58	BX	141	
59	BY	126	
60	BZ	135	
61	Ba	148	
62	Bb	58	
63	Bc	104	
64	Bd	112	
65	Be	129	
66	Bf	106	
67	Bg	120	
68	Bh	119	
69	Bi	99	
70	Bj	87	
71	Bk	77	
72	Bl	50	
73	Bm	128	
74	Bn	25	
75	Bo	105	
76	Bq	312	
77	Br	47	
78	Bs	46	

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Mol	Chain	Length	Quality of chain
79	By	229	
79	CL	229	
80	B2	1800	
81	B5	3396	
82	B7	121	
83	B8	158	
84	CN	87	
85	CP	339	
86	CW	76	

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
89	OHX	A3	102	-	-	X	-
89	OHX	AC	301	-	-	X	-
89	OHX	B2	1907	-	-	X	-
89	OHX	B2	1915	-	-	X	-
89	OHX	B2	1918	-	-	X	-
89	OHX	B2	1921	-	-	X	-
89	OHX	B2	1922	-	-	X	-
89	OHX	B2	1940	-	-	X	-
89	OHX	B2	1954	-	-	X	-
89	OHX	B2	1961	-	-	X	-
89	OHX	B2	1963	-	-	X	-
89	OHX	B2	1964	-	-	X	-
89	OHX	B2	1968	-	-	X	-
89	OHX	B2	1969	-	-	X	-
89	OHX	B2	1974	-	-	X	-
89	OHX	B2	1977	-	-	X	-
89	OHX	B2	1982	-	-	X	-
89	OHX	B2	1988	-	-	X	-
89	OHX	B2	2013	-	-	X	-
89	OHX	B2	2016	-	-	X	-
89	OHX	B2	2027	-	-	X	-
89	OHX	B2	2046	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	OHX	B2	2050	-	-	X	-
89	OHX	B2	2064	-	-	X	-
89	OHX	B2	2068	-	-	X	-
89	OHX	B2	2071	-	-	X	-
89	OHX	B2	2073	-	-	X	-
89	OHX	B2	2079	-	-	X	-
89	OHX	B2	2083	-	-	X	-
89	OHX	BR	201	-	-	X	-
90	GCP	CP	401	-	-	X	-

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 222555 atoms, of which 8300 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S RIBOSOMAL PROTEIN S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 6 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A5	71	Total	C	N	O	S	0	0
			516	328	93	91	4		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	82	UNK	LYS	SEE REMARK 999	UNP P05759
A5	83	UNK	LYS	SEE REMARK 999	UNP P05759
A5	84	UNK	VAL	SEE REMARK 999	UNP P05759
A5	85	UNK	TYR	SEE REMARK 999	UNP P05759
A5	86	UNK	THR	SEE REMARK 999	UNP P05759
A5	87	UNK	THR	SEE REMARK 999	UNP P05759
A5	88	UNK	PRO	SEE REMARK 999	UNP P05759
A5	89	UNK	LYS	SEE REMARK 999	UNP P05759
A5	90	UNK	LYS	SEE REMARK 999	UNP P05759
A5	91	UNK	ILE	SEE REMARK 999	UNP P05759
A5	92	UNK	LYS	SEE REMARK 999	UNP P05759
A5	93	UNK	HIS	SEE REMARK 999	UNP P05759
A5	94	UNK	LYS	SEE REMARK 999	UNP P05759
A5	95	UNK	HIS	SEE REMARK 999	UNP P05759
A5	96	UNK	LYS	SEE REMARK 999	UNP P05759
A5	97	UNK	LYS	SEE REMARK 999	UNP P05759
A5	98	UNK	VAL	SEE REMARK 999	UNP P05759
A5	99	UNK	LYS	SEE REMARK 999	UNP P05759
A5	100	UNK	LEU	SEE REMARK 999	UNP P05759
A5	101	UNK	ALA	SEE REMARK 999	UNP P05759

- Molecule 7 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 8 is a protein called SUPPRESSOR PROTEIN STM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	A7	159	Total	C	N	O	0	0
			1105	653	221	231		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A7	9	UNK	GLY	SEE REMARK 999	UNP P39015
A7	10	UNK	ASN	SEE REMARK 999	UNP P39015
A7	11	UNK	ASP	SEE REMARK 999	UNP P39015
A7	12	UNK	VAL	SEE REMARK 999	UNP P39015

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Chain	Residue	Modelled	Actual	Comment	Reference
A7	13	UNK	GLU	SEE REMARK 999	UNP P39015
A7	14	UNK	ASP	SEE REMARK 999	UNP P39015
A7	15	UNK	ALA	SEE REMARK 999	UNP P39015
A7	16	UNK	ASP	SEE REMARK 999	UNP P39015
A7	17	UNK	VAL	SEE REMARK 999	UNP P39015
A7	18	UNK	VAL	SEE REMARK 999	UNP P39015
A7	19	UNK	VAL	SEE REMARK 999	UNP P39015
A7	20	UNK	LEU	SEE REMARK 999	UNP P39015
A7	151	UNK	LEU	SEE REMARK 999	UNP P39015
A7	152	UNK	GLN	SEE REMARK 999	UNP P39015
A7	153	UNK	ASP	SEE REMARK 999	UNP P39015
A7	154	UNK	TYR	SEE REMARK 999	UNP P39015
A7	155	UNK	LEU	SEE REMARK 999	UNP P39015
A7	156	UNK	ASN	SEE REMARK 999	UNP P39015
A7	157	UNK	GLN	SEE REMARK 999	UNP P39015
A7	158	UNK	GLN	SEE REMARK 999	UNP P39015
A7	159	UNK	ALA	SEE REMARK 999	UNP P39015
A7	160	UNK	ASN	SEE REMARK 999	UNP P39015
A7	161	UNK	ASN	SEE REMARK 999	UNP P39015
A7	162	UNK	GLN	SEE REMARK 999	UNP P39015
A7	163	UNK	PHE	SEE REMARK 999	UNP P39015
A7	164	UNK	ASN	SEE REMARK 999	UNP P39015
A7	165	UNK	LYS	SEE REMARK 999	UNP P39015
A7	166	UNK	VAL	SEE REMARK 999	UNP P39015
A7	167	UNK	PRO	SEE REMARK 999	UNP P39015
A7	168	UNK	GLU	SEE REMARK 999	UNP P39015
A7	169	UNK	ALA	SEE REMARK 999	UNP P39015
A7	170	UNK	LYS	SEE REMARK 999	UNP P39015
A7	171	UNK	LYS	SEE REMARK 999	UNP P39015
A7	172	UNK	VAL	SEE REMARK 999	UNP P39015
A7	173	UNK	GLU	SEE REMARK 999	UNP P39015
A7	174	UNK	LEU	SEE REMARK 999	UNP P39015
A7	175	UNK	ASP	SEE REMARK 999	UNP P39015

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AA	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AG	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AH	184	Total	C	N	O		0	0
			1481	951	265	265			

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AK	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AL	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AM	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AO	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AP	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AR	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AT	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 33 is a protein called 40S RIBOSOMAL PROTEIN S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AY	134	Total	C	N	O		0	0
			1073	676	208	189			

- Molecule 34 is a protein called 40S RIBOSOMAL PROTEIN S25-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AZ	70	Total	C	N	O		0	0
			563	360	104	99			

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	252	Total	C	N	O	S	0	0
			1912	1190	388	333	1		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	213	Total	C	N	O	S	0	0
			1722	1094	325	297	6		

- Molecule 44 is a protein called 60S RIBOSOMAL PROTEIN L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BK	151	Total	C	H	N	O	0	1
			1507	450	756	151	150		

- Molecule 46 is a protein called 60S RIBOSOMAL PROTEIN L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BL	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 47 is a protein called 60S RIBOSOMAL PROTEIN L14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	89	ALA	GLY	conflict	UNP P38754

- Molecule 48 is a protein called 60S RIBOSOMAL PROTEIN L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 49 is a protein called 60S RIBOSOMAL PROTEIN L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BO	197	Total	C	N	O	S	197	0
			3119	2008	581	528	2		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	3	VAL	SER	microheterogeneity	UNP P26784
BO	4	GLU	GLN	microheterogeneity	UNP P26784
BO	11	GLY	ALA	microheterogeneity	UNP P26784
BO	13	GLY	ASP	microheterogeneity	UNP P26784
BO	16	VAL	LEU	microheterogeneity	UNP P26784
BO	22	VAL	THR	microheterogeneity	UNP P26784
BO	23	VAL	ILE	microheterogeneity	UNP P26784

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Chain	Residue	Modelled	Actual	Comment	Reference
BO	27	LEU	VAL	microheterogeneity	UNP P26784
BO	40	GLU	ALA	microheterogeneity	UNP P26784
BO	80	PHE	LEU	microheterogeneity	UNP P26784
BO	84	LEU	ILE	microheterogeneity	UNP P26784
BO	104	VAL	ILE	microheterogeneity	UNP P26784
BO	158	ALA	ASP	microheterogeneity	UNP P26784
BO	163	SER	ARG	microheterogeneity	UNP P26784
BO	179	ALA	SER	microheterogeneity	UNP P26784
BO	182	ASN	SER	microheterogeneity	UNP P26784
BO	184	THR	ALA	microheterogeneity	UNP P26784
BO	186	ALA	SER	microheterogeneity	UNP P26784
BO	196	ALA	SER	microheterogeneity	UNP P26784
BO	197	LEU	PHE	microheterogeneity	UNP P26784

- Molecule 50 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BP	155	Total	C	N	O	0	0
			1227	764	238	225		

- Molecule 51 is a protein called 60S RIBOSOMAL PROTEIN L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 52 is a protein called 60S RIBOSOMAL PROTEIN L19-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	BR	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 53 is a protein called 60S RIBOSOMAL PROTEIN L20-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 54 is a protein called 60S RIBOSOMAL PROTEIN L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 55 is a protein called 60S RIBOSOMAL PROTEIN L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BU	98	Total	C	N	O		0	0
			778	505	127	146			

- Molecule 56 is a protein called 60S RIBOSOMAL PROTEIN L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 57 is a protein called 60S RIBOSOMAL PROTEIN L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BW	135	Total	C	N	O	S	0	0
			1038	651	206	180	1		

- Molecule 58 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BX	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 59 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BY	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 60 is a protein called 60S RIBOSOMAL PROTEIN L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BZ	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 61 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ba	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 62 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bb	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 63 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bc	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 64 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bd	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 65 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Be	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 66 is a protein called 60S RIBOSOMAL PROTEIN L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bf	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 67 is a protein called 60S RIBOSOMAL PROTEIN L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bg	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 68 is a protein called 60S RIBOSOMAL PROTEIN L35-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bh	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 69 is a protein called 60S RIBOSOMAL PROTEIN L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bi	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 70 is a protein called 60S RIBOSOMAL PROTEIN L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 71 is a protein called 60S RIBOSOMAL PROTEIN L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bk	77	Total	C	N	O		0	0
			608	388	114	106			

- Molecule 72 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bl	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 73 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bm	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 74 is a protein called 60S RIBOSOMAL PROTEIN L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bn	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 75 is a protein called 60S RIBOSOMAL PROTEIN L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bo	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 76 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P0.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	Bq	143	Total	C	H	N	O	S	0	0
			2187	687	1110	192	195	3		

- Molecule 77 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Br	47	Total	C	H	N	O	0	0
			473	141	237	47	48		

- Molecule 78 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P2.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bs	46	Total	C	H	N	O	0	0
			463	138	232	46	47		

- Molecule 79 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	By	225	Total	C	H	N	O	S	0	0
			3492	1086	1773	315	316	2		
79	CL	225	Total	C	N	O	S		0	0
			1719	1086	315	316	2			

- Molecule 80 is a RNA chain called 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	B2	1781	Total	C	N	O	P	1	0
			37835	16910	6661	12482	1782		

- Molecule 81 is a RNA chain called 25S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	B5	3147	Total	C	H	N	O	P	0	0
			67972	30066	664	12132	21965	3145		

- Molecule 82 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	B7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 83 is a RNA chain called 5.8S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	B8	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 84 is a RNA chain called EUKARYOTIC RIBOSOMAL L1_RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	CN	87	Total	C	N	O	P	0	0
			1875	832	347	609	87		

- Molecule 85 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
85	CP	339	Total	C	H	N	O	S	0	0
			5380	1679	2725	457	507	12		

- Molecule 86 is a RNA chain called EUKARYOTIC RIBOSOMAL P_E TRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	CW	74	Total	C	H	N	O	P	0	0
			2379	705	803	285	514	72		

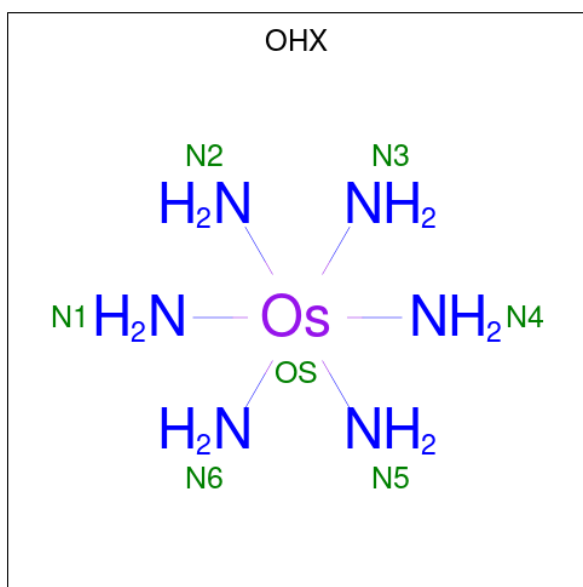
- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	A0	1	Total	Zn	0
			1	1	
87	A1	1	Total	Zn	0
			1	1	
87	A3	1	Total	Zn	0
			1	1	
87	A5	1	Total	Zn	0
			1	1	
87	Bj	1	Total	Zn	0
			1	1	
87	Bm	1	Total	Zn	0
			1	1	

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A0	2	Total 2	Mg 2	0
88	A3	3	Total 3	Mg 3	0
88	A5	1	Total 1	Mg 1	0
88	AB	1	Total 1	Mg 1	0
88	AC	2	Total 2	Mg 2	0
88	AE	1	Total 1	Mg 1	0
88	AG	1	Total 1	Mg 1	0
88	AI	1	Total 1	Mg 1	0
88	AJ	1	Total 1	Mg 1	0
88	AL	2	Total 2	Mg 2	0
88	AN	1	Total 1	Mg 1	0
88	AP	1	Total 1	Mg 1	0
88	AS	1	Total 1	Mg 1	0
88	AU	1	Total 1	Mg 1	0
88	B2	169	Total 169	Mg 169	0
88	B5	3	Total 3	Mg 3	0

- Molecule 89 is osmium (III) hexammine (CCD ID: OHX) (formula: H₁₂N₆Os).



Mol	Chain	Residues	Atoms			AltConf
89	A3	1	Total	N	Os	0
			7	6	1	
89	A6	1	Total	N	Os	0
			7	6	1	
89	AC	1	Total	N	Os	0
			7	6	1	
89	AI	1	Total	N	Os	0
			7	6	1	
89	AI	1	Total	N	Os	0
			7	6	1	
89	AL	1	Total	N	Os	0
			7	6	1	
89	AN	1	Total	N	Os	0
			7	6	1	
89	AP	1	Total	N	Os	0
			7	6	1	
89	BR	1	Total	N	Os	0
			7	6	1	
89	Bn	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	

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Mol	Chain	Residues	Atoms			AltConf
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	

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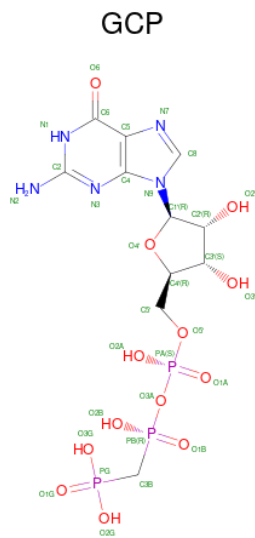
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[illegible]

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Mol	Chain	Residues	Atoms			AltConf
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B2	1	Total	N	Os	0
			7	6	1	
89	B5	1	Total	N	Os	0
			7	6	1	
89	B5	1	Total	N	Os	0
			7	6	1	
89	B5	1	Total	N	Os	0
			7	6	1	

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

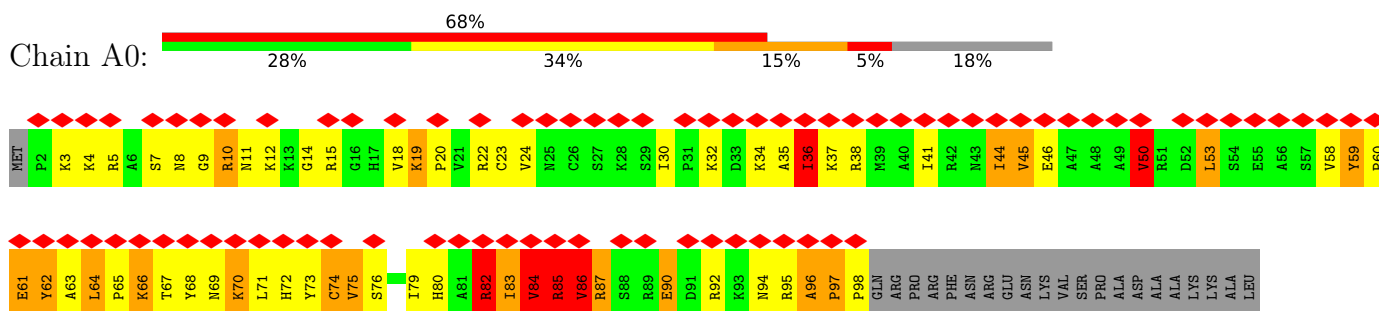


Mol	Chain	Residues	Atoms					AltConf
90	CP	1	Total 32	C 11	N 5	O 13	P 3	0

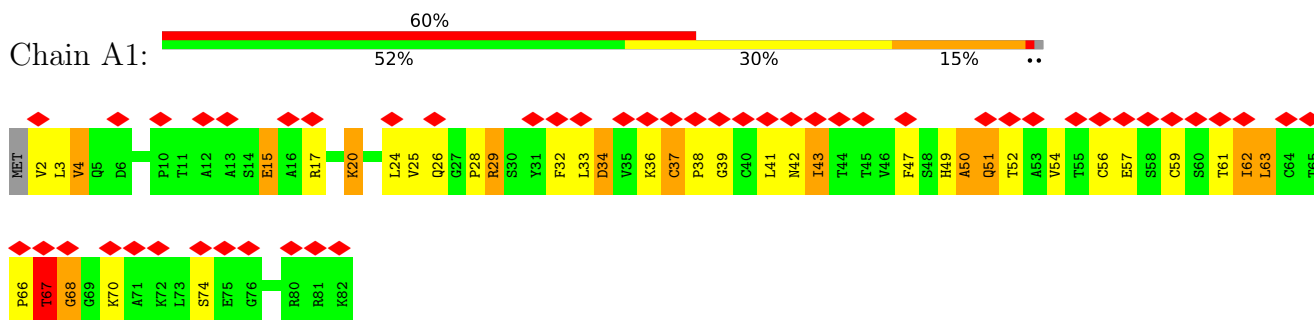
3 Residue-property plots

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.

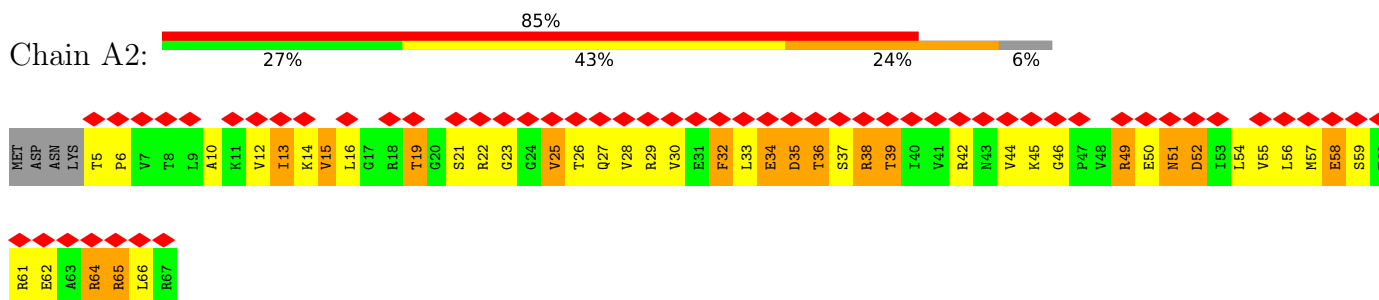
• Molecule 1: 40S RIBOSOMAL PROTEIN S26-A



• Molecule 2: 40S RIBOSOMAL PROTEIN S27-A



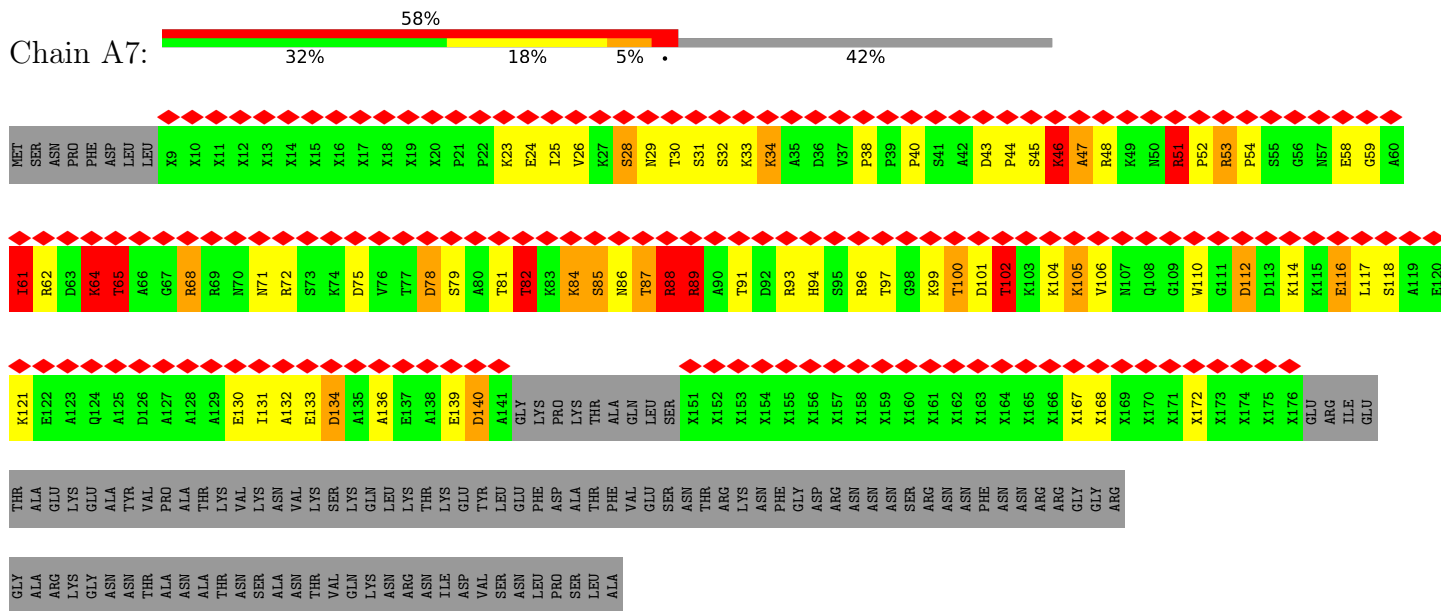
• Molecule 3: 40S RIBOSOMAL PROTEIN S28-A



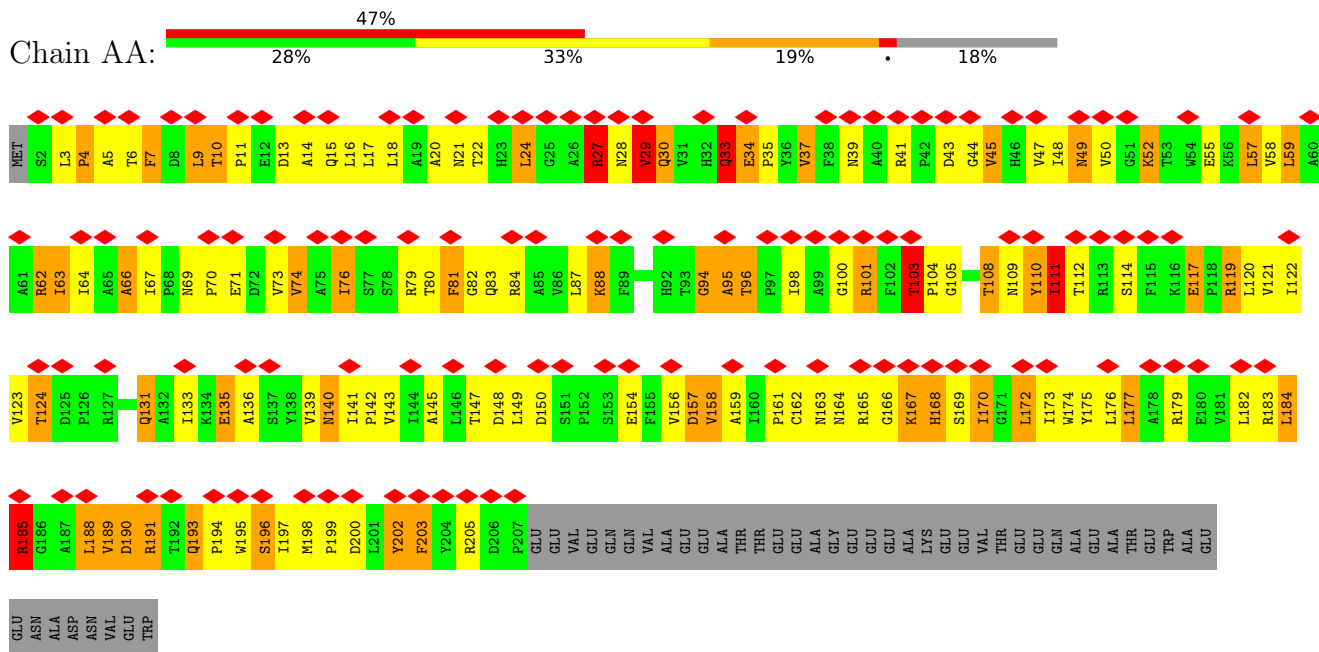
• Molecule 4: 40S RIBOSOMAL PROTEIN S29-A



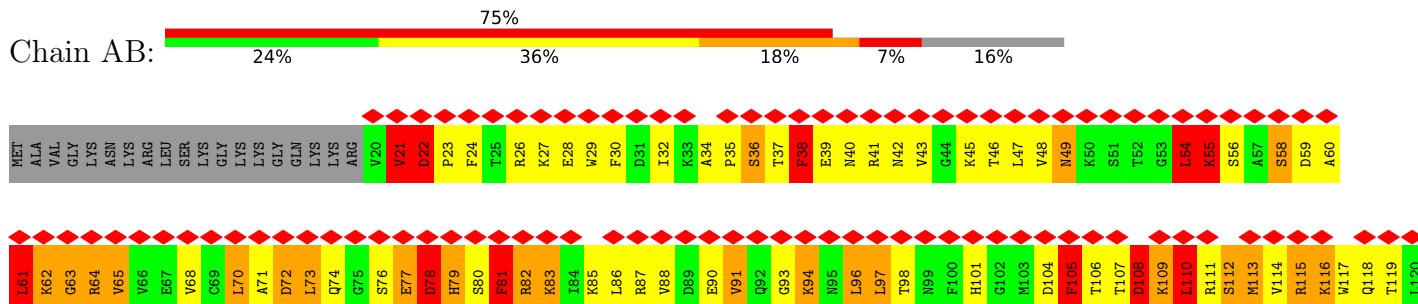
Chain A7:



Chain AA:

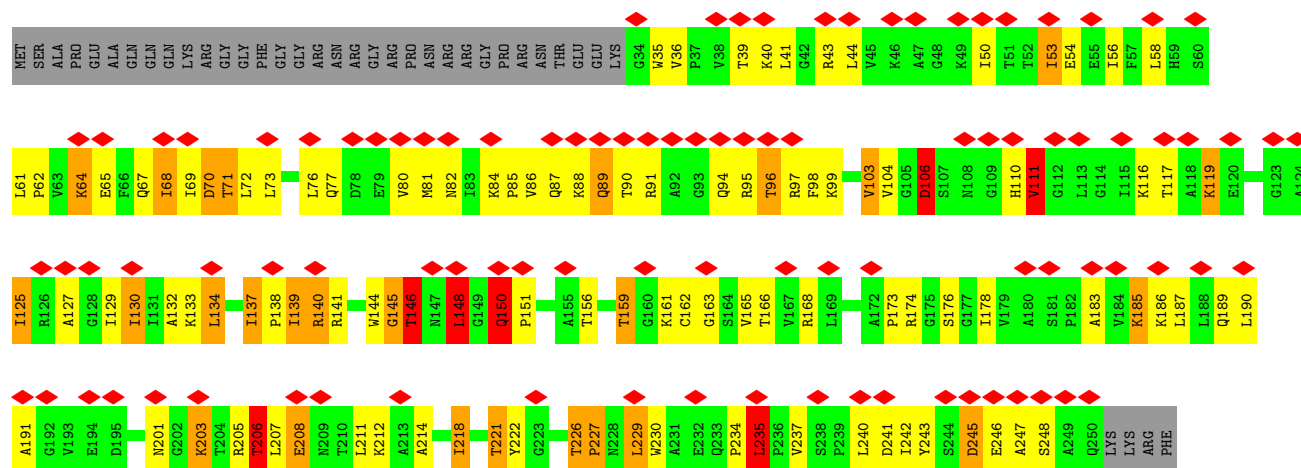
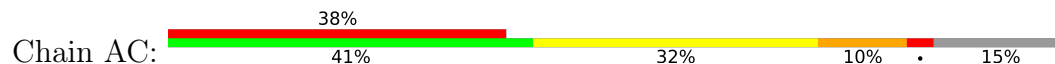


Chain AB:

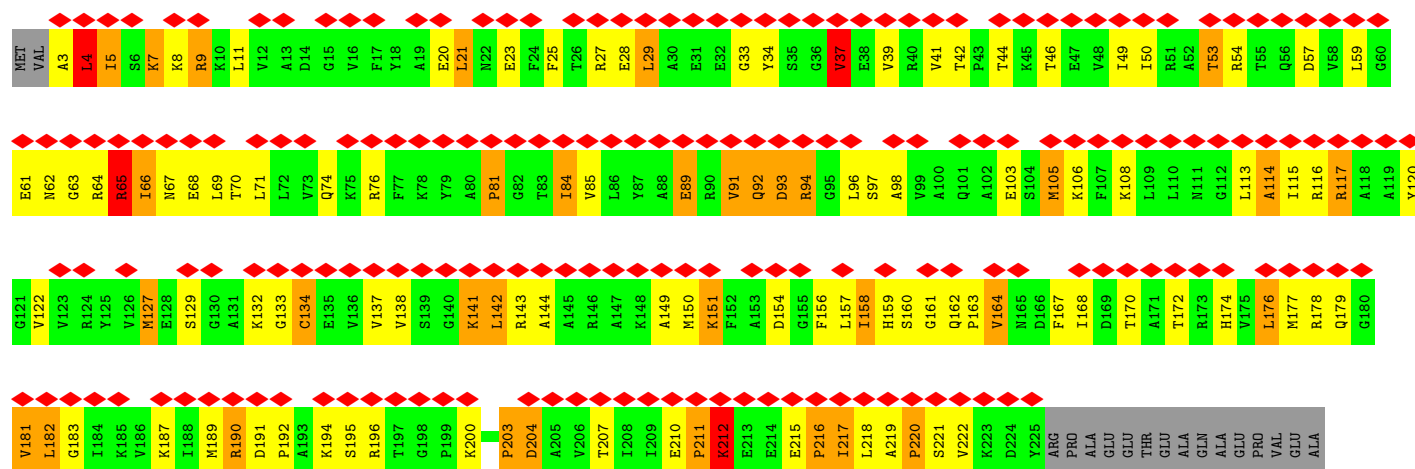
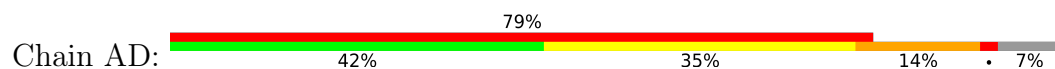




• Molecule 11: 40S RIBOSOMAL PROTEIN S2

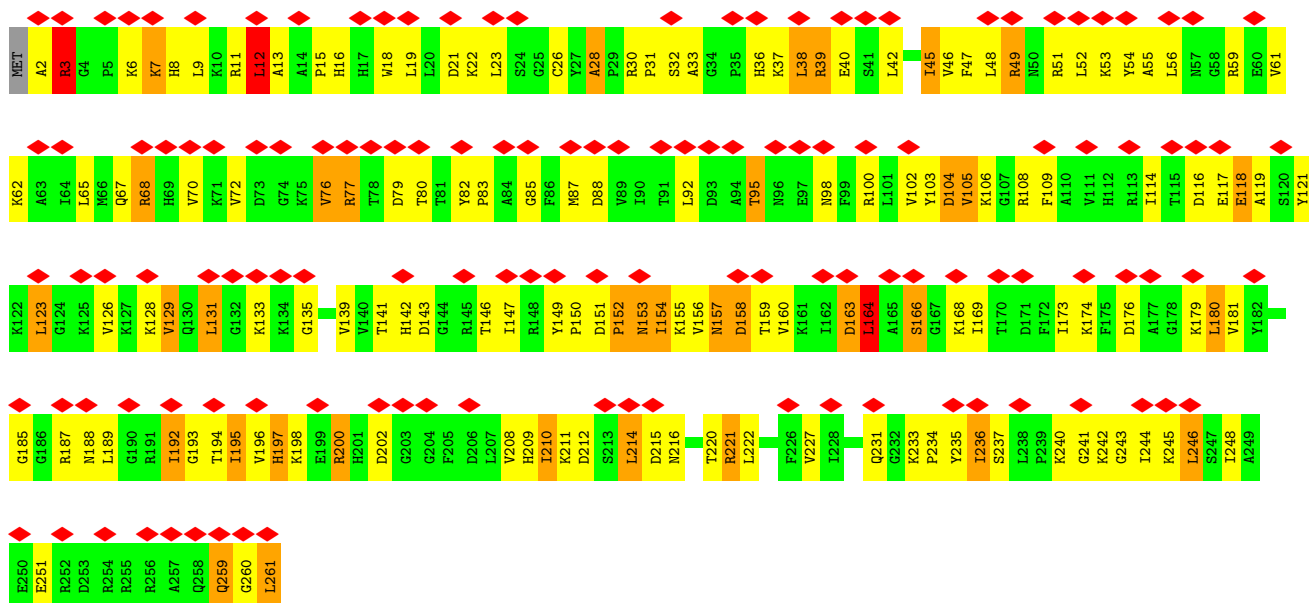


• Molecule 12: 40S RIBOSOMAL PROTEIN S3

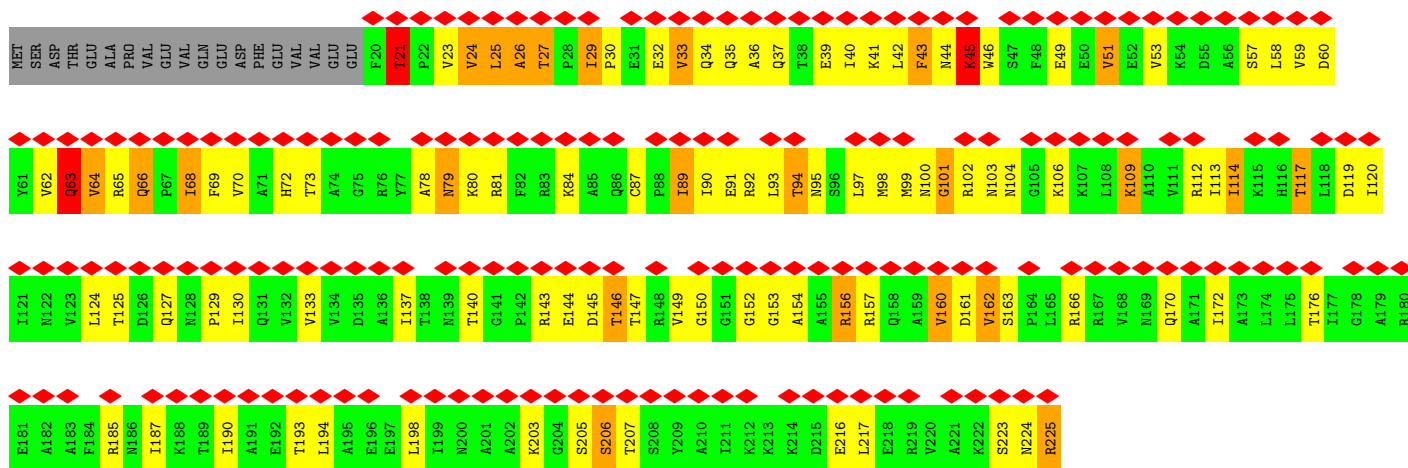
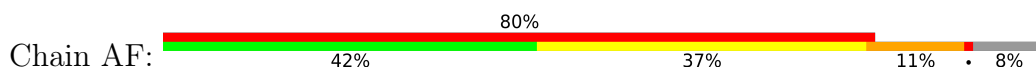


• Molecule 13: 40S RIBOSOMAL PROTEIN S4-A

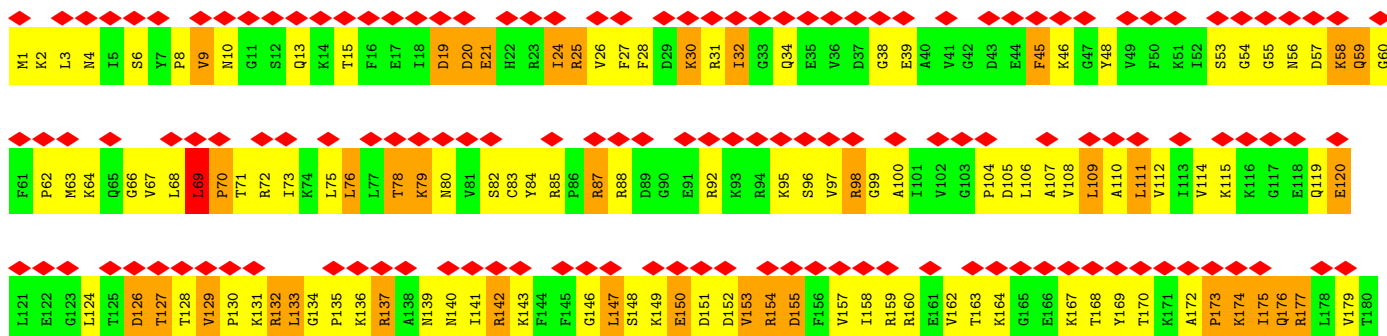
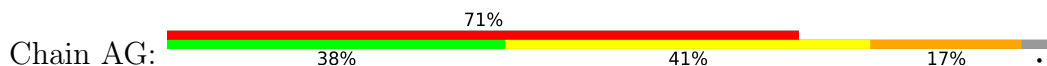




• Molecule 14: 40S RIBOSOMAL PROTEIN S5

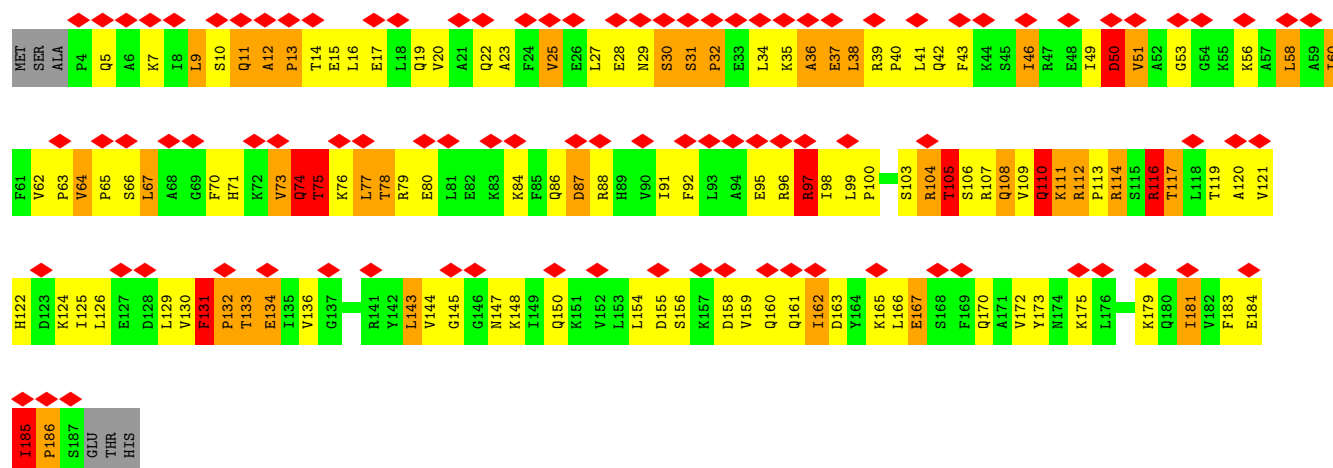


• Molecule 15: 40S RIBOSOMAL PROTEIN S6-A

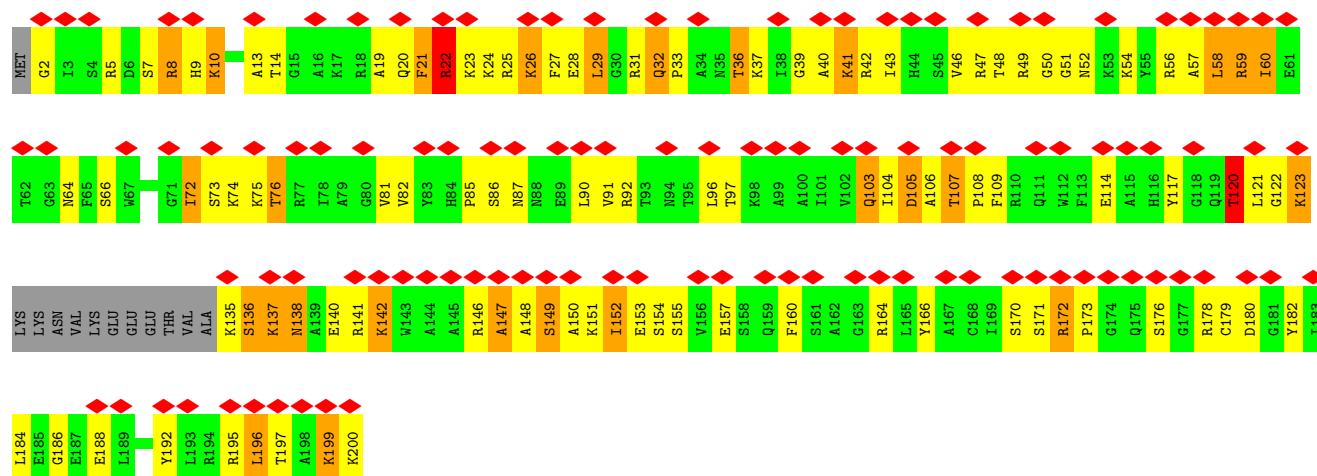




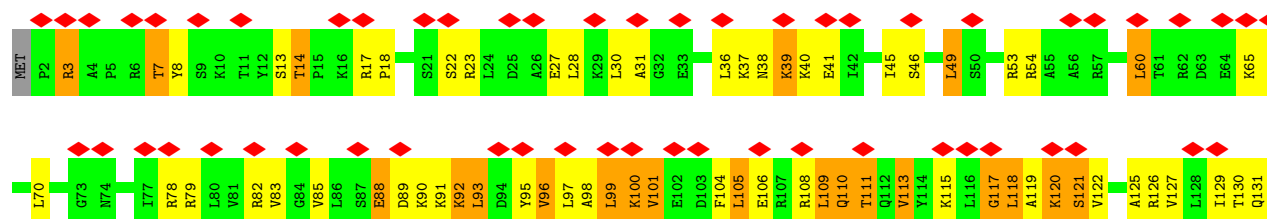
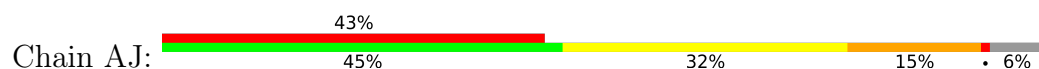
• Molecule 16: 40S RIBOSOMAL PROTEIN S7-A

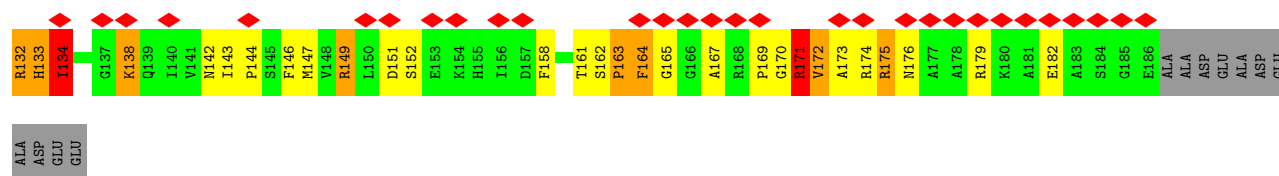


• Molecule 17: 40S RIBOSOMAL PROTEIN S8-A

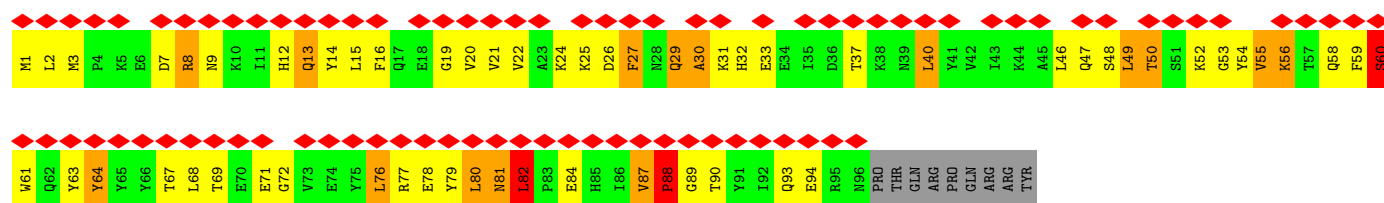
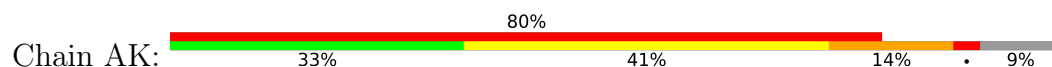


• Molecule 18: 40S RIBOSOMAL PROTEIN S9-A

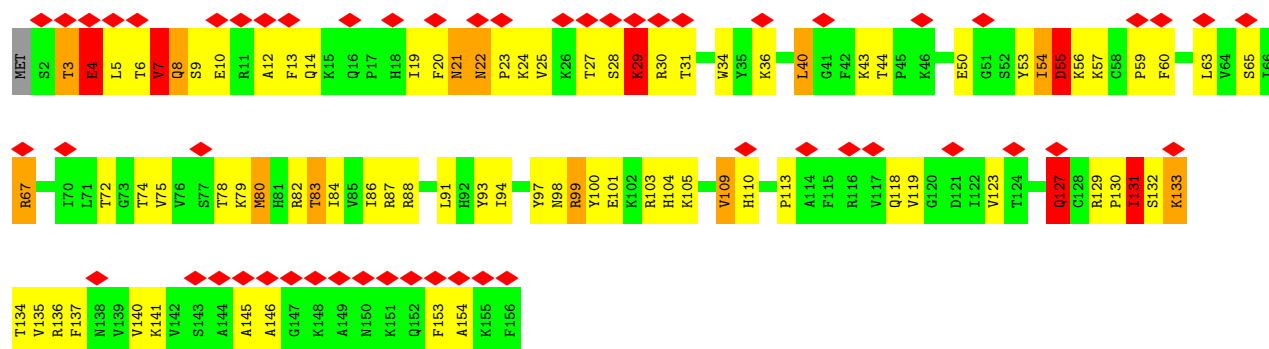




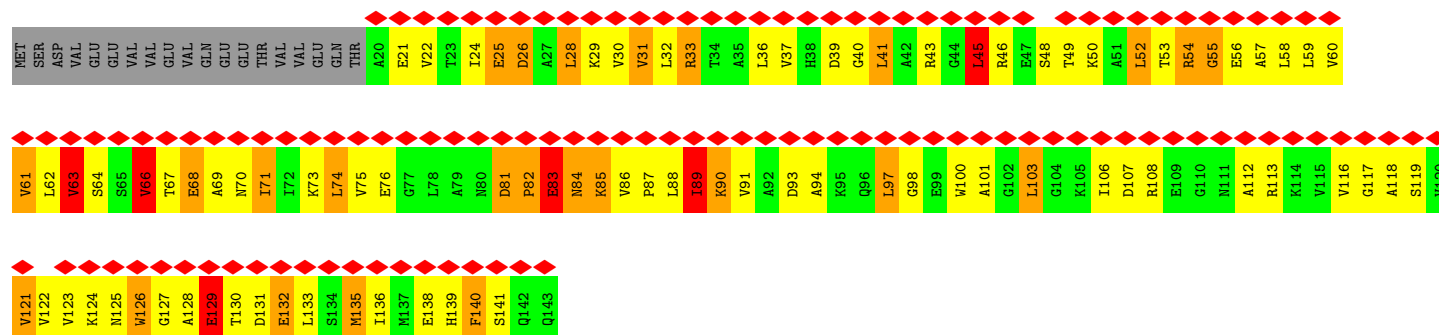
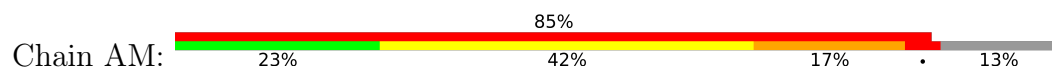
• Molecule 19: 40S RIBOSOMAL PROTEIN S10-A



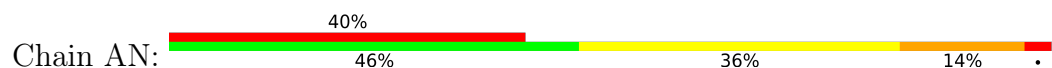
• Molecule 20: 40S RIBOSOMAL PROTEIN S11-A

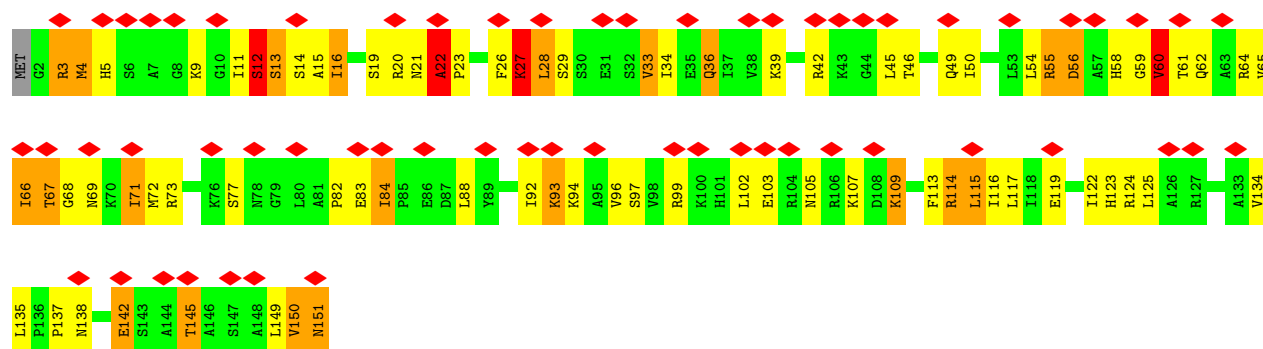


• Molecule 21: 40S RIBOSOMAL PROTEIN S12

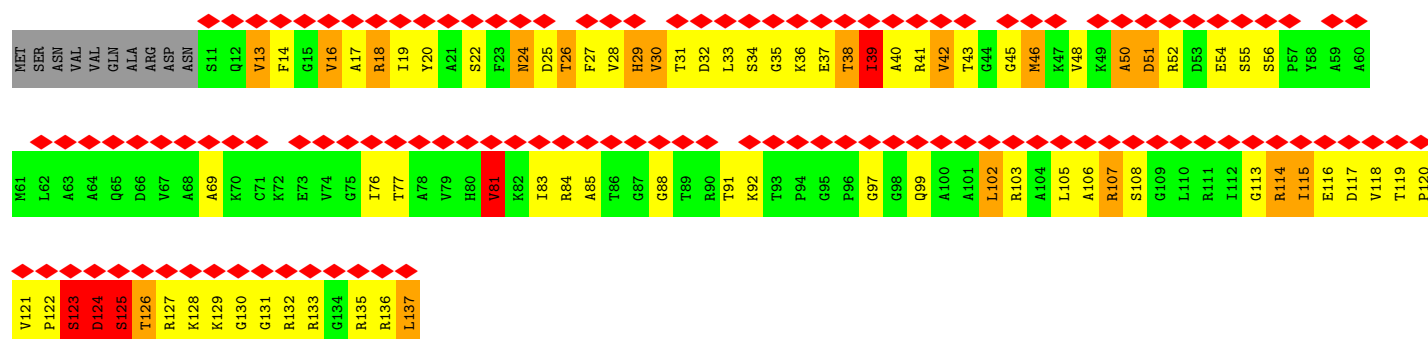
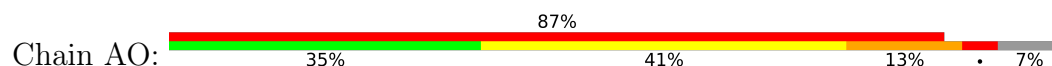


• Molecule 22: 40S RIBOSOMAL PROTEIN S13

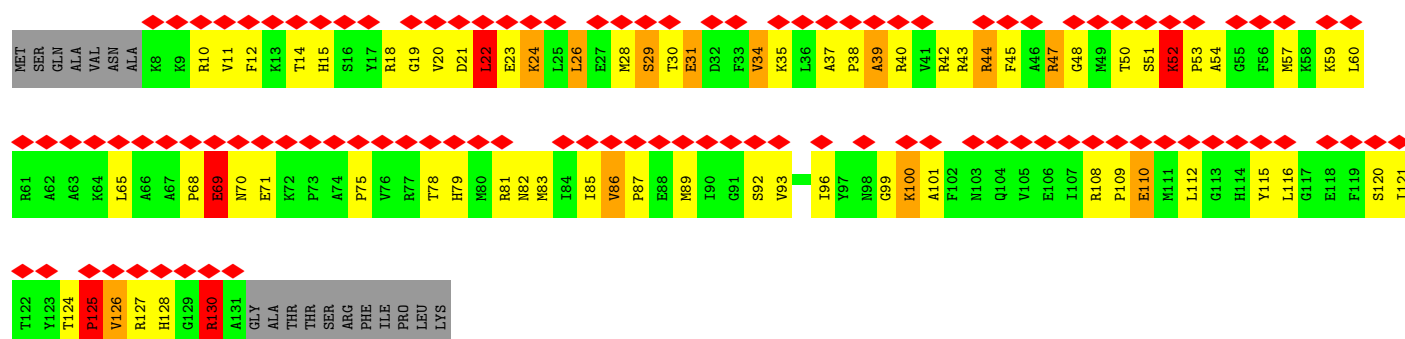
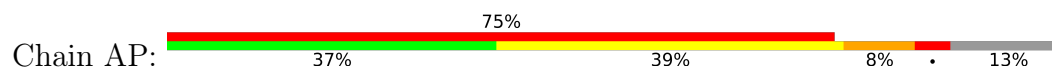




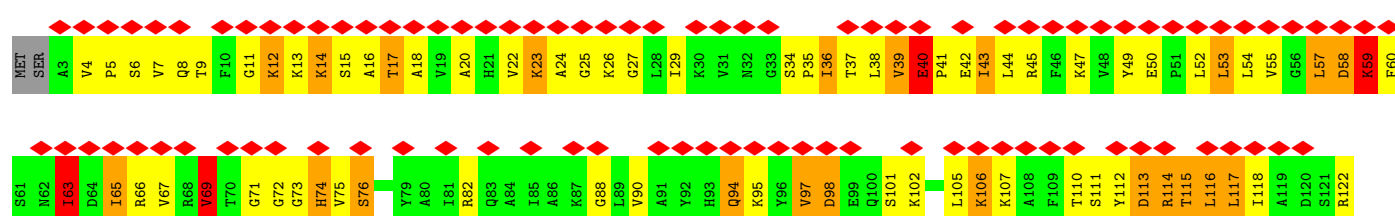
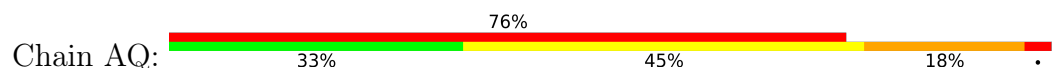
• Molecule 23: 40S RIBOSOMAL PROTEIN S14-A

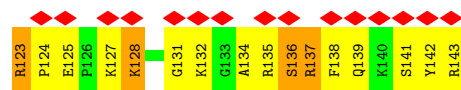


• Molecule 24: 40S RIBOSOMAL PROTEIN S15

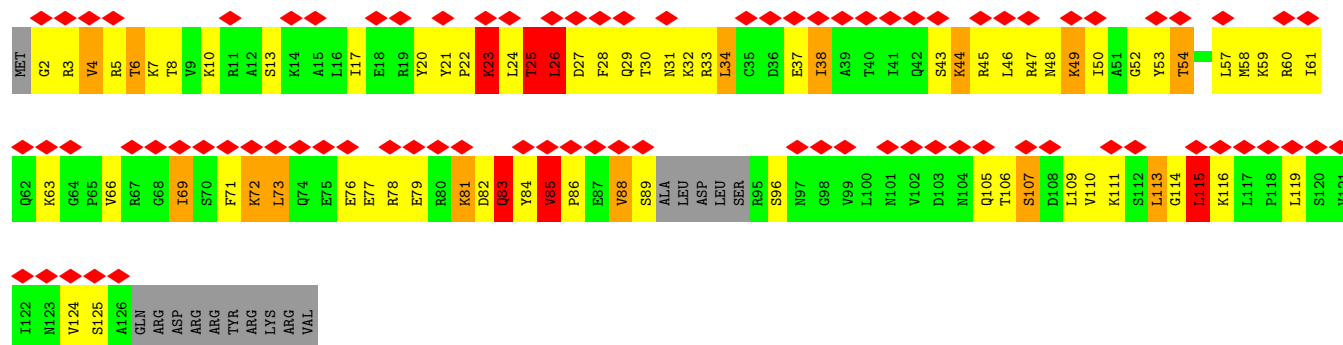


• Molecule 25: 40S RIBOSOMAL PROTEIN S16-A

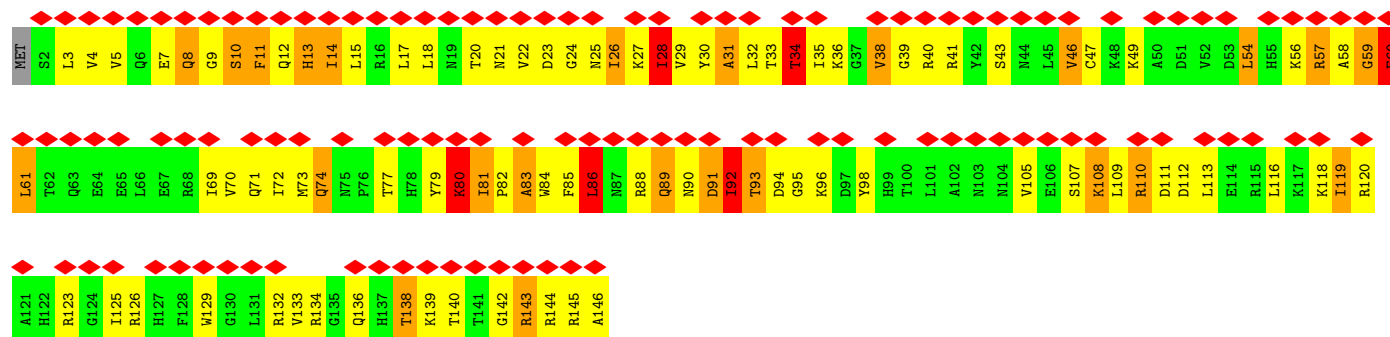
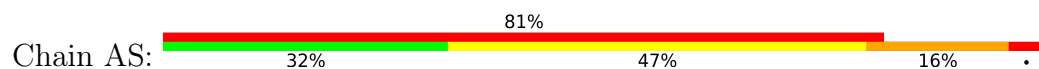




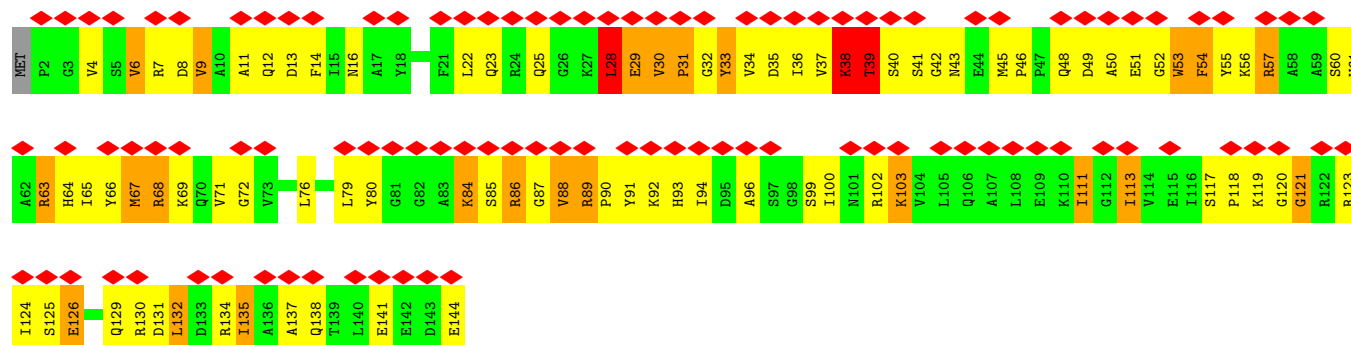
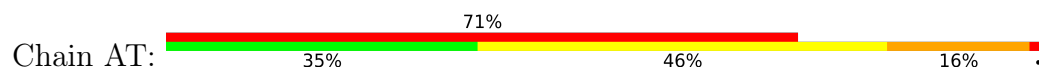
• Molecule 26: 40S RIBOSOMAL PROTEIN S17-A



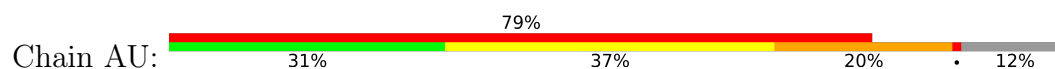
• Molecule 27: 40S RIBOSOMAL PROTEIN S18-A

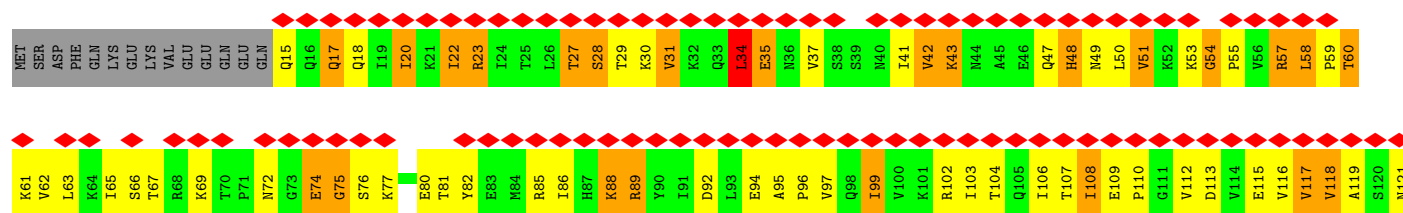


• Molecule 28: 40S RIBOSOMAL PROTEIN S19-A

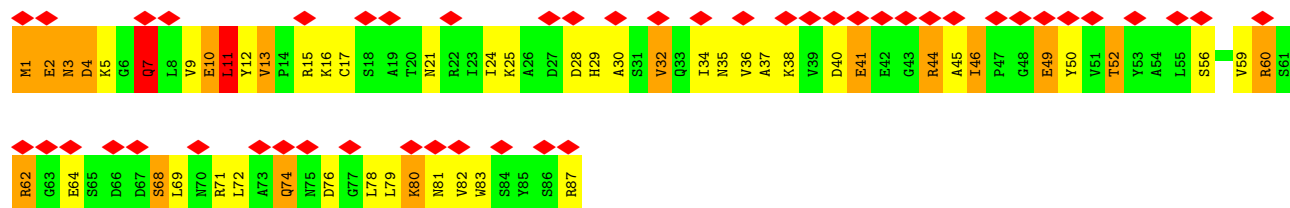


• Molecule 29: 40S RIBOSOMAL PROTEIN S20

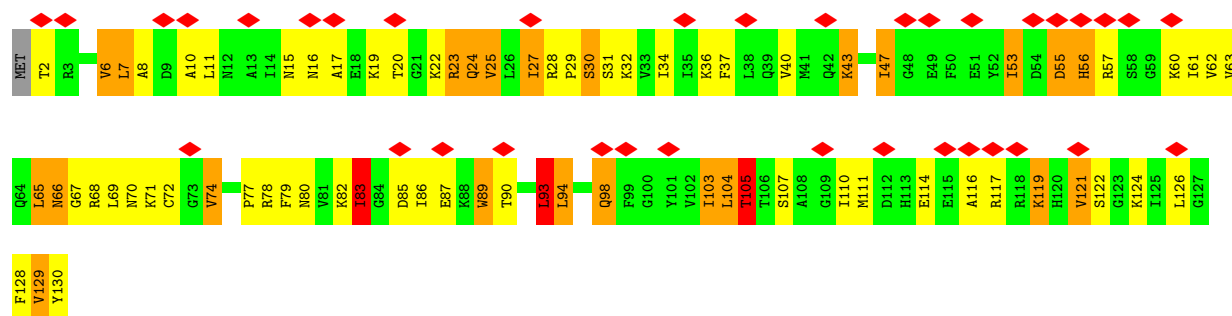
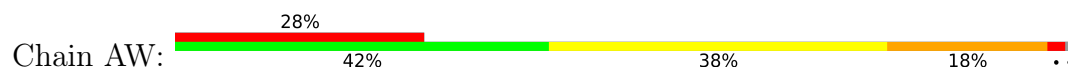




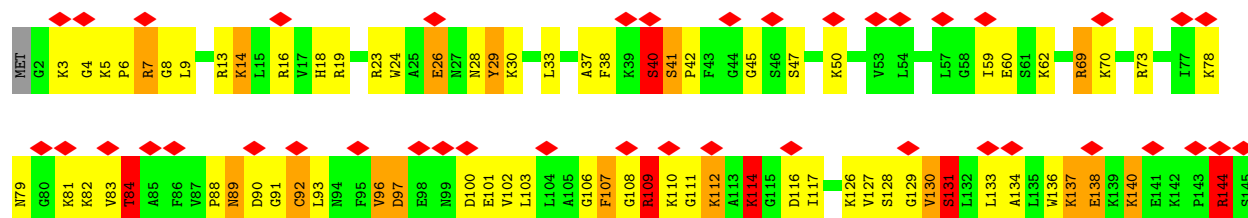
• Molecule 30: 40S RIBOSOMAL PROTEIN S21-A



• Molecule 31: 40S RIBOSOMAL PROTEIN S22-A



• Molecule 32: 40S RIBOSOMAL PROTEIN S23-A

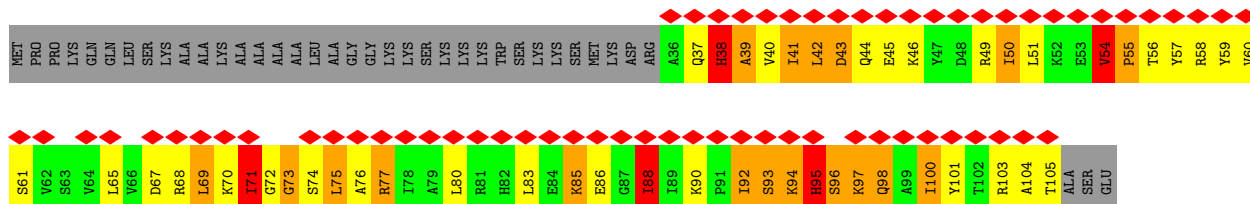


• Molecule 33: 40S RIBOSOMAL PROTEIN S24-A

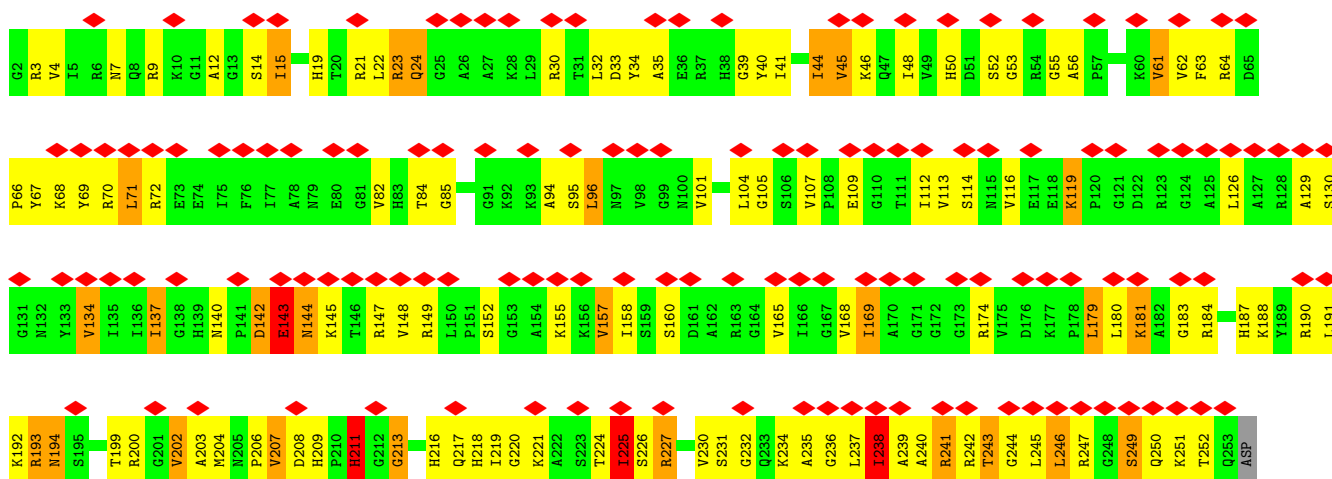




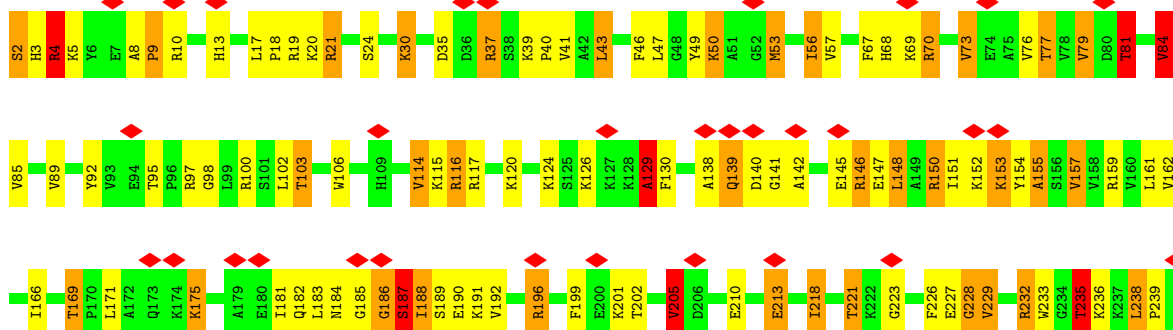
• Molecule 34: 40S RIBOSOMAL PROTEIN S25-A

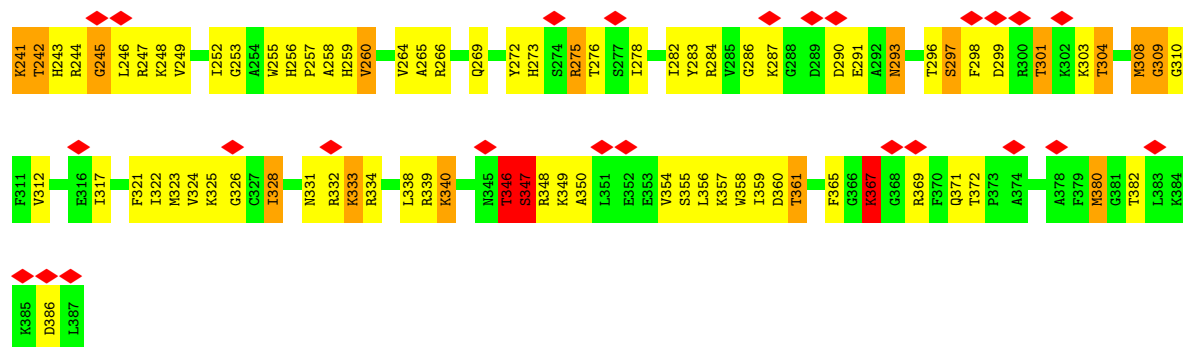


• Molecule 35: 60S RIBOSOMAL PROTEIN L2-B

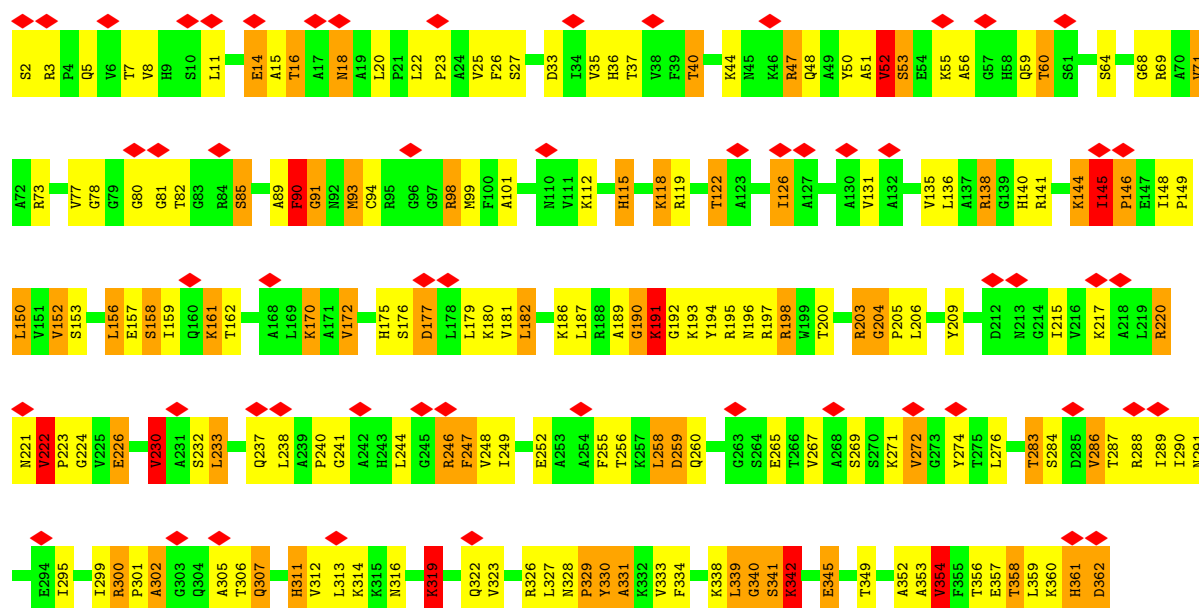


• Molecule 36: 60S RIBOSOMAL PROTEIN L3

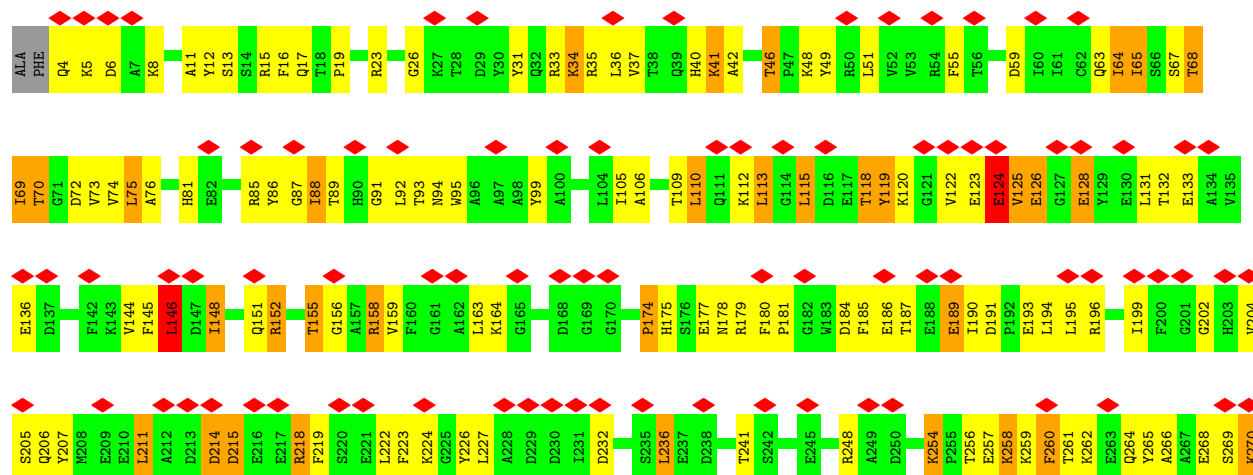


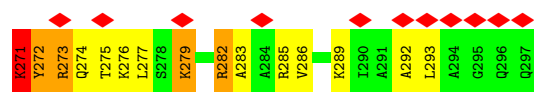


• Molecule 37: 60S RIBOSOMAL PROTEIN L4-A

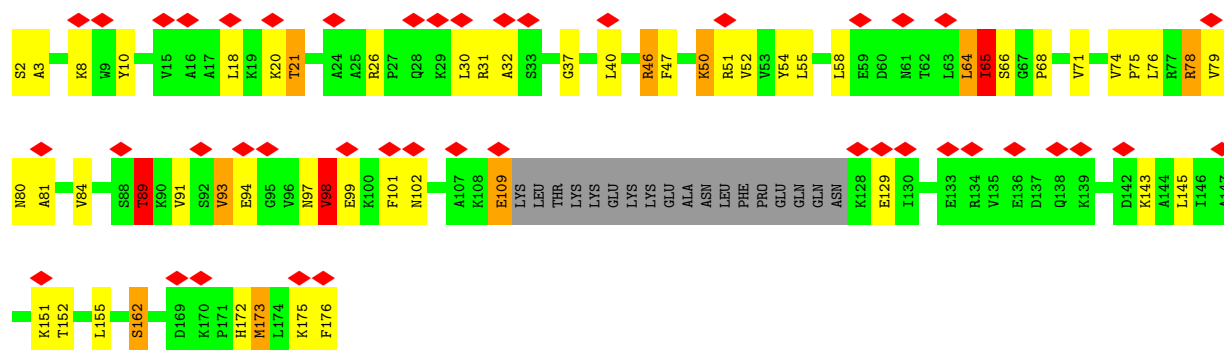


• Molecule 38: 60S RIBOSOMAL PROTEIN L5

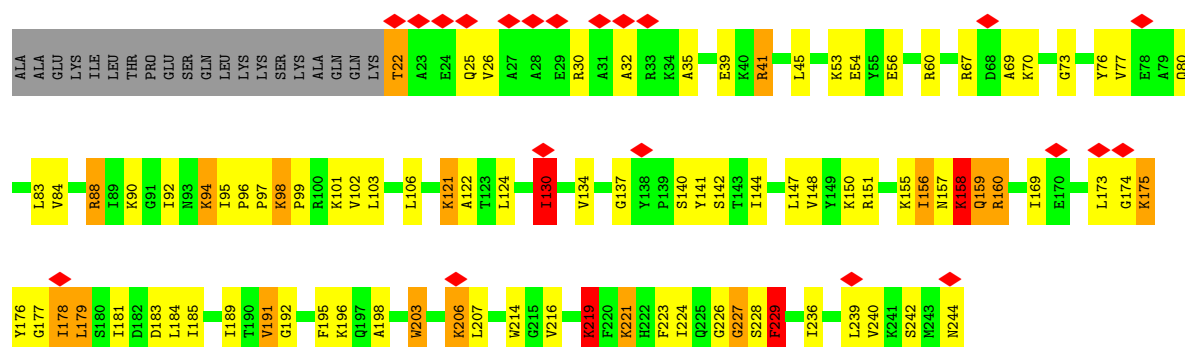




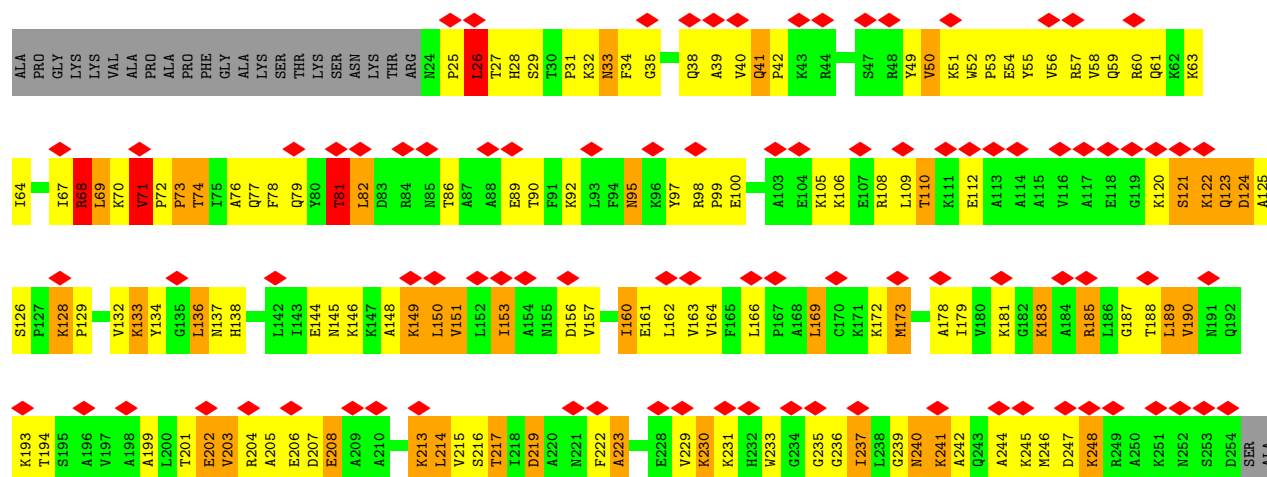
• Molecule 39: 60S RIBOSOMAL PROTEIN L6-A



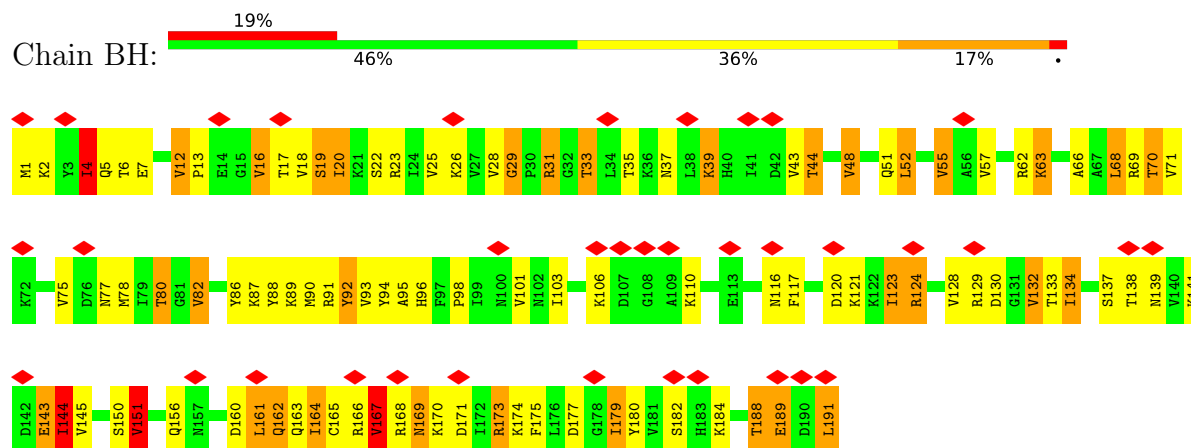
• Molecule 40: 60S RIBOSOMAL PROTEIN L7-A



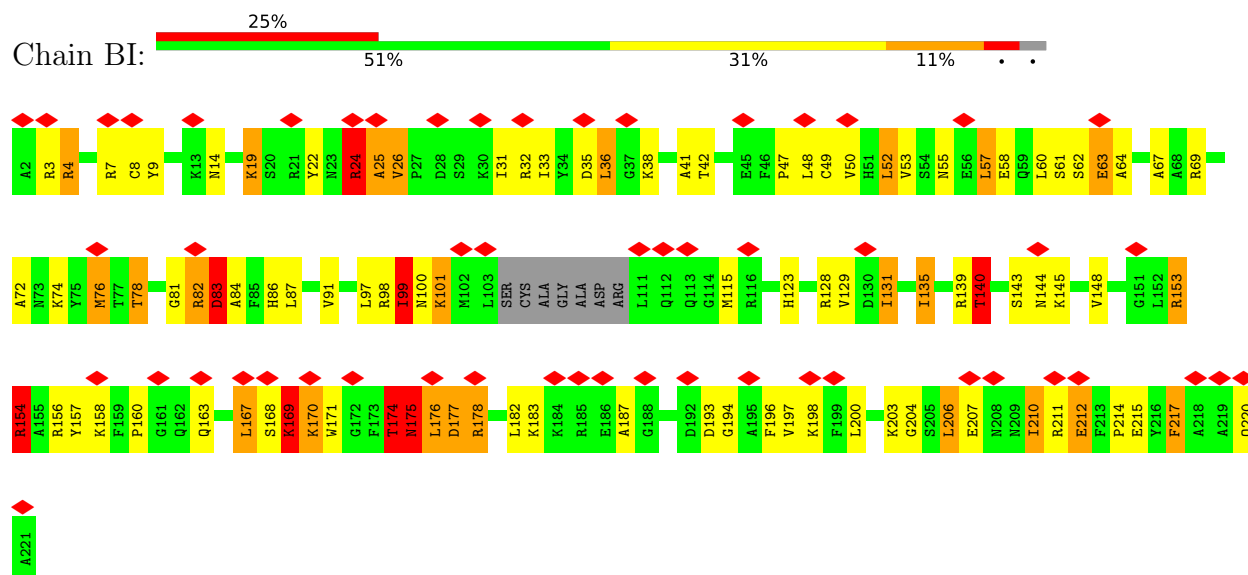
• Molecule 41: 60S RIBOSOMAL PROTEIN L8-A



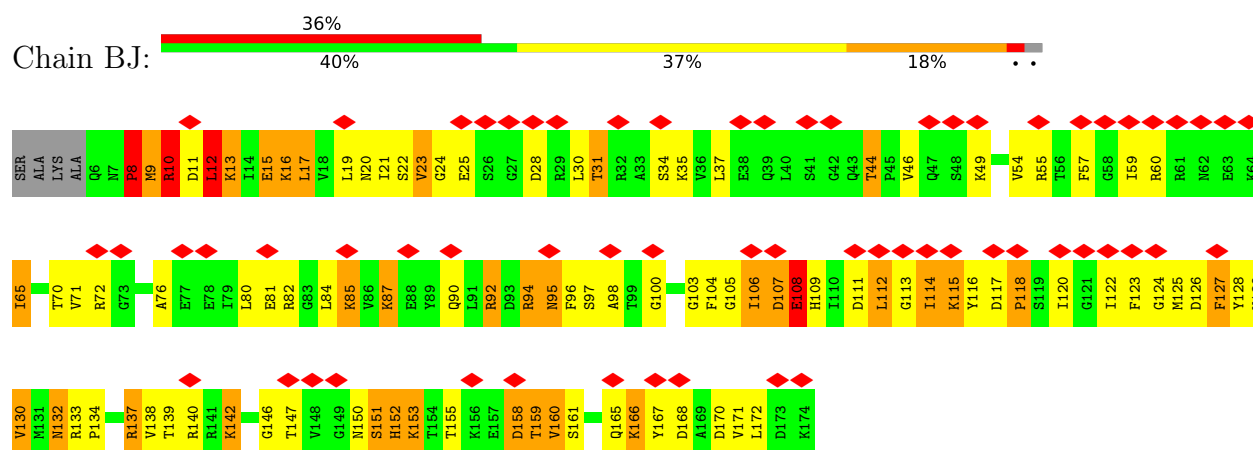
- Molecule 42: 60S RIBOSOMAL PROTEIN L9-A



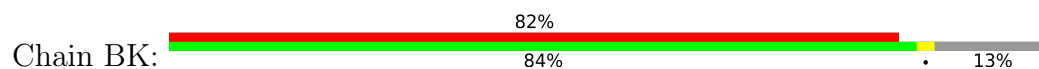
- Molecule 43: 60S RIBOSOMAL PROTEIN L10

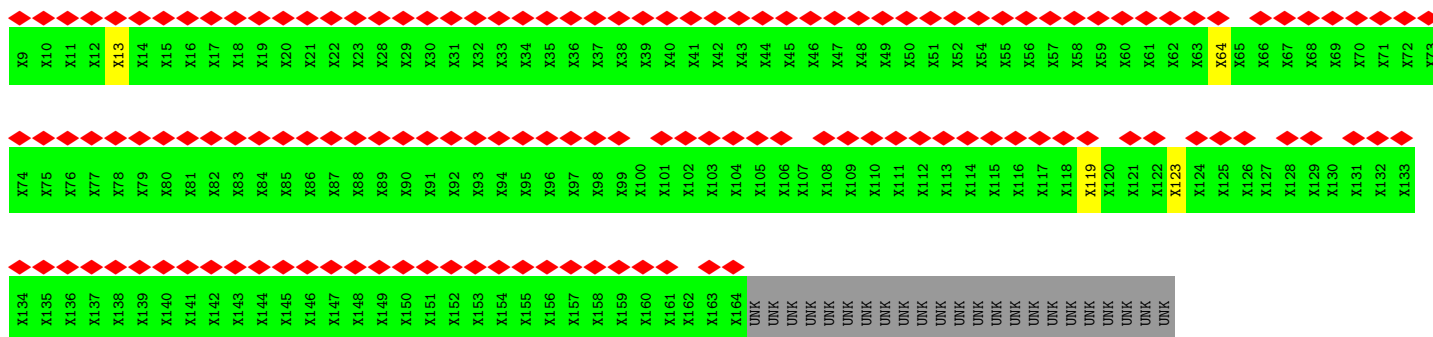


- Molecule 44: 60S RIBOSOMAL PROTEIN L11-A

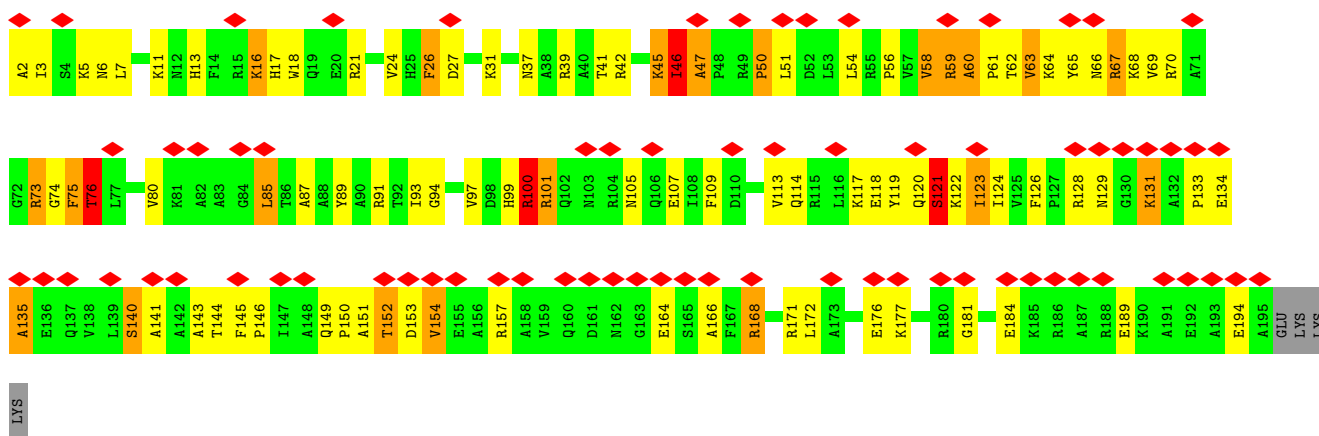
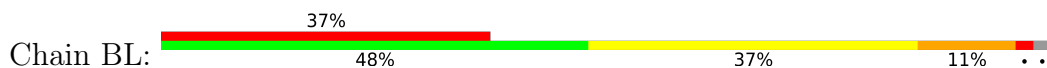


- Molecule 45: 60S RIBOSOMAL PROTEIN L11-A

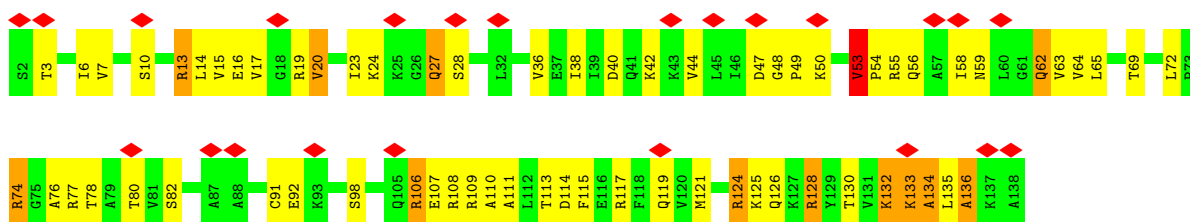




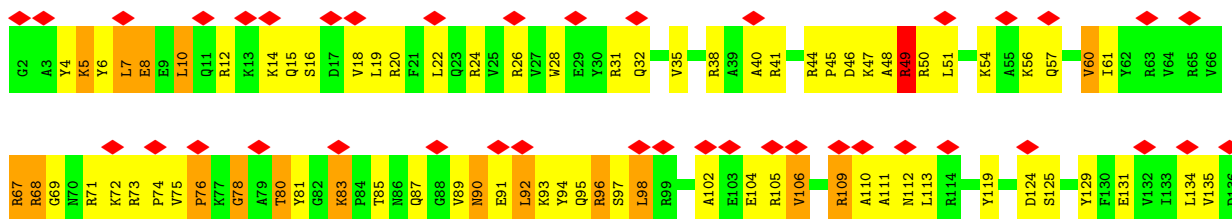
• Molecule 46: 60S RIBOSOMAL PROTEIN L13-A

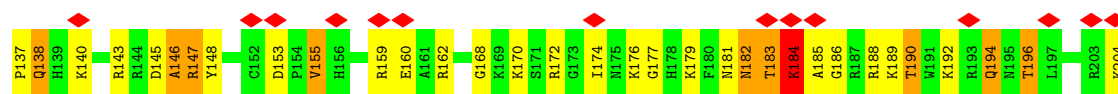


• Molecule 47: 60S RIBOSOMAL PROTEIN L14-B

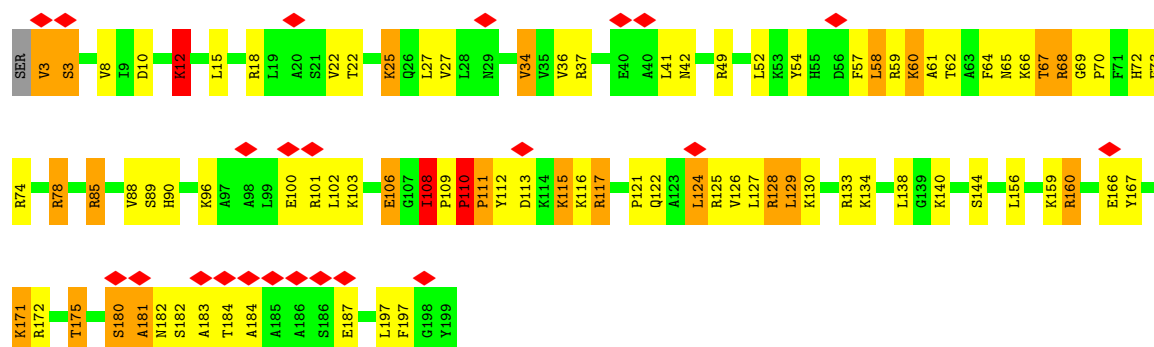


• Molecule 48: 60S RIBOSOMAL PROTEIN L15-A

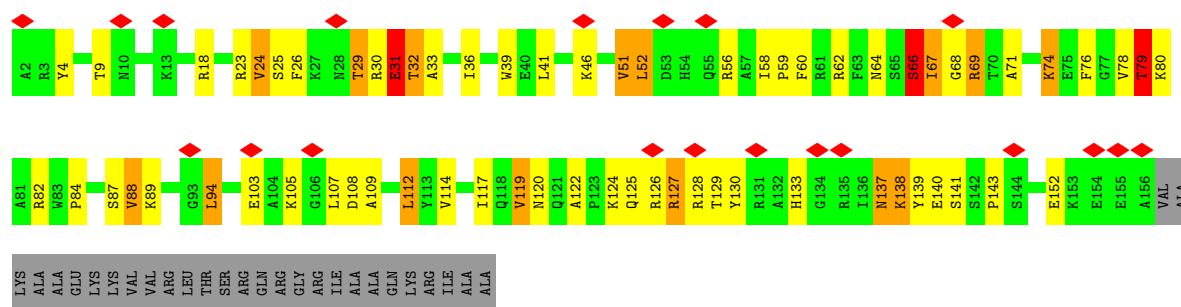




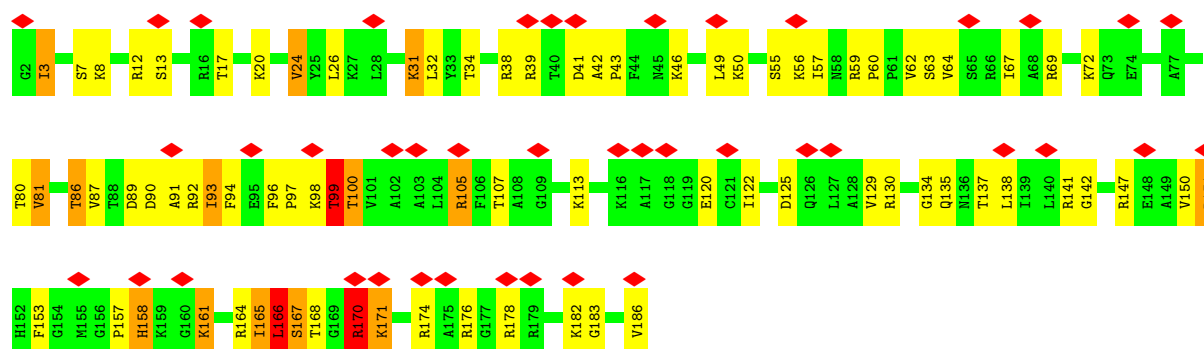
• Molecule 49: 60S RIBOSOMAL PROTEIN L16-A



• Molecule 50: 60S RIBOSOMAL PROTEIN L17-A

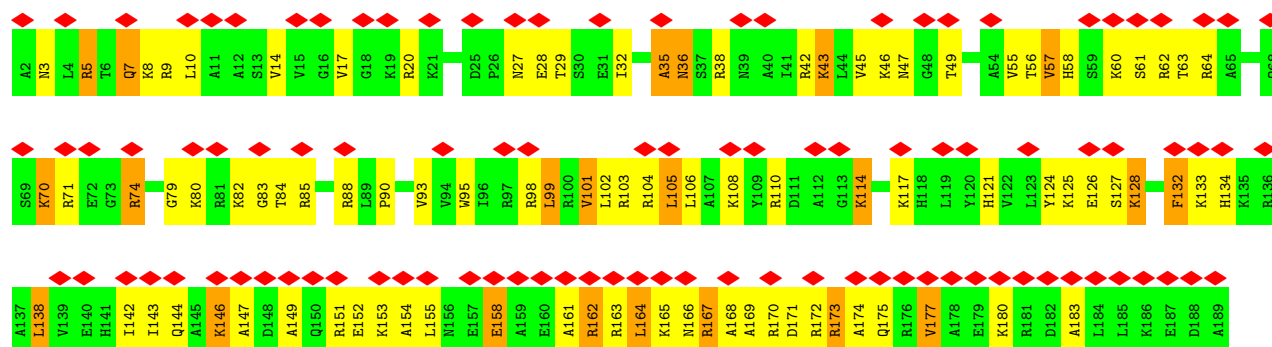


• Molecule 51: 60S RIBOSOMAL PROTEIN L18-A

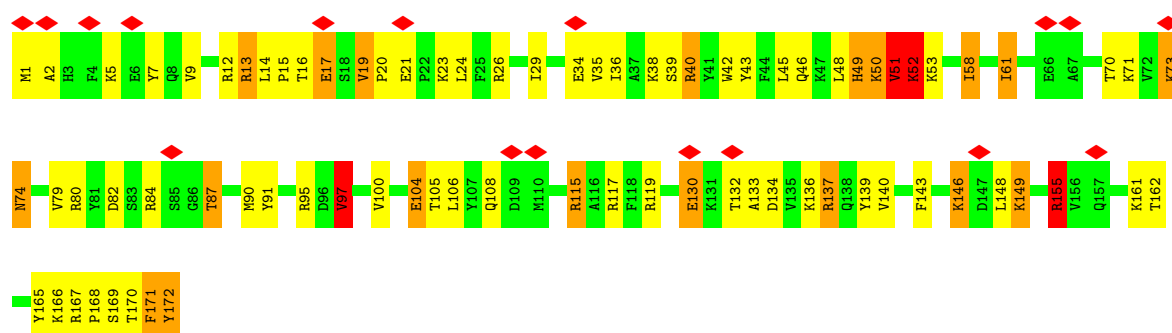


• Molecule 52: 60S RIBOSOMAL PROTEIN L19-B

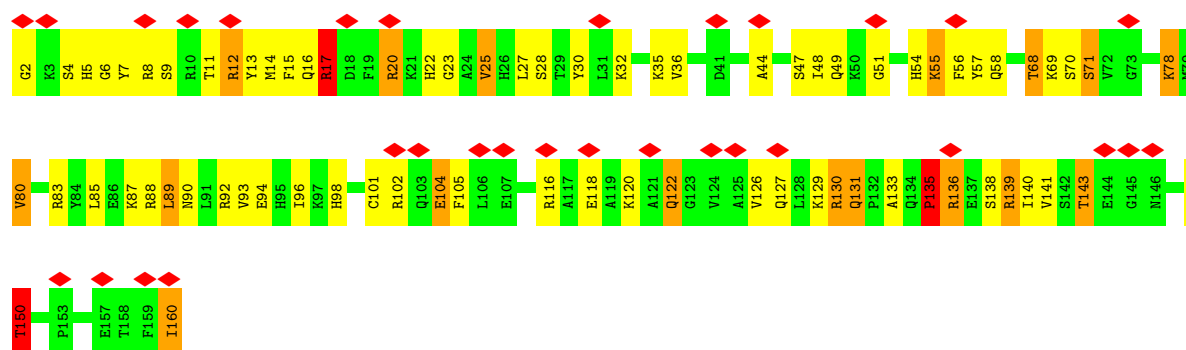




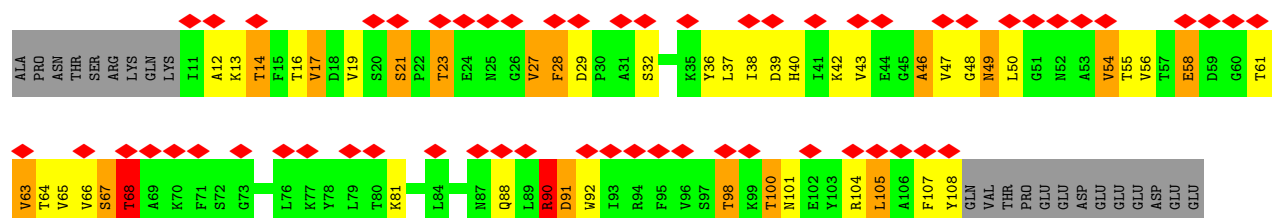
• Molecule 53: 60S RIBOSOMAL PROTEIN L20-B



• Molecule 54: 60S RIBOSOMAL PROTEIN L21-A

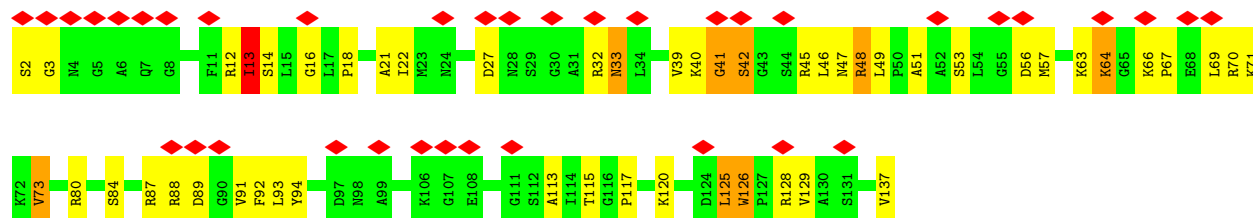


• Molecule 55: 60S RIBOSOMAL PROTEIN L22-A



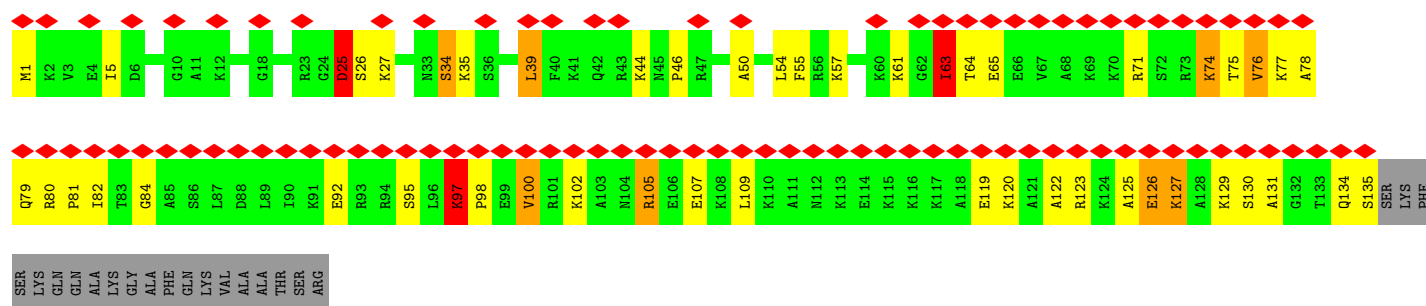
- Molecule 56: 60S RIBOSOMAL PROTEIN L23-A

Chain BV: 

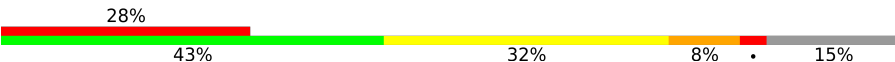


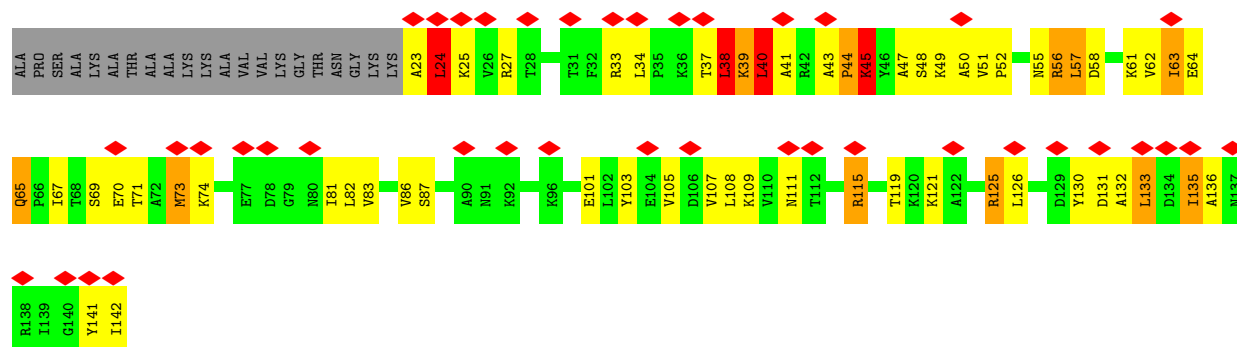
- Molecule 57: 60S RIBOSOMAL PROTEIN L24-A

Chain BW: 



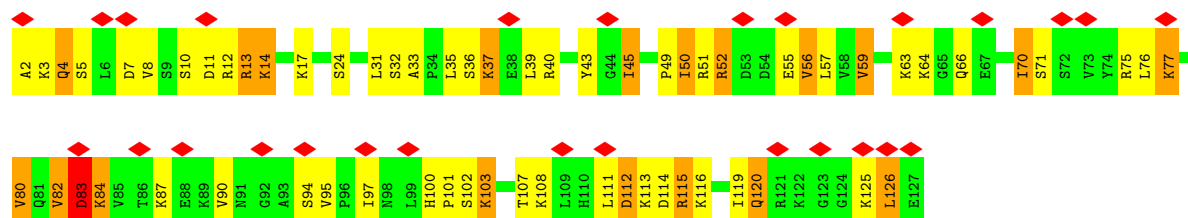
- Molecule 58: 60S RIBOSOMAL PROTEIN L25

Chain BX: 

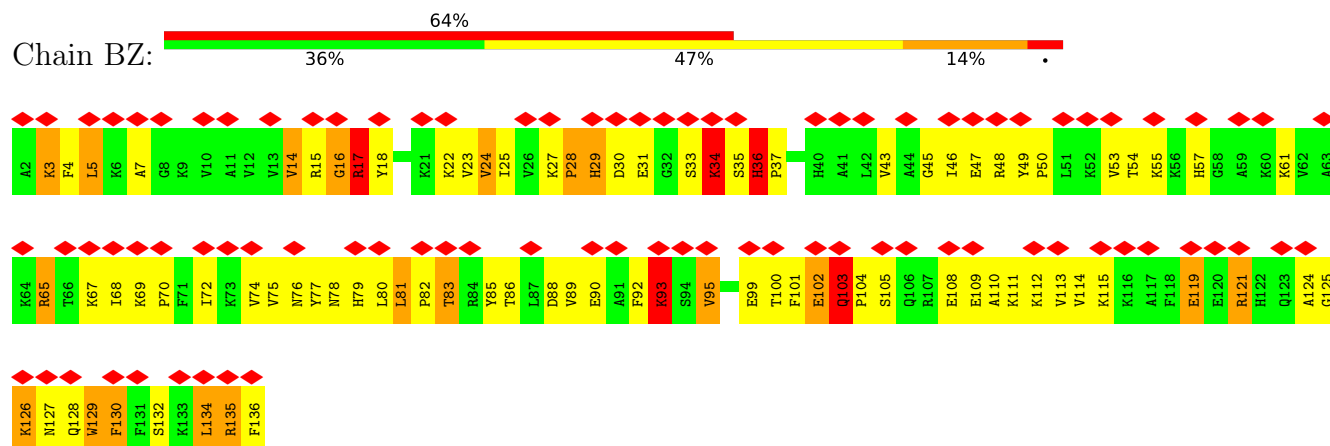


- Molecule 59: 60S RIBOSOMAL PROTEIN L26-A

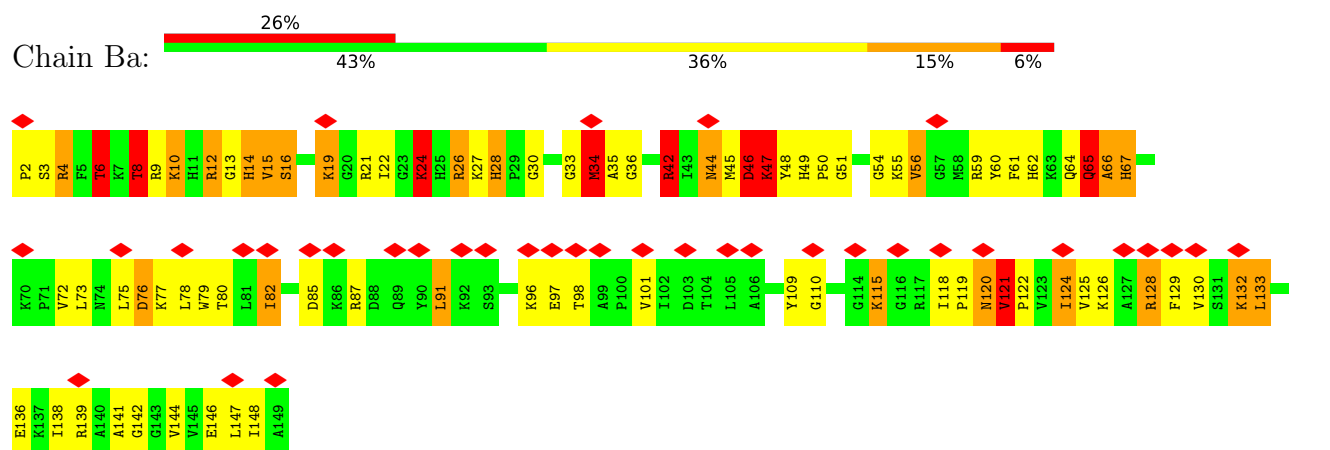
Chain BY: 



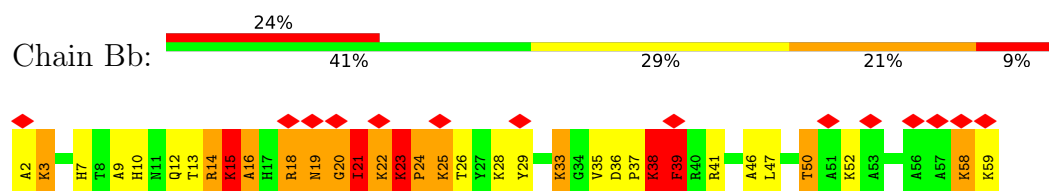
- Molecule 60: 60S RIBOSOMAL PROTEIN L27-A



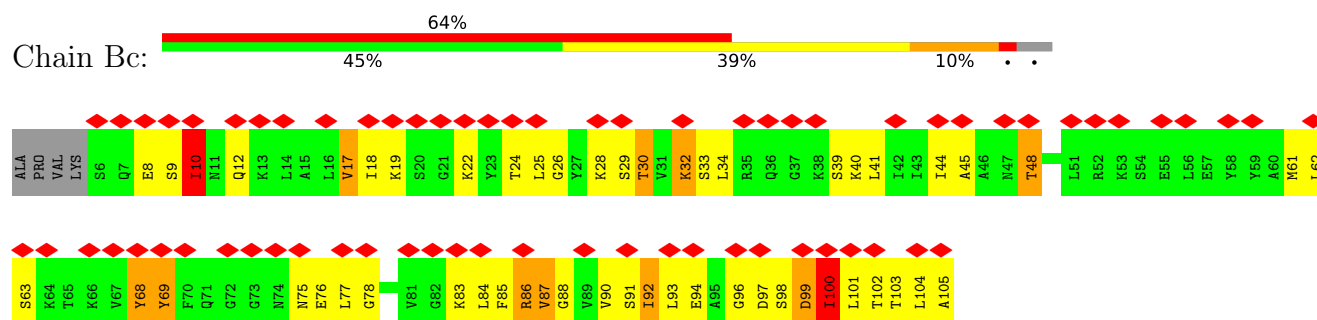
- Molecule 61: 60S RIBOSOMAL PROTEIN L28



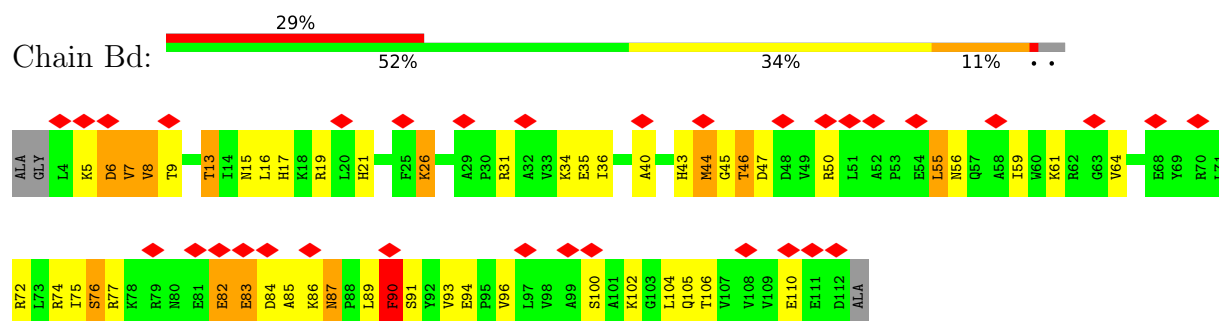
- Molecule 62: 60S RIBOSOMAL PROTEIN L29



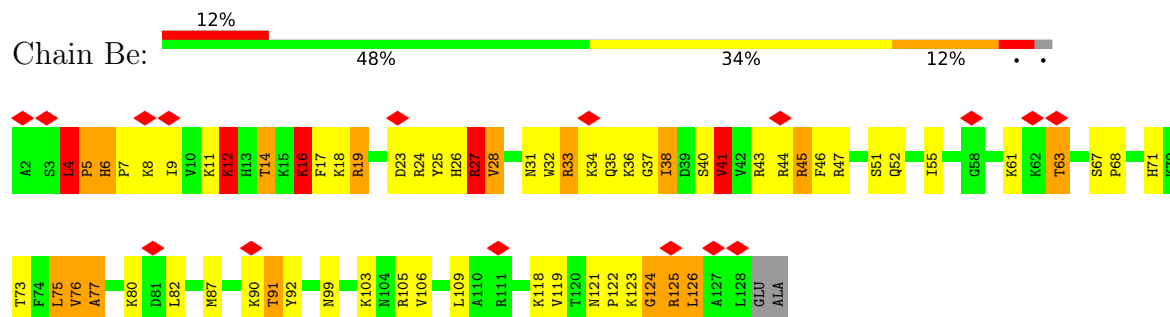
- Molecule 63: 60S RIBOSOMAL PROTEIN L30



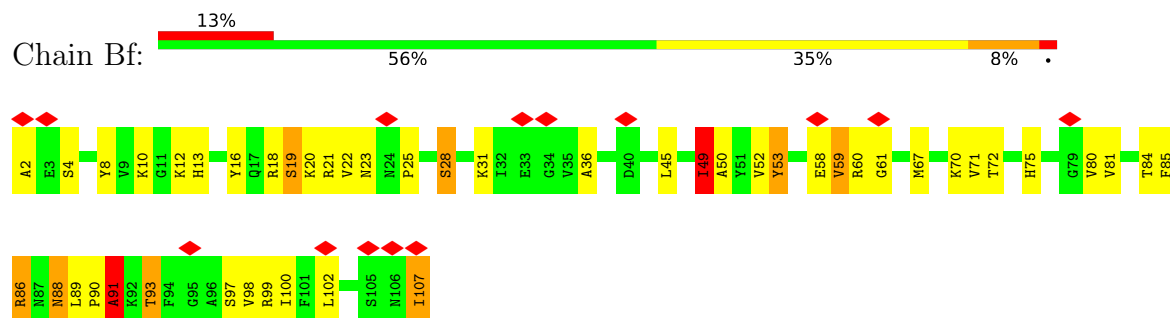
- Molecule 64: 60S RIBOSOMAL PROTEIN L31-A



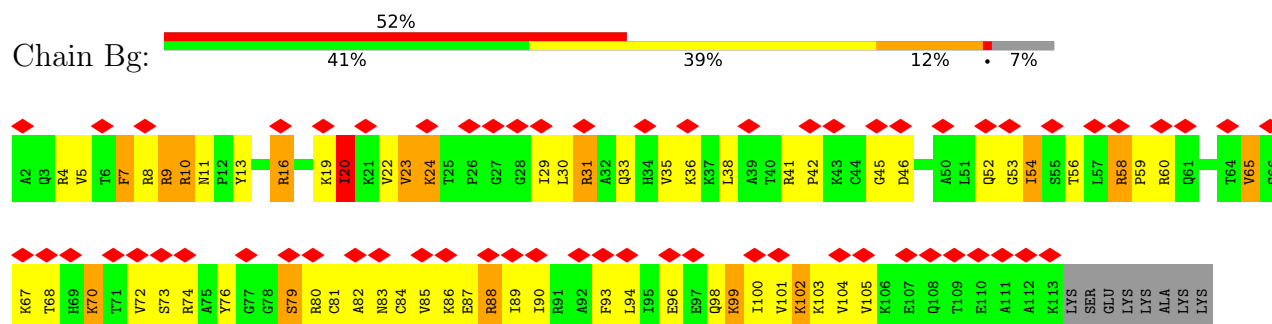
• Molecule 65: 60S RIBOSOMAL PROTEIN L32



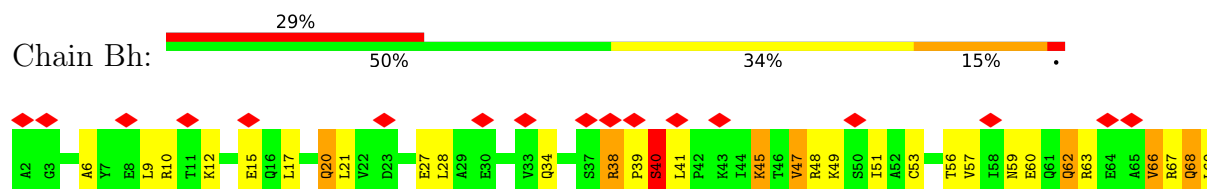
• Molecule 66: 60S RIBOSOMAL PROTEIN L33-A

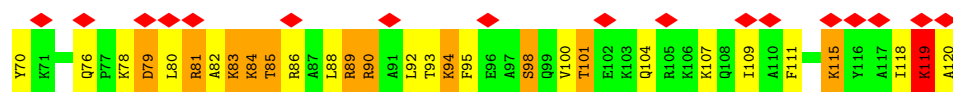


• Molecule 67: 60S RIBOSOMAL PROTEIN L34-A

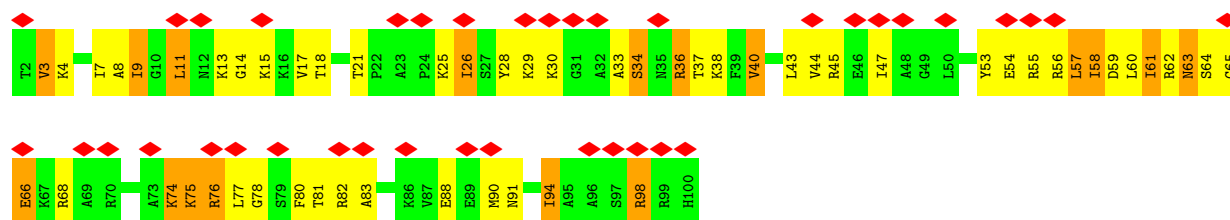
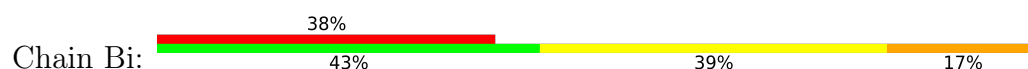


• Molecule 68: 60S RIBOSOMAL PROTEIN L35-B

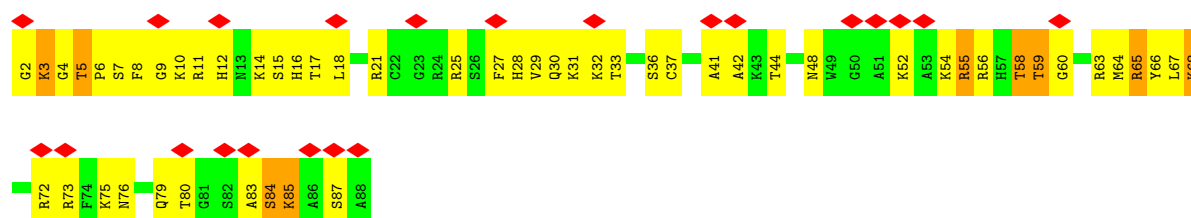




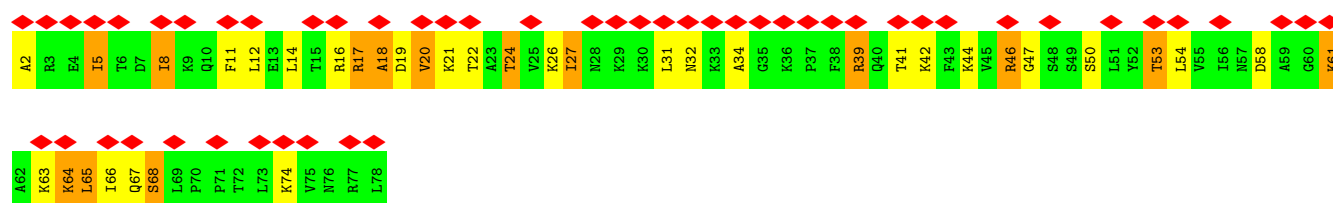
• Molecule 69: 60S RIBOSOMAL PROTEIN L36-A



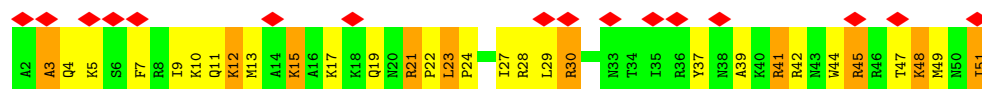
• Molecule 70: 60S RIBOSOMAL PROTEIN L37-A



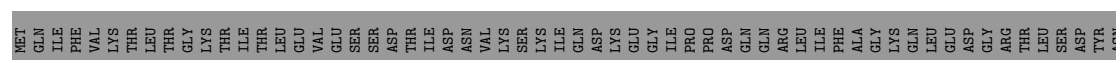
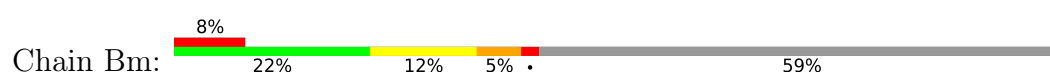
• Molecule 71: 60S RIBOSOMAL PROTEIN L38

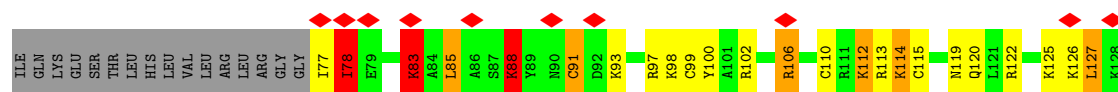


• Molecule 72: 60S RIBOSOMAL PROTEIN L39

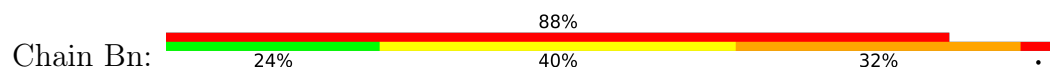


• Molecule 73: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

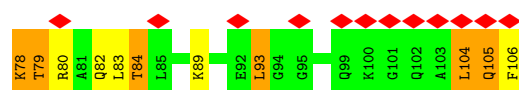
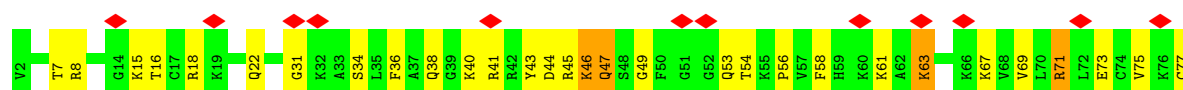




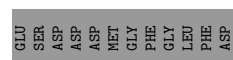
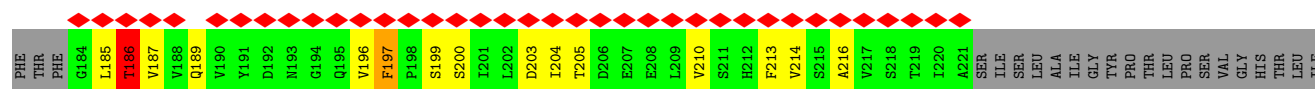
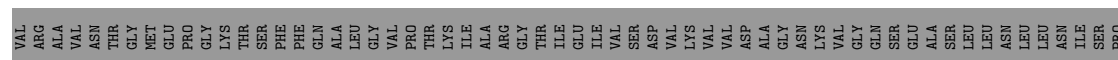
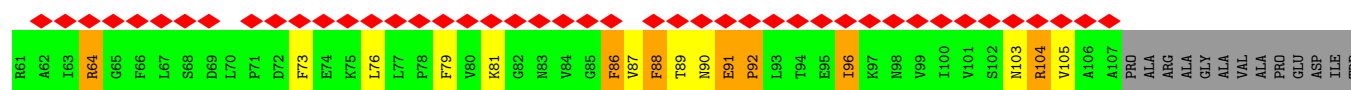
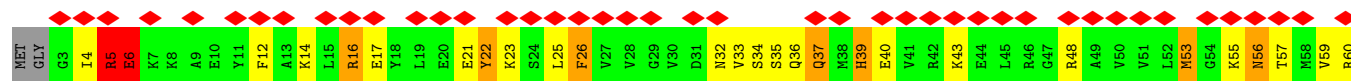
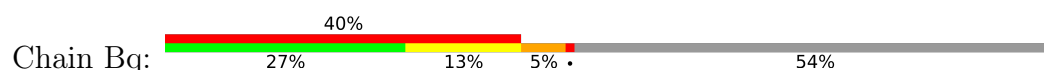
- Molecule 74: 60S RIBOSOMAL PROTEIN L41-B



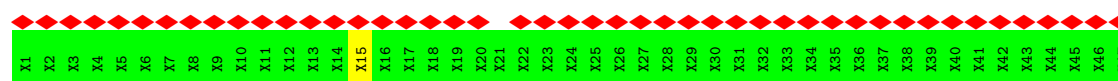
- Molecule 75: 60S RIBOSOMAL PROTEIN L42-A



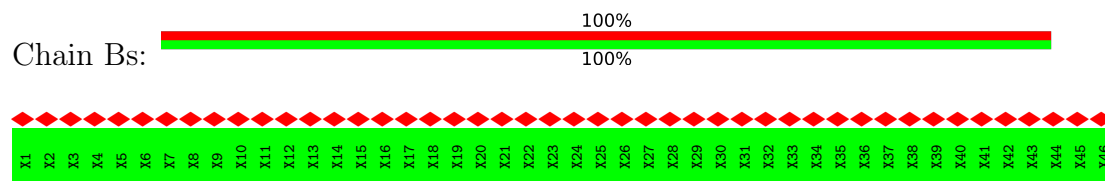
- Molecule 76: 60S ACIDIC RIBOSOMAL PROTEIN P0



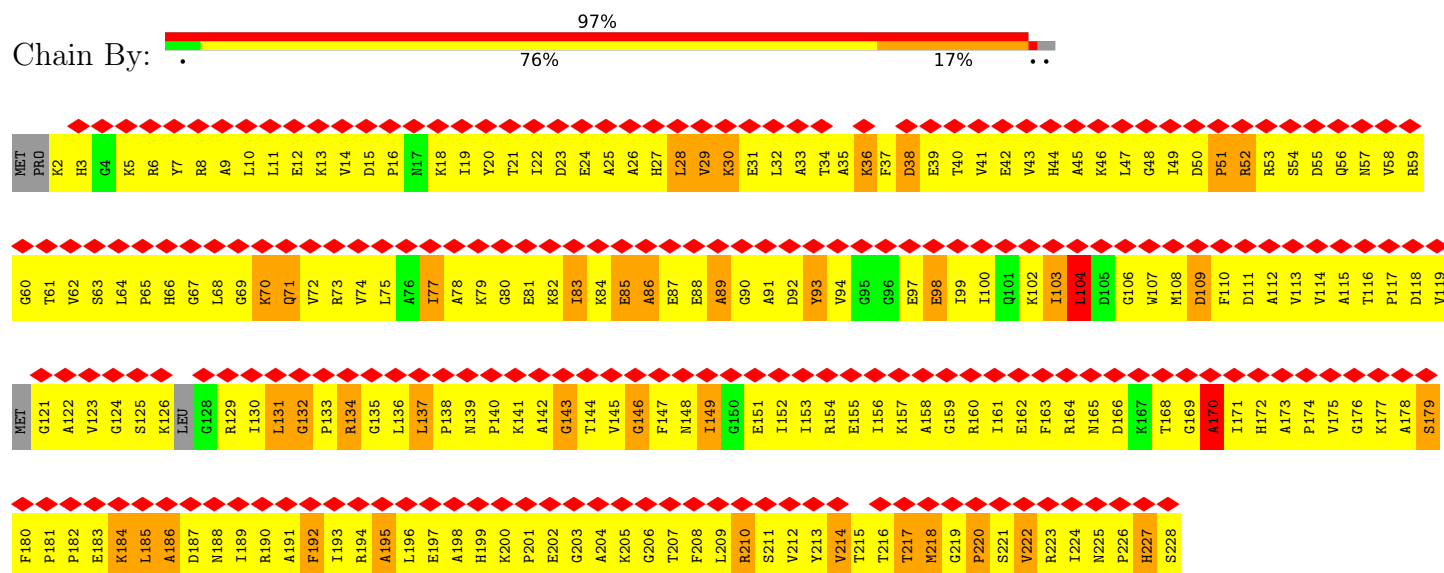
- Molecule 77: 60S ACIDIC RIBOSOMAL PROTEIN P1



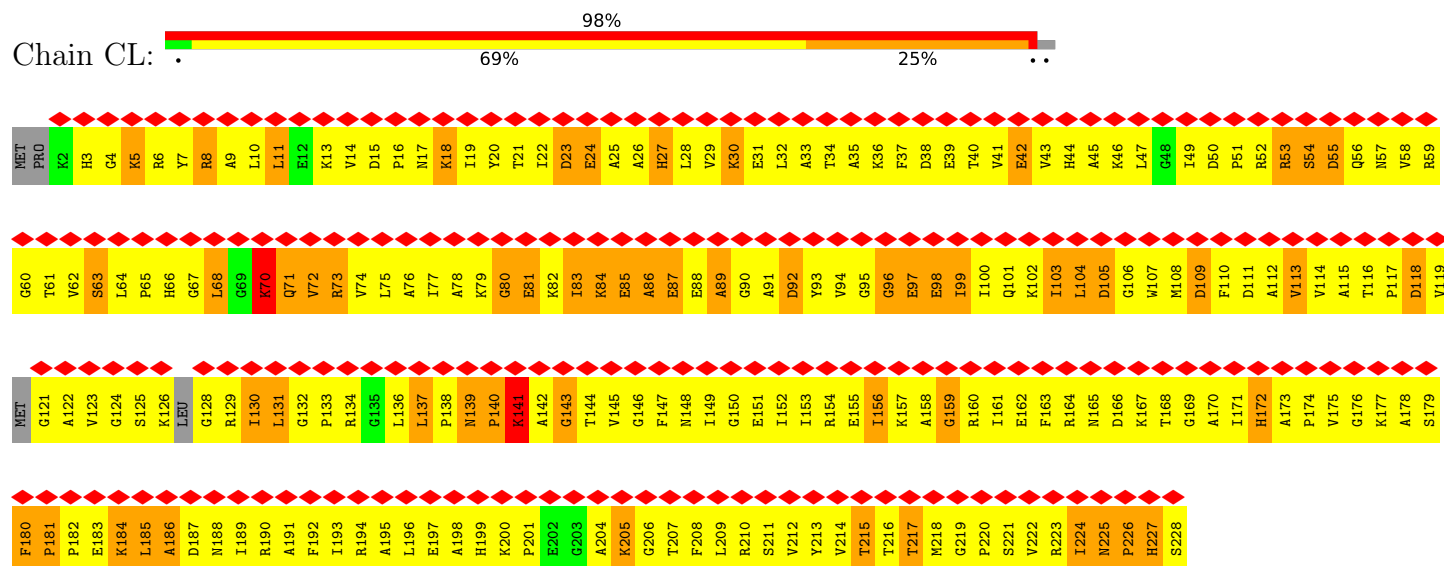
• Molecule 78: 60S ACIDIC RIBOSOMAL PROTEIN P2



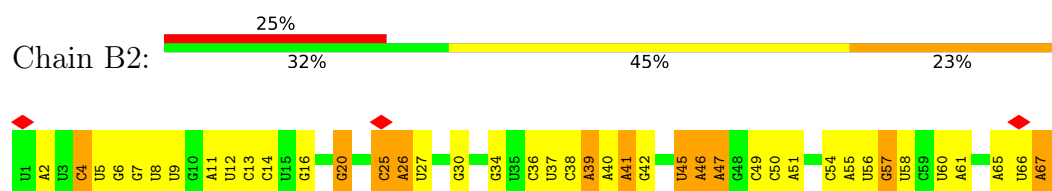
• Molecule 79: 50S RIBOSOMAL PROTEIN L1

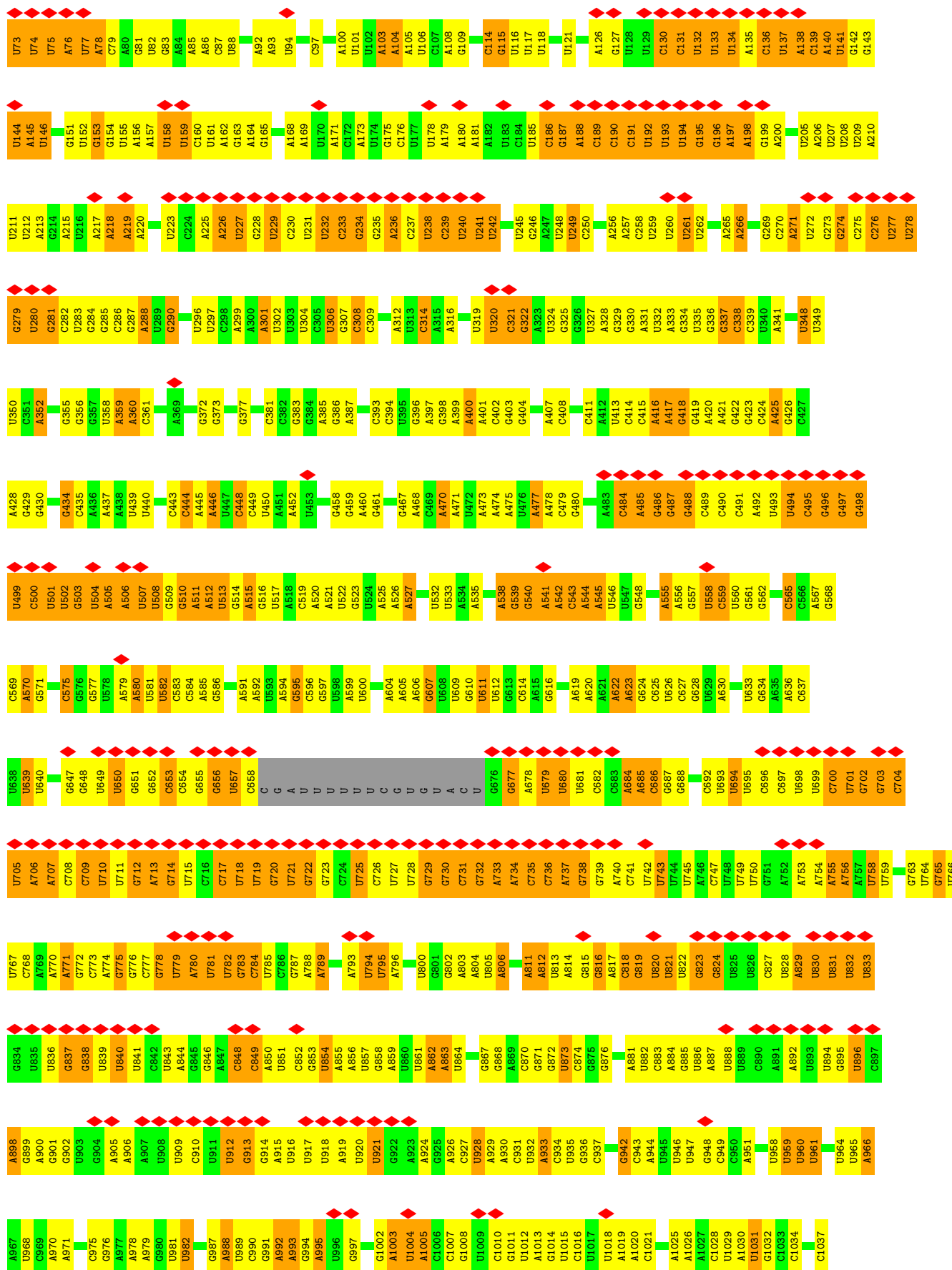


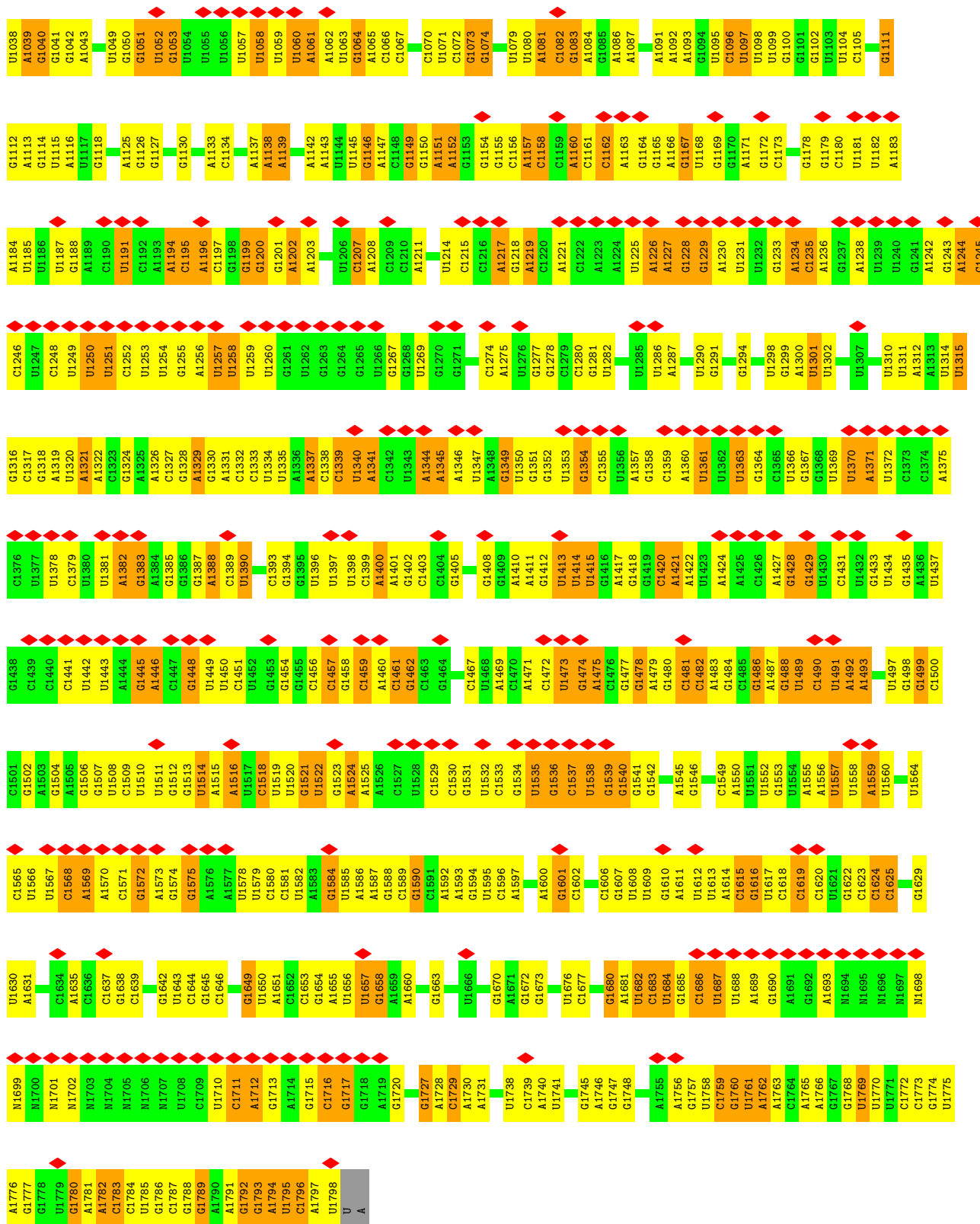
• Molecule 79: 50S RIBOSOMAL PROTEIN L1



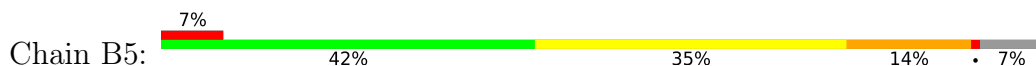
• Molecule 80: 18S RIBOSOMAL RNA

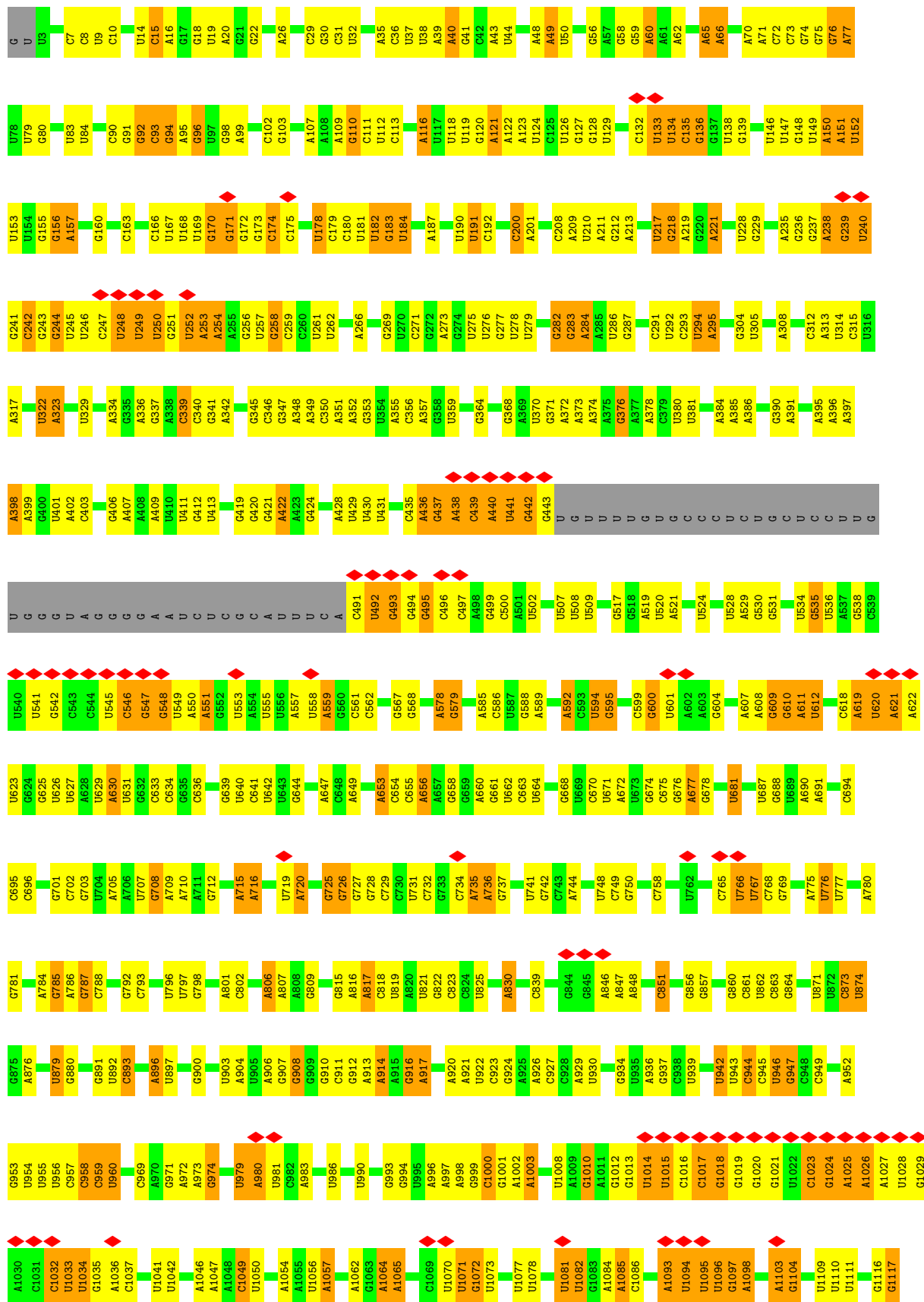




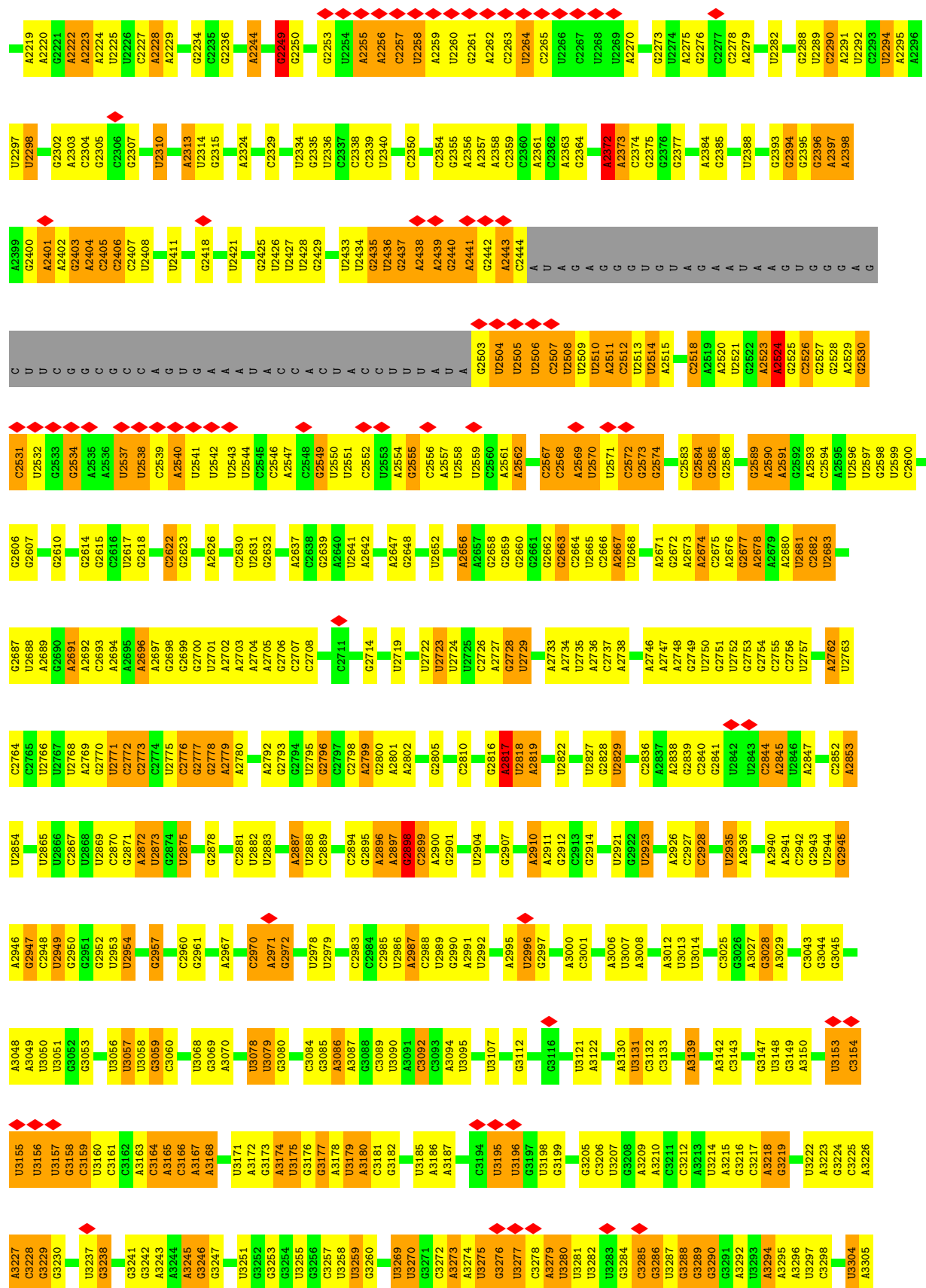


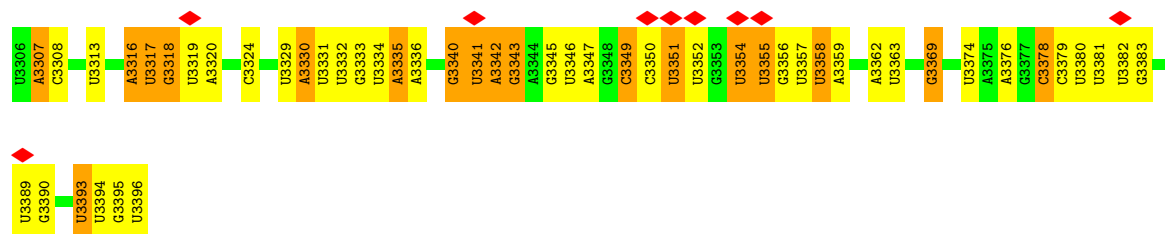
- Molecule 81: 25S RIBOSOMAL RNA



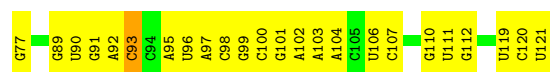




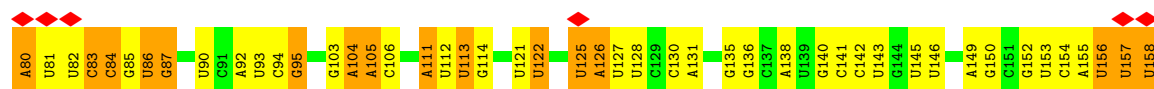




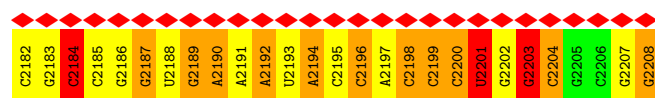
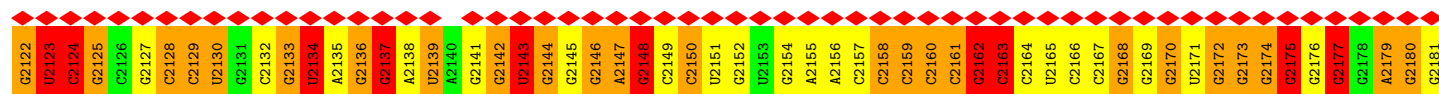
• Molecule 82: 5S RIBOSOMAL RNA



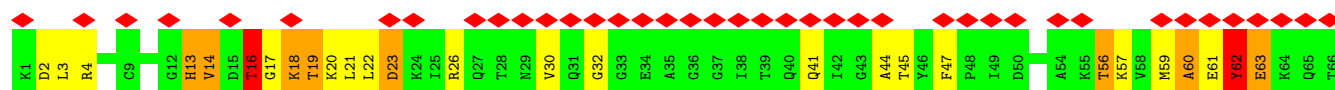
• Molecule 83: 5.8S RIBOSOMAL RNA

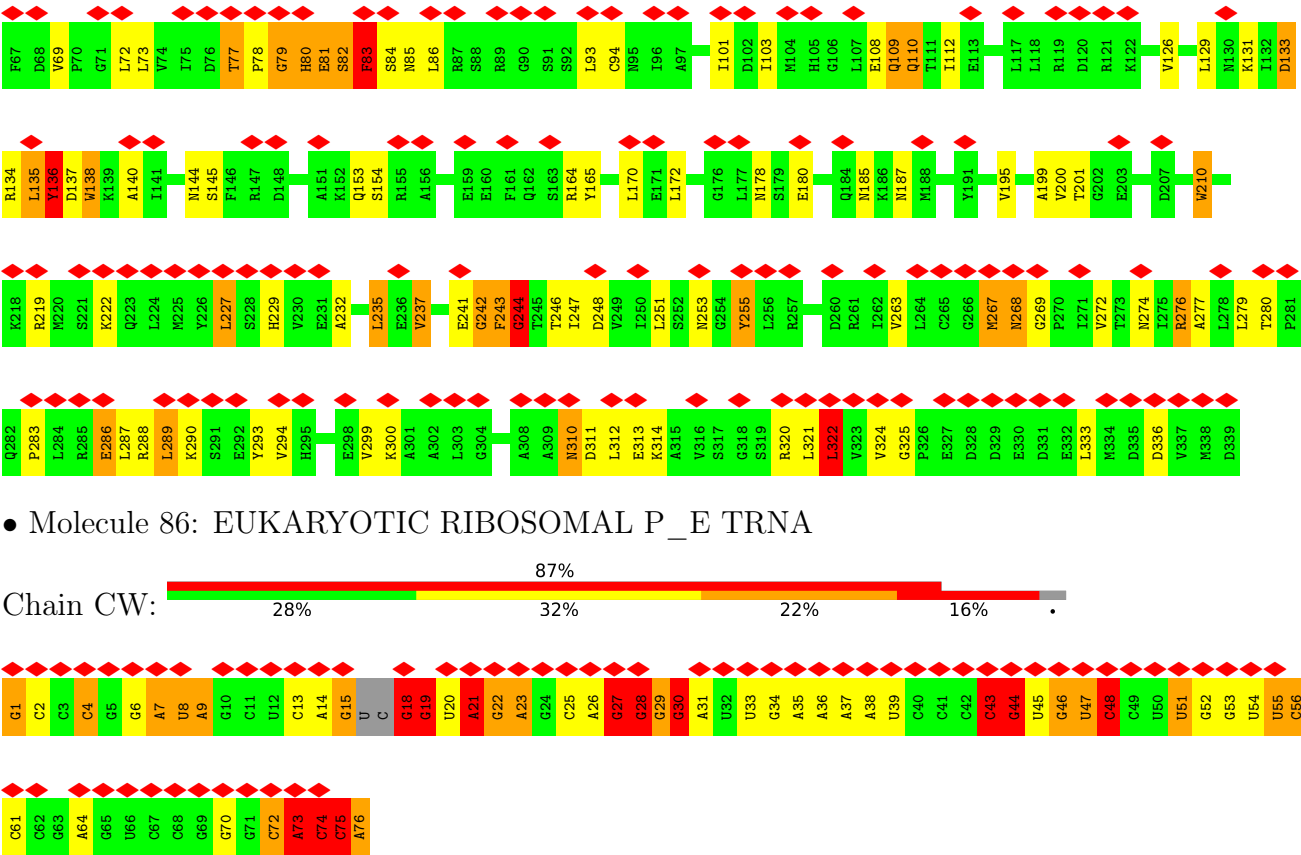


• Molecule 84: EUKARYOTIC RIBOSOMAL L1_RRNA



• Molecule 85: EUKARYOTIC TRANSLATION INITIATION FACTOR 5B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40729	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	79096	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	1.374	Depositor
Minimum map value	-0.930	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	424.8, 424.8, 424.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.77, 1.77, 1.77	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OHX, GCP, MG

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	A0	0.76	0/782	1.15	4/1047 (0.4%)
2	A1	0.69	0/620	1.23	7/838 (0.8%)
3	A2	0.54	0/499	1.08	0/670
4	A3	0.85	1/452 (0.2%)	1.24	2/600 (0.3%)
5	A4	0.61	0/483	1.13	2/643 (0.3%)
6	A5	0.72	0/404	1.37	5/542 (0.9%)
7	A6	0.63	0/2490	1.03	7/3389 (0.2%)
8	A7	1.09	3/925 (0.3%)	1.29	8/1240 (0.6%)
9	AA	0.71	1/1617 (0.1%)	1.22	18/2215 (0.8%)
10	AB	0.62	0/1735	1.13	11/2335 (0.5%)
11	AC	0.81	3/1665 (0.2%)	1.19	6/2263 (0.3%)
12	AD	0.76	0/1759	1.15	11/2368 (0.5%)
13	AE	0.74	0/2109	1.20	17/2839 (0.6%)
14	AF	0.65	0/1629	1.10	7/2202 (0.3%)
15	AG	0.70	0/1823	1.12	7/2439 (0.3%)
16	AH	0.68	0/1506	1.15	12/2028 (0.6%)
17	AI	0.84	0/1514	1.17	7/2021 (0.3%)
18	AJ	0.73	0/1519	1.18	7/2035 (0.3%)
19	AK	0.71	0/789	1.20	7/1067 (0.7%)
20	AL	0.85	0/1239	1.17	6/1673 (0.4%)
21	AM	0.70	0/898	1.13	4/1220 (0.3%)
22	AN	0.79	0/1215	1.17	7/1638 (0.4%)
23	AO	0.69	0/901	1.24	7/1217 (0.6%)
24	AP	0.75	0/998	1.20	8/1341 (0.6%)
25	AQ	0.70	0/1125	1.18	8/1510 (0.5%)
26	AR	0.73	0/935	1.25	7/1254 (0.6%)
27	AS	0.74	0/1211	1.14	5/1628 (0.3%)
28	AT	0.72	1/1130 (0.1%)	1.09	5/1517 (0.3%)
29	AU	0.71	0/865	1.18	8/1169 (0.7%)
30	AV	0.68	1/693 (0.1%)	1.07	3/935 (0.3%)
31	AW	0.83	0/1038	1.23	8/1395 (0.6%)
32	AX	0.91	1/1139 (0.1%)	1.26	6/1518 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AY	0.70	1/1087 (0.1%)	1.08	2/1449 (0.1%)
34	AZ	0.65	0/571	1.22	4/768 (0.5%)
35	BA	1.11	4/1946 (0.2%)	1.43	18/2614 (0.7%)
36	BB	1.23	5/3146 (0.2%)	1.44	26/4228 (0.6%)
37	BC	1.12	6/2800 (0.2%)	1.43	34/3790 (0.9%)
38	BD	1.02	1/2408 (0.0%)	1.27	21/3248 (0.6%)
39	BE	1.07	0/1269	1.37	11/1705 (0.6%)
40	BF	1.17	2/1828 (0.1%)	1.43	26/2461 (1.1%)
41	BG	0.78	0/1795	1.18	14/2429 (0.6%)
42	BH	1.18	0/1539	1.45	13/2073 (0.6%)
43	BI	1.11	0/1758	1.38	12/2358 (0.5%)
44	BJ	0.99	1/1374 (0.1%)	1.36	17/1842 (0.9%)
46	BL	1.06	3/1573 (0.2%)	1.40	19/2113 (0.9%)
47	BM	1.19	0/1074	1.36	9/1446 (0.6%)
48	BN	0.99	2/1757 (0.1%)	1.30	14/2354 (0.6%)
49	BO	0.64	0/3159	0.95	14/4205 (0.3%)
50	BP	1.34	4/1250 (0.3%)	1.41	6/1683 (0.4%)
51	BQ	1.08	1/1465 (0.1%)	1.42	10/1965 (0.5%)
52	BR	0.95	0/1538	1.21	5/2050 (0.2%)
53	BS	1.20	3/1481 (0.2%)	1.43	17/1990 (0.9%)
54	BT	1.16	2/1300 (0.2%)	1.35	6/1743 (0.3%)
55	BU	0.67	0/794	1.20	8/1076 (0.7%)
56	BV	1.25	2/1018 (0.2%)	1.42	6/1369 (0.4%)
57	BW	0.99	0/1052	1.22	7/1398 (0.5%)
58	BX	0.88	0/974	1.24	7/1314 (0.5%)
59	BY	0.94	0/1004	1.31	6/1341 (0.4%)
60	BZ	0.65	0/1118	1.18	9/1497 (0.6%)
61	Ba	1.20	7/1204 (0.6%)	1.59	28/1612 (1.7%)
62	Bb	1.20	2/473 (0.4%)	1.61	10/629 (1.6%)
63	Bc	0.72	0/775	1.11	3/1040 (0.3%)
64	Bd	1.11	1/897 (0.1%)	1.32	8/1205 (0.7%)
65	Be	1.23	3/1041 (0.3%)	1.58	9/1394 (0.6%)
66	Bf	1.34	6/868 (0.7%)	1.40	6/1168 (0.5%)
67	Bg	0.87	0/890	1.26	3/1189 (0.3%)
68	Bh	0.81	0/974	1.15	2/1297 (0.2%)
69	Bi	0.84	0/777	1.17	2/1033 (0.2%)
70	Bj	1.03	0/696	1.35	4/923 (0.4%)
71	Bk	0.66	0/614	1.07	1/822 (0.1%)
72	Bl	1.03	0/443	1.28	0/588
73	Bm	1.29	0/423	1.42	5/562 (0.9%)
74	Bn	1.05	0/234	1.25	2/300 (0.7%)
75	Bo	0.95	0/860	1.24	0/1136
76	Bq	1.51	4/1092 (0.4%)	1.82	30/1474 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
79	By	1.31	0/1749	1.74	28/2355 (1.2%)
79	CL	1.08	5/1749 (0.3%)	1.34	14/2355 (0.6%)
80	B2	0.53	1/42128 (0.0%)	0.58	0/65642
81	B5	0.84	29/75336 (0.0%)	0.72	69/117449 (0.1%)
82	B7	0.78	0/2883	0.63	0/4491
83	B8	0.66	0/3746	0.61	0/5832
84	CN	0.67	1/2097 (0.0%)	1.35	39/3273 (1.2%)
85	CP	2.73	18/2694 (0.7%)	1.91	93/3637 (2.6%)
86	CW	1.13	2/1761 (0.1%)	1.50	32/2743 (1.2%)
All	All	0.88	127/226189 (0.1%)	0.99	956/331454 (0.3%)

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
2	A1	0	1
6	A5	0	2
8	A7	0	1
10	AB	0	1
16	AH	0	1
20	AL	0	1
23	AO	0	1
26	AR	0	2
34	AZ	0	3
35	BA	0	2
37	BC	0	1
38	BD	0	1
39	BE	0	1
40	BF	0	2
49	BO	0	2
53	BS	0	1
56	BV	0	1
59	BY	0	1
60	BZ	0	1
61	Ba	0	3
62	Bb	0	1
76	Bq	0	7
77	Br	0	1
79	By	0	4
79	CL	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
81	B5	0	35
85	CP	0	8
86	CW	0	19
All	All	0	107

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	CP	63	GLU	N-CA	99.89	2.84	1.46
85	CP	210	TRP	CD2-CE3	32.65	1.92	1.40
85	CP	210	TRP	CE2-CZ2	25.81	1.94	1.39
85	CP	210	TRP	CZ2-CH2	23.93	1.82	1.37
85	CP	210	TRP	CD2-CE2	23.30	1.80	1.41

The worst 5 of 956 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B5	1256	G	P-O3'-C3'	25.89	159.04	120.20
81	B5	1238	C	P-O3'-C3'	17.46	146.38	120.20
65	Be	4	LEU	CA-C-N	-17.04	98.54	119.84
65	Be	4	LEU	C-N-CA	-17.04	98.54	119.84
81	B5	1226	G	C5'-C4'-C3'	16.80	141.20	116.00

There are no chirality outliers.

5 of 107 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A1	42	ASN	Peptide
6	A5	105	TYR	Peptide
6	A5	138	ARG	Peptide
8	A7	134	ASP	Sidechain
10	AB	131	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	769	0	814	122	0
2	A1	610	0	630	53	0
3	A2	497	0	535	32	0
4	A3	442	0	428	57	0
5	A4	475	0	525	21	0
6	A5	516	0	517	41	0
7	A6	2437	0	2386	86	0
8	A7	1105	0	959	207	0
9	AA	1577	0	1567	101	0
10	AB	1709	0	1784	200	0
11	AC	1635	0	1723	82	0
12	AD	1734	0	1817	123	0
13	AE	2068	0	2154	95	0
14	AF	1609	0	1675	118	0
15	AG	1799	0	1874	442	0
16	AH	1481	0	1572	84	0
17	AI	1489	0	1523	193	0
18	AJ	1494	0	1573	98	0
19	AK	772	0	727	48	0
20	AL	1213	0	1257	104	0
21	AM	890	0	887	53	0
22	AN	1192	0	1252	66	0
23	AO	891	0	880	300	0
24	AP	977	0	1002	73	0
25	AQ	1105	0	1166	142	0
26	AR	926	0	930	135	0
27	AS	1192	0	1220	118	0
28	AT	1112	0	1123	111	0
29	AU	855	0	917	118	0
30	AV	684	0	672	47	0
31	AW	1021	0	1060	70	0
32	AX	1121	0	1196	75	0
33	AY	1073	0	1132	115	0
34	AZ	563	0	602	54	0
35	BA	1912	0	1973	284	0
36	BB	3075	0	3142	153	0
37	BC	2748	0	2859	137	0
38	BD	2359	0	2311	272	0
39	BE	1248	0	1339	41	0
40	BF	1791	0	1869	60	0
41	BG	1763	0	1819	152	0
42	BH	1518	0	1587	85	0
43	BI	1722	0	1755	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BJ	1353	0	1380	110	0
45	BK	751	756	195	3	0
46	BL	1548	0	1613	99	0
47	BM	1059	0	1154	45	0
48	BN	1720	0	1779	139	0
49	BO	3119	0	3302	99	0
50	BP	1227	0	1236	43	0
51	BQ	1441	0	1543	78	0
52	BR	1521	0	1605	196	0
53	BS	1445	0	1487	67	0
54	BT	1276	0	1323	141	0
55	BU	778	0	791	24	0
56	BV	1003	0	1048	52	0
57	BW	1038	0	1071	45	0
58	BX	959	0	1023	41	0
59	BY	993	0	1081	46	0
60	BZ	1092	0	1154	119	0
61	Ba	1173	0	1215	108	0
62	Bb	462	0	491	39	0
63	Bc	767	0	816	78	0
64	Bd	883	0	918	32	0
65	Be	1020	0	1090	62	0
66	Bf	850	0	880	36	0
67	Bg	880	0	944	106	0
68	Bh	965	0	1067	56	0
69	Bi	770	0	846	61	0
70	Bj	681	0	683	71	0
71	Bk	608	0	671	23	0
72	Bl	436	0	475	46	0
73	Bm	417	0	455	26	0
74	Bn	233	0	271	71	0
75	Bo	847	0	916	49	0
76	Bq	1077	1110	1041	37	0
77	Br	236	237	65	0	0
78	Bs	231	232	67	0	0
79	By	1719	1773	1619	3762	0
79	CL	1719	0	1652	3462	0
80	B2	37835	0	19048	3055	0
81	B5	67308	664	33793	2713	0
82	B7	2579	0	1303	190	0
83	B8	3353	0	1695	158	0
84	CN	1875	0	926	459	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	CP	2655	2725	2709	241	0
86	CW	1576	803	797	93	0
87	A0	1	0	0	0	0
87	A1	1	0	0	0	0
87	A3	1	0	0	0	0
87	A5	1	0	0	0	0
87	Bj	1	0	0	0	0
87	Bm	1	0	0	0	0
88	A0	2	0	0	0	0
88	A3	3	0	0	0	0
88	A5	1	0	0	0	0
88	AB	1	0	0	0	0
88	AC	2	0	0	0	0
88	AE	1	0	0	0	0
88	AG	1	0	0	0	0
88	AI	1	0	0	0	0
88	AJ	1	0	0	0	0
88	AL	2	0	0	0	0
88	AN	1	0	0	0	0
88	AP	1	0	0	0	0
88	AS	1	0	0	0	0
88	AU	1	0	0	0	0
88	B2	169	0	0	0	0
88	B5	3	0	0	0	0
89	A3	7	0	0	4	0
89	A6	7	0	0	2	0
89	AC	7	0	0	5	0
89	AI	14	0	0	2	0
89	AL	7	0	0	3	0
89	AN	7	0	0	2	0
89	AP	7	0	0	3	0
89	B2	1288	0	0	224	0
89	B5	21	0	0	4	0
89	BR	7	0	0	9	0
89	Bn	7	0	0	0	0
90	CP	32	0	7	62	0
All	All	214255	8300	157978	13207	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 36.

The worst 5 of 13207 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)
79:By:77:ILE:CG2	79:CL:99:ILE:HD11	1.18	1.66
79:By:116:THR:HA	79:CL:115:ALA:CB	1.24	1.66
15:AG:175:ILE:HG12	80:B2:78:A:C4	1.29	1.65
79:By:30:LYS:HG2	79:CL:31:GLU:CA	1.22	1.65
79:By:208:PHE:CZ	79:CL:58:VAL:HG21	1.16	1.65

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	
1	A0	95/119 (80%)	57 (60%)	21 (22%)	17 (18%)	0	2
2	A1	79/82 (96%)	62 (78%)	13 (16%)	4 (5%)	1	15
3	A2	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	0	9
4	A3	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	2	19
5	A4	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	3	21
6	A5	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0	1
7	A6	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	2	18
8	A7	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	0	8
9	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0	4
10	AB	212/255 (83%)	132 (62%)	42 (20%)	38 (18%)	0	2
11	AC	215/254 (85%)	187 (87%)	16 (7%)	12 (6%)	1	15
12	AD	221/240 (92%)	180 (81%)	27 (12%)	14 (6%)	1	13
13	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1	9
14	AF	204/225 (91%)	155 (76%)	30 (15%)	19 (9%)	0	8
15	AG	224/236 (95%)	190 (85%)	23 (10%)	11 (5%)	1	16
16	AH	182/190 (96%)	128 (70%)	27 (15%)	27 (15%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	0	9
18	AJ	183/197 (93%)	153 (84%)	18 (10%)	12 (7%)	1	12
19	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	0	6
20	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	1	14
21	AM	122/143 (85%)	66 (54%)	23 (19%)	33 (27%)	0	0
22	AN	148/151 (98%)	125 (84%)	15 (10%)	8 (5%)	1	15
23	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	0	4
24	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	0	4
25	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1	9
26	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0	6
27	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	0	7
28	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	0	9
29	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	2	16
30	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	4
31	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	4	27
32	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0	4
33	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	0	7
34	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0	2
35	BA	250/253 (99%)	213 (85%)	30 (12%)	7 (3%)	4	24
36	BB	384/386 (100%)	341 (89%)	34 (9%)	9 (2%)	5	28
37	BC	359/361 (99%)	306 (85%)	32 (9%)	21 (6%)	1	14
38	BD	292/296 (99%)	267 (91%)	19 (6%)	6 (2%)	5	30
39	BE	153/175 (87%)	134 (88%)	15 (10%)	4 (3%)	4	25
40	BF	221/243 (91%)	201 (91%)	16 (7%)	4 (2%)	6	33
41	BG	229/255 (90%)	180 (79%)	28 (12%)	21 (9%)	0	8
42	BH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	5	30
43	BI	209/220 (95%)	175 (84%)	22 (10%)	12 (6%)	1	14
44	BJ	167/173 (96%)	135 (81%)	19 (11%)	13 (8%)	1	10
46	BL	192/198 (97%)	161 (84%)	20 (10%)	11 (6%)	1	14
47	BM	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	18	55
48	BN	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	BO	352/218 (162%)	324 (92%)	18 (5%)	10 (3%)	4	24
50	BP	153/183 (84%)	142 (93%)	9 (6%)	2 (1%)	9	41
51	BQ	183/185 (99%)	168 (92%)	9 (5%)	6 (3%)	3	21
52	BR	186/188 (99%)	167 (90%)	16 (9%)	3 (2%)	7	37
53	BS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	21	58
54	BT	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	9	41
55	BU	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	3	22
56	BV	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	8	38
57	BW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	1	13
58	BX	118/141 (84%)	104 (88%)	6 (5%)	8 (7%)	1	12
59	BY	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	2	18
60	BZ	133/135 (98%)	107 (80%)	13 (10%)	13 (10%)	0	7
61	Ba	146/148 (99%)	123 (84%)	18 (12%)	5 (3%)	3	21
62	Bb	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	0	8
63	Bc	98/104 (94%)	87 (89%)	8 (8%)	3 (3%)	3	22
64	Bd	107/112 (96%)	88 (82%)	13 (12%)	6 (6%)	1	15
65	Be	125/129 (97%)	110 (88%)	9 (7%)	6 (5%)	2	16
66	Bf	104/106 (98%)	96 (92%)	5 (5%)	3 (3%)	3	23
67	Bg	110/120 (92%)	93 (84%)	13 (12%)	4 (4%)	2	20
68	Bh	117/119 (98%)	99 (85%)	14 (12%)	4 (3%)	3	21
69	Bi	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	11
70	Bj	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	4	27
71	Bk	75/77 (97%)	61 (81%)	10 (13%)	4 (5%)	1	15
72	Bl	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	5	30
73	Bm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	6	31
74	Bn	23/25 (92%)	22 (96%)	0	1 (4%)	2	17
75	Bo	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	6	32
76	Bq	139/312 (45%)	104 (75%)	14 (10%)	21 (15%)	0	2
79	By	219/229 (96%)	178 (81%)	24 (11%)	17 (8%)	1	10
79	CL	219/229 (96%)	165 (75%)	35 (16%)	19 (9%)	0	9
85	CP	337/339 (99%)	280 (83%)	34 (10%)	23 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	12057/13155 (92%)	10005 (83%)	1277 (11%)	775 (6%)	2 13

5 of 775 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	19	LYS
1	A0	45	VAL
1	A0	46	GLU
1	A0	62	TYR
1	A0	65	PRO

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
1	A0	83/101 (82%)	61 (74%)	22 (26%)	0 3
2	A1	70/71 (99%)	60 (86%)	10 (14%)	3 15
3	A2	56/60 (93%)	36 (64%)	20 (36%)	0 1
4	A3	47/49 (96%)	40 (85%)	7 (15%)	3 14
5	A4	51/54 (94%)	41 (80%)	10 (20%)	1 8
6	A5	43/116 (37%)	31 (72%)	12 (28%)	0 3
7	A6	259/262 (99%)	215 (83%)	44 (17%)	2 12
8	A7	97/195 (50%)	71 (73%)	26 (27%)	0 3
9	AA	164/210 (78%)	114 (70%)	50 (30%)	0 2
10	AB	191/224 (85%)	137 (72%)	54 (28%)	0 3
11	AC	176/205 (86%)	124 (70%)	52 (30%)	0 2
12	AD	182/195 (93%)	133 (73%)	49 (27%)	0 3
13	AE	221/222 (100%)	160 (72%)	61 (28%)	0 3
14	AF	173/191 (91%)	139 (80%)	34 (20%)	1 8
15	AG	188/201 (94%)	145 (77%)	43 (23%)	1 6
16	AH	165/170 (97%)	116 (70%)	49 (30%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
17	AI	150/161 (93%)	114 (76%)	36 (24%)	1	4	
18	AJ	158/166 (95%)	121 (77%)	37 (23%)	1	5	
19	AK	77/98 (79%)	57 (74%)	20 (26%)	0	3	
20	AL	129/137 (94%)	102 (79%)	27 (21%)	1	7	
21	AM	88/119 (74%)	53 (60%)	35 (40%)	0	1	
22	AN	127/128 (99%)	86 (68%)	41 (32%)	0	2	
23	AO	81/105 (77%)	57 (70%)	24 (30%)	0	2	
24	AP	101/118 (86%)	81 (80%)	20 (20%)	1	8	
25	AQ	117/119 (98%)	82 (70%)	35 (30%)	0	2	
26	AR	94/124 (76%)	72 (77%)	22 (23%)	1	5	
27	AS	128/129 (99%)	87 (68%)	41 (32%)	0	2	
28	AT	115/116 (99%)	84 (73%)	31 (27%)	0	3	
29	AU	100/114 (88%)	69 (69%)	31 (31%)	0	2	
30	AV	74/74 (100%)	54 (73%)	20 (27%)	0	3	
31	AW	110/111 (99%)	82 (74%)	28 (26%)	0	3	
32	AX	119/120 (99%)	93 (78%)	26 (22%)	1	6	
33	AY	112/113 (99%)	81 (72%)	31 (28%)	0	3	
34	AZ	61/89 (68%)	42 (69%)	19 (31%)	0	2	
35	BA	192/195 (98%)	149 (78%)	43 (22%)	1	6	
36	BB	320/322 (99%)	241 (75%)	79 (25%)	1	4	
37	BC	288/288 (100%)	213 (74%)	75 (26%)	0	3	
38	BD	243/244 (100%)	185 (76%)	58 (24%)	1	5	
39	BE	135/152 (89%)	113 (84%)	22 (16%)	2	12	
40	BF	187/204 (92%)	158 (84%)	29 (16%)	2	13	
41	BG	177/207 (86%)	136 (77%)	41 (23%)	1	5	
42	BH	171/171 (100%)	128 (75%)	43 (25%)	0	4	
43	BI	179/186 (96%)	134 (75%)	45 (25%)	0	4	
44	BJ	147/149 (99%)	113 (77%)	34 (23%)	1	5	
46	BL	154/158 (98%)	126 (82%)	28 (18%)	2	10	
47	BM	108/108 (100%)	80 (74%)	28 (26%)	0	3	
48	BN	175/175 (100%)	139 (79%)	36 (21%)	1	7	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BO	323/178 (182%)	254 (79%)	69 (21%)	1	6
50	BP	125/145 (86%)	98 (78%)	27 (22%)	1	6
51	BQ	150/150 (100%)	121 (81%)	29 (19%)	1	8
52	BR	153/153 (100%)	113 (74%)	40 (26%)	0	3
53	BS	156/156 (100%)	119 (76%)	37 (24%)	1	5
54	BT	136/136 (100%)	107 (79%)	29 (21%)	1	6
55	BU	85/106 (80%)	60 (71%)	25 (29%)	0	2
56	BV	104/104 (100%)	93 (89%)	11 (11%)	6	22
57	BW	100/129 (78%)	83 (83%)	17 (17%)	2	12
58	BX	104/117 (89%)	77 (74%)	27 (26%)	0	3
59	BY	109/109 (100%)	81 (74%)	28 (26%)	0	3
60	BZ	115/115 (100%)	87 (76%)	28 (24%)	1	4
61	Ba	118/118 (100%)	90 (76%)	28 (24%)	1	5
62	Bb	46/46 (100%)	32 (70%)	14 (30%)	0	2
63	Bc	84/87 (97%)	65 (77%)	19 (23%)	1	6
64	Bd	94/96 (98%)	72 (77%)	22 (23%)	1	5
65	Be	109/110 (99%)	85 (78%)	24 (22%)	1	6
66	Bf	90/90 (100%)	80 (89%)	10 (11%)	6	21
67	Bg	95/102 (93%)	70 (74%)	25 (26%)	0	3
68	Bh	103/104 (99%)	75 (73%)	28 (27%)	0	3
69	Bi	80/81 (99%)	51 (64%)	29 (36%)	0	1
70	Bj	70/70 (100%)	55 (79%)	15 (21%)	1	6
71	Bk	67/68 (98%)	50 (75%)	17 (25%)	0	3
72	Bl	45/45 (100%)	30 (67%)	15 (33%)	0	2
73	Bm	47/116 (40%)	35 (74%)	12 (26%)	0	3
74	Bn	23/23 (100%)	13 (56%)	10 (44%)	0	0
75	Bo	90/90 (100%)	72 (80%)	18 (20%)	1	8
76	Bq	105/254 (41%)	94 (90%)	11 (10%)	6	23
79	By	177/181 (98%)	174 (98%)	3 (2%)	53	67
79	CL	177/181 (98%)	147 (83%)	30 (17%)	2	12
85	CP	296/296 (100%)	276 (93%)	20 (7%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10159/10982 (92%)	7814 (77%)	2345 (23%)	2 5

5 of 2345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BT	139	ARG
79	By	104	LEU
57	BW	105	ARG
54	BT	131	GLN
65	Be	14	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
54	BT	49	GLN
72	Bl	11	GLN
57	BW	42	GLN
62	Bb	19	ASN
79	By	3	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
80	B2	1763/1800 (97%)	548 (31%)	86 (4%)
81	B5	3140/3396 (92%)	756 (24%)	131 (4%)
82	B7	120/121 (99%)	18 (15%)	0
83	B8	157/158 (99%)	33 (21%)	3 (1%)
84	CN	86/87 (98%)	41 (47%)	8 (9%)
86	CW	73/76 (96%)	28 (38%)	7 (9%)
All	All	5339/5638 (94%)	1424 (26%)	235 (4%)

5 of 1424 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
80	B2	2	A
80	B2	4	C
80	B2	8	U
80	B2	16	G
80	B2	20	G

5 of 235 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
81	B5	908	G
84	CN	2162	G
81	B5	1434	G
83	B8	156	U
81	B5	2996	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 395 ligands modelled in this entry, 197 are monoatomic - leaving 198 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	OHX	B2	2028	-	0,6,6	-	-	-		
89	OHX	B2	1946	-	0,6,6	-	-	-		
89	OHX	AC	301	-	0,6,6	-	-	-		
89	OHX	B2	1931	-	0,6,6	-	-	-		
89	OHX	B2	2060	-	0,6,6	-	-	-		
89	OHX	B2	2006	-	0,6,6	-	-	-		
89	OHX	B2	1947	-	0,6,6	-	-	-		
89	OHX	B2	2013	-	0,6,6	-	-	-		
89	OHX	B2	2020	-	0,6,6	-	-	-		
89	OHX	B2	2029	-	0,6,6	-	-	-		
89	OHX	B2	1914	-	0,6,6	-	-	-		
89	OHX	B2	1974	-	0,6,6	-	-	-		
89	OHX	B2	2067	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	1942	-	0,6,6	-	-	-		
89	OHX	B2	2001	-	0,6,6	-	-	-		
89	OHX	B2	2081	-	0,6,6	-	-	-		
89	OHX	B2	1926	-	0,6,6	-	-	-		
89	OHX	B2	2082	-	0,6,6	-	-	-		
89	OHX	B2	1986	-	0,6,6	-	-	-		
89	OHX	B2	1994	-	0,6,6	-	-	-		
89	OHX	B2	2030	-	0,6,6	-	-	-		
89	OHX	B2	1944	-	0,6,6	-	-	-		
89	OHX	B2	1964	-	0,6,6	-	-	-		
89	OHX	B2	1925	-	0,6,6	-	-	-		
89	OHX	B2	1904	-	0,6,6	-	-	-		
89	OHX	B2	2026	-	0,6,6	-	-	-		
89	OHX	B2	1917	-	0,6,6	-	-	-		
89	OHX	B2	2019	-	0,6,6	-	-	-		
89	OHX	B2	2038	-	0,6,6	-	-	-		
89	OHX	AP	201	-	0,6,6	-	-	-		
89	OHX	B2	1954	-	0,6,6	-	-	-		
89	OHX	B2	1966	-	0,6,6	-	-	-		
89	OHX	B2	1998	-	0,6,6	-	-	-		
89	OHX	AN	201	-	0,6,6	-	-	-		
89	OHX	B2	1965	-	0,6,6	-	-	-		
89	OHX	B2	1950	-	0,6,6	-	-	-		
89	OHX	B2	2025	-	0,6,6	-	-	-		
89	OHX	B2	2033	-	0,6,6	-	-	-		
89	OHX	B2	1909	89	0,6,6	-	-	-		
89	OHX	B2	1976	-	0,6,6	-	-	-		
89	OHX	B2	2055	-	0,6,6	-	-	-		
89	OHX	B2	1959	-	0,6,6	-	-	-		
89	OHX	B2	1915	-	0,6,6	-	-	-		
89	OHX	B5	3401	-	0,6,6	-	-	-		
89	OHX	B2	1952	-	0,6,6	-	-	-		
89	OHX	B2	1981	-	0,6,6	-	-	-		
89	OHX	B2	2007	-	0,6,6	-	-	-		
89	OHX	B2	2063	-	0,6,6	-	-	-		
89	OHX	B2	2032	-	0,6,6	-	-	-		
89	OHX	B2	2080	-	0,6,6	-	-	-		
89	OHX	B2	2054	-	0,6,6	-	-	-		
89	OHX	BR	201	-	0,6,6	-	-	-		
89	OHX	B5	3402	-	0,6,6	-	-	-		
89	OHX	B2	2004	-	0,6,6	-	-	-		
89	OHX	B2	2062	-	0,6,6	-	-	-		
89	OHX	B2	2010	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	A3	102	-	0,6,6	-	-	-		
89	OHX	B2	2068	-	0,6,6	-	-	-		
89	OHX	B2	2078	-	0,6,6	-	-	-		
89	OHX	A6	401	-	0,6,6	-	-	-		
89	OHX	B2	1932	-	0,6,6	-	-	-		
89	OHX	B2	2003	-	0,6,6	-	-	-		
89	OHX	B2	2058	-	0,6,6	-	-	-		
89	OHX	B2	2031	89	0,6,6	-	-	-		
89	OHX	B2	1902	-	0,6,6	-	-	-		
89	OHX	B2	1919	-	0,6,6	-	-	-		
89	OHX	B2	2070	-	0,6,6	-	-	-		
89	OHX	B2	1993	-	0,6,6	-	-	-		
89	OHX	B2	2023	-	0,6,6	-	-	-		
89	OHX	B2	1928	-	0,6,6	-	-	-		
89	OHX	B2	2046	-	0,6,6	-	-	-		
89	OHX	B2	2037	-	0,6,6	-	-	-		
89	OHX	B2	1916	-	0,6,6	-	-	-		
89	OHX	B2	2039	-	0,6,6	-	-	-		
89	OHX	B2	1933	-	0,6,6	-	-	-		
89	OHX	B2	1955	-	0,6,6	-	-	-		
89	OHX	B2	2056	-	0,6,6	-	-	-		
89	OHX	B2	1967	-	0,6,6	-	-	-		
89	OHX	B2	1901	-	0,6,6	-	-	-		
89	OHX	B2	1913	-	0,6,6	-	-	-		
89	OHX	B2	2005	-	0,6,6	-	-	-		
89	OHX	B2	1969	-	0,6,6	-	-	-		
89	OHX	B2	2009	-	0,6,6	-	-	-		
89	OHX	B2	2008	-	0,6,6	-	-	-		
89	OHX	B2	1990	-	0,6,6	-	-	-		
89	OHX	B2	1963	-	0,6,6	-	-	-		
89	OHX	B2	1940	-	0,6,6	-	-	-		
89	OHX	B2	1905	-	0,6,6	-	-	-		
89	OHX	B2	1920	-	0,6,6	-	-	-		
89	OHX	B2	1941	-	0,6,6	-	-	-		
89	OHX	B2	1906	88	0,6,6	-	-	-		
89	OHX	B2	2034	-	0,6,6	-	-	-		
89	OHX	B2	1962	-	0,6,6	-	-	-		
89	OHX	B2	1975	-	0,6,6	-	-	-		
89	OHX	B2	2053	-	0,6,6	-	-	-		
89	OHX	B2	1924	-	0,6,6	-	-	-		
89	OHX	B2	1961	-	0,6,6	-	-	-		
89	OHX	B2	1980	-	0,6,6	-	-	-		
89	OHX	B2	1939	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	1987	-	0,6,6	-	-	-		
89	OHX	B2	1983	-	0,6,6	-	-	-		
89	OHX	B2	1938	-	0,6,6	-	-	-		
89	OHX	B2	2047	-	0,6,6	-	-	-		
89	OHX	B2	2052	-	0,6,6	-	-	-		
89	OHX	B2	2050	88	0,6,6	-	-	-		
89	OHX	B2	1930	-	0,6,6	-	-	-		
89	OHX	B2	2059	-	0,6,6	-	-	-		
89	OHX	B2	1982	-	0,6,6	-	-	-		
89	OHX	AI	301	-	0,6,6	-	-	-		
89	OHX	B2	2024	-	0,6,6	-	-	-		
89	OHX	B2	2061	-	0,6,6	-	-	-		
89	OHX	B2	1937	-	0,6,6	-	-	-		
89	OHX	B2	2084	-	0,6,6	-	-	-		
89	OHX	B2	2057	-	0,6,6	-	-	-		
89	OHX	B2	2015	-	0,6,6	-	-	-		
89	OHX	B2	1910	-	0,6,6	-	-	-		
89	OHX	B2	2076	-	0,6,6	-	-	-		
89	OHX	B2	1988	-	0,6,6	-	-	-		
89	OHX	B2	1996	-	0,6,6	-	-	-		
89	OHX	B2	2051	-	0,6,6	-	-	-		
89	OHX	B2	1945	-	0,6,6	-	-	-		
89	OHX	B2	2077	-	0,6,6	-	-	-		
89	OHX	B2	2040	-	0,6,6	-	-	-		
89	OHX	B2	2022	-	0,6,6	-	-	-		
89	OHX	B2	1979	-	0,6,6	-	-	-		
89	OHX	B2	2071	80	0,6,6	-	-	-		
89	OHX	B2	2014	-	0,6,6	-	-	-		
89	OHX	B2	1953	-	0,6,6	-	-	-		
89	OHX	B2	1912	-	0,6,6	-	-	-		
89	OHX	B2	1992	-	0,6,6	-	-	-		
89	OHX	B2	1999	-	0,6,6	-	-	-		
89	OHX	B2	1911	-	0,6,6	-	-	-		
89	OHX	B2	1907	-	0,6,6	-	-	-		
89	OHX	B2	2075	-	0,6,6	-	-	-		
89	OHX	B2	1984	-	0,6,6	-	-	-		
89	OHX	B2	1958	-	0,6,6	-	-	-		
89	OHX	B2	2073	-	0,6,6	-	-	-		
89	OHX	B2	2074	-	0,6,6	-	-	-		
89	OHX	B2	2083	-	0,6,6	-	-	-		
89	OHX	B2	2017	-	0,6,6	-	-	-		
89	OHX	B2	2044	-	0,6,6	-	-	-		
89	OHX	B2	1989	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	1970	-	0,6,6	-	-	-		
89	OHX	B2	2027	-	0,6,6	-	-	-		
89	OHX	B2	1949	-	0,6,6	-	-	-		
89	OHX	B2	2048	-	0,6,6	-	-	-		
89	OHX	B2	1985	-	0,6,6	-	-	-		
89	OHX	B2	1943	-	0,6,6	-	-	-		
89	OHX	B2	2035	-	0,6,6	-	-	-		
89	OHX	B2	2045	-	0,6,6	-	-	-		
89	OHX	B2	1973	-	0,6,6	-	-	-		
89	OHX	AL	201	-	0,6,6	-	-	-		
89	OHX	B2	2036	-	0,6,6	-	-	-		
89	OHX	B2	2072	-	0,6,6	-	-	-		
89	OHX	B2	1948	-	0,6,6	-	-	-		
89	OHX	B2	1929	-	0,6,6	-	-	-		
89	OHX	B2	2066	-	0,6,6	-	-	-		
89	OHX	B2	1957	-	0,6,6	-	-	-		
89	OHX	B2	1951	-	0,6,6	-	-	-		
89	OHX	B2	1960	-	0,6,6	-	-	-		
89	OHX	B2	2065	-	0,6,6	-	-	-		
89	OHX	B2	1918	89	0,6,6	-	-	-		
90	GCP	CP	401	-	32,34,34	1.73	4 (12%)	49,54,54	1.62	5 (10%)
89	OHX	B2	1921	-	0,6,6	-	-	-		
89	OHX	B2	2011	-	0,6,6	-	-	-		
89	OHX	B2	1997	-	0,6,6	-	-	-		
89	OHX	B2	1927	-	0,6,6	-	-	-		
89	OHX	B2	1995	-	0,6,6	-	-	-		
89	OHX	B2	1903	-	0,6,6	-	-	-		
89	OHX	B2	1972	-	0,6,6	-	-	-		
89	OHX	B2	1971	-	0,6,6	-	-	-		
89	OHX	B2	1991	-	0,6,6	-	-	-		
89	OHX	B2	1977	-	0,6,6	-	-	-		
89	OHX	B2	1923	-	0,6,6	-	-	-		
89	OHX	B5	3403	-	0,6,6	-	-	-		
89	OHX	B2	2016	-	0,6,6	-	-	-		
89	OHX	B2	2000	-	0,6,6	-	-	-		
89	OHX	B2	1922	-	0,6,6	-	-	-		
89	OHX	B2	1968	-	0,6,6	-	-	-		
89	OHX	B2	1936	-	0,6,6	-	-	-		
89	OHX	B2	1908	-	0,6,6	-	-	-		
89	OHX	B2	2064	89,88	0,6,6	-	-	-		
89	OHX	B2	1956	-	0,6,6	-	-	-		
89	OHX	B2	2049	-	0,6,6	-	-	-		
89	OHX	B2	1935	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	2079	-	0,6,6	-	-	-		
89	OHX	B2	2069	-	0,6,6	-	-	-		
89	OHX	B2	1978	-	0,6,6	-	-	-		
89	OHX	B2	2021	-	0,6,6	-	-	-		
89	OHX	B2	2018	-	0,6,6	-	-	-		
89	OHX	B2	2042	-	0,6,6	-	-	-		
89	OHX	B2	2041	-	0,6,6	-	-	-		
89	OHX	B2	1934	-	0,6,6	-	-	-		
89	OHX	B2	2002	-	0,6,6	-	-	-		
89	OHX	B2	2012	-	0,6,6	-	-	-		
89	OHX	B2	2043	-	0,6,6	-	-	-		
89	OHX	AI	302	-	0,6,6	-	-	-		
89	OHX	Bn	101	-	0,6,6	-	-	-		

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
90	GCP	CP	401	-	-	1/19/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	CP	401	GCP	PA-O3A	-6.63	1.52	1.59
90	CP	401	GCP	C2'-C1'	-3.04	1.43	1.53
90	CP	401	GCP	C4-N3	2.54	1.40	1.34
90	CP	401	GCP	PB-O3A	-2.36	1.55	1.58

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	CP	401	GCP	O3G-PG-C3B	-7.36	88.55	106.40
90	CP	401	GCP	O2A-PA-O3A	3.08	115.59	107.27
90	CP	401	GCP	O1B-PB-C3B	2.91	116.72	109.05
90	CP	401	GCP	O2G-PG-O1G	2.77	119.54	112.39
90	CP	401	GCP	C1'-N9-C8	2.21	133.00	126.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	CP	401	GCP	PB-C3B-PG-O1G

There are no ring outliers.

121 monomers are involved in 313 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	B2	1946	OHX	1	0
89	AC	301	OHX	5	0
89	B2	2060	OHX	1	0
89	B2	2013	OHX	11	0
89	B2	1914	OHX	3	0
89	B2	1974	OHX	7	0
89	B2	1942	OHX	1	0
89	B2	2001	OHX	3	0
89	B2	1926	OHX	1	0
89	B2	1986	OHX	3	0
89	B2	2030	OHX	1	0
89	B2	1964	OHX	6	0
89	B2	1925	OHX	1	0
89	B2	2026	OHX	2	0
89	B2	1917	OHX	2	0
89	B2	2038	OHX	1	0
89	AP	201	OHX	3	0
89	B2	1954	OHX	6	0
89	AN	201	OHX	2	0
89	B2	1965	OHX	2	0
89	B2	1950	OHX	2	0
89	B2	2025	OHX	2	0
89	B2	1909	OHX	2	0
89	B2	1915	OHX	6	0
89	B5	3401	OHX	1	0
89	B2	1952	OHX	2	0
89	B2	2063	OHX	1	0
89	B2	2080	OHX	1	0
89	BR	201	OHX	9	0
89	B5	3402	OHX	3	0
89	B2	2004	OHX	1	0
89	A3	102	OHX	4	0
89	B2	2068	OHX	6	0
89	B2	2078	OHX	1	0
89	A6	401	OHX	2	0
89	B2	2058	OHX	1	0
89	B2	2031	OHX	1	0

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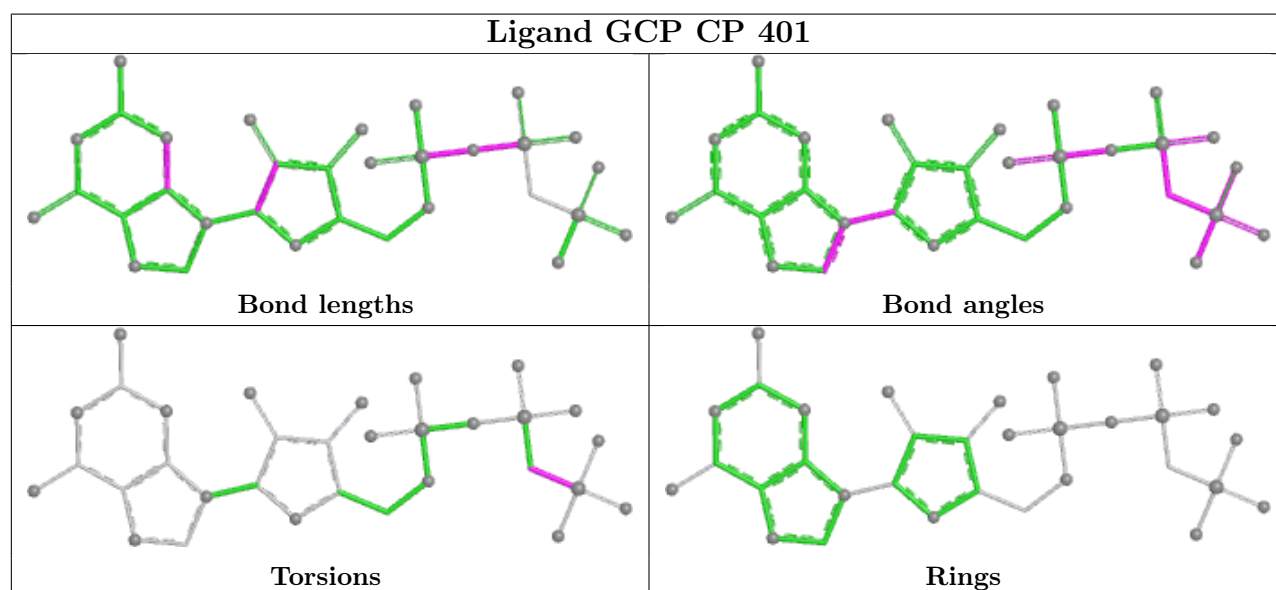
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	B2	1919	OHX	1	0
89	B2	2070	OHX	1	0
89	B2	1928	OHX	1	0
89	B2	2046	OHX	5	0
89	B2	1916	OHX	1	0
89	B2	2039	OHX	1	0
89	B2	1955	OHX	1	0
89	B2	1901	OHX	1	0
89	B2	1969	OHX	7	0
89	B2	2009	OHX	2	0
89	B2	2008	OHX	1	0
89	B2	1990	OHX	1	0
89	B2	1963	OHX	4	0
89	B2	1940	OHX	5	0
89	B2	1906	OHX	3	0
89	B2	2034	OHX	1	0
89	B2	1962	OHX	1	0
89	B2	1975	OHX	3	0
89	B2	2053	OHX	1	0
89	B2	1924	OHX	1	0
89	B2	1961	OHX	4	0
89	B2	1987	OHX	1	0
89	B2	1983	OHX	1	0
89	B2	1938	OHX	1	0
89	B2	2047	OHX	1	0
89	B2	2050	OHX	7	0
89	B2	1930	OHX	1	0
89	B2	2059	OHX	1	0
89	B2	1982	OHX	5	0
89	B2	2024	OHX	1	0
89	B2	2061	OHX	1	0
89	B2	1937	OHX	1	0
89	B2	2084	OHX	1	0
89	B2	2015	OHX	1	0
89	B2	1910	OHX	2	0
89	B2	2076	OHX	1	0
89	B2	1988	OHX	8	0
89	B2	1996	OHX	1	0
89	B2	1945	OHX	1	0
89	B2	2077	OHX	2	0
89	B2	2040	OHX	1	0
89	B2	2022	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	B2	1979	OHX	1	0
89	B2	2071	OHX	17	0
89	B2	2014	OHX	1	0
89	B2	1953	OHX	2	0
89	B2	1907	OHX	6	0
89	B2	2075	OHX	1	0
89	B2	2073	OHX	6	0
89	B2	2083	OHX	11	0
89	B2	1989	OHX	1	0
89	B2	1970	OHX	1	0
89	B2	2027	OHX	7	0
89	B2	1949	OHX	1	0
89	B2	2048	OHX	1	0
89	B2	2035	OHX	2	0
89	B2	2045	OHX	1	0
89	B2	1973	OHX	1	0
89	AL	201	OHX	3	0
89	B2	1948	OHX	1	0
89	B2	1929	OHX	1	0
89	B2	1957	OHX	1	0
89	B2	1960	OHX	1	0
89	B2	2065	OHX	2	0
89	B2	1918	OHX	8	0
90	CP	401	GCP	62	0
89	B2	1921	OHX	6	0
89	B2	2011	OHX	2	0
89	B2	1972	OHX	2	0
89	B2	1991	OHX	3	0
89	B2	1977	OHX	7	0
89	B2	1923	OHX	1	0
89	B2	2016	OHX	7	0
89	B2	1922	OHX	7	0
89	B2	1968	OHX	5	0
89	B2	2064	OHX	6	0
89	B2	2049	OHX	3	0
89	B2	2079	OHX	5	0
89	B2	2069	OHX	2	0
89	B2	1978	OHX	1	0
89	B2	2042	OHX	1	0
89	B2	2012	OHX	1	0
89	B2	2043	OHX	1	0
89	AI	302	OHX	2	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
45	BK	2
81	B5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BK	52:UNK	C	54:UNK	N	9.71

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BK	23:UNK	C	28:UNK	N	8.84
1	B5	1285:G	O3'	1286:A	P	6.77

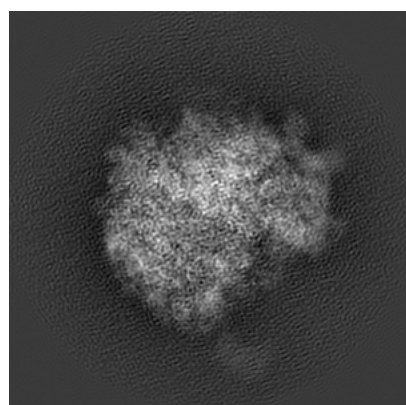
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2421. These allow visual inspection of the internal detail of the map and identification of artifacts.

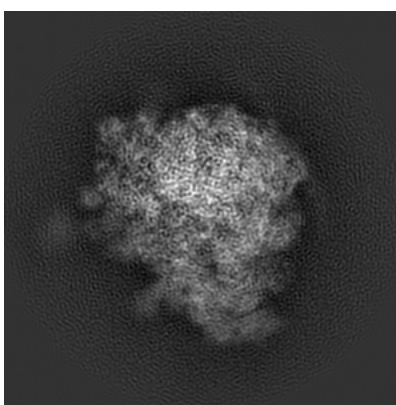
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

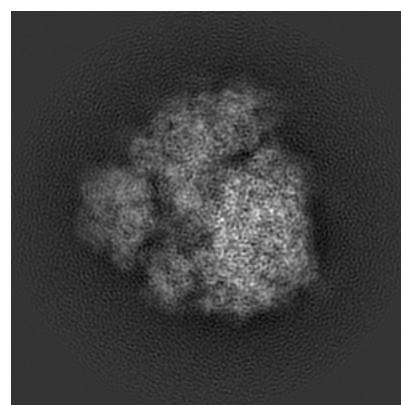
6.1.1 Primary map



X



Y

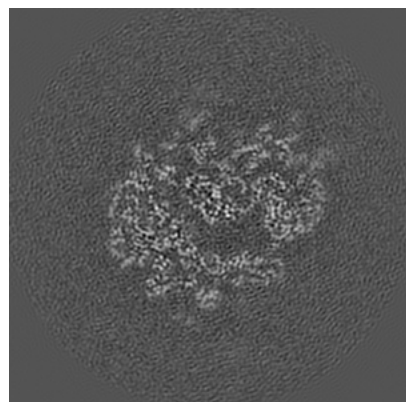


Z

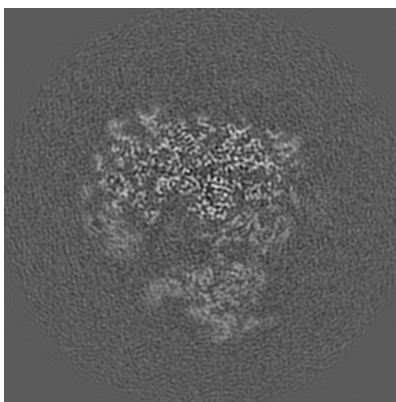
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

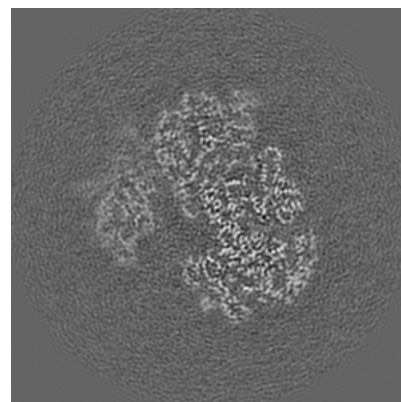
6.2.1 Primary map



X Index: 120



Y Index: 120

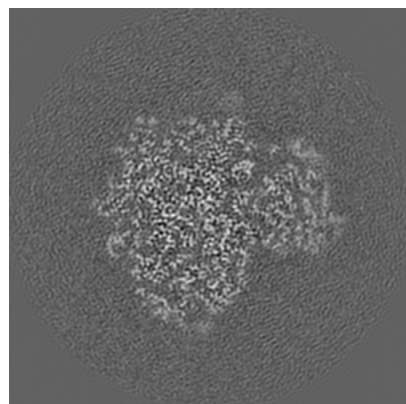


Z Index: 120

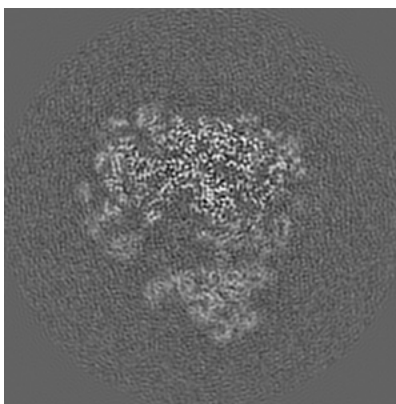
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

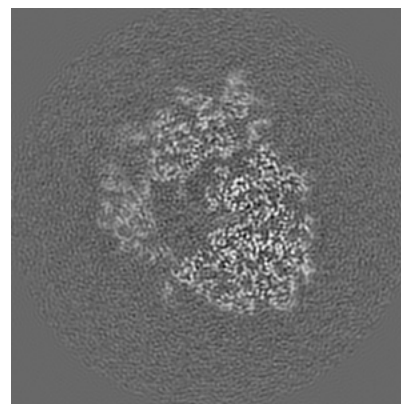
6.3.1 Primary map



X Index: 133



Y Index: 118

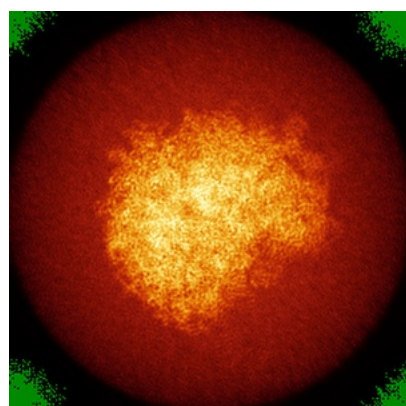


Z Index: 112

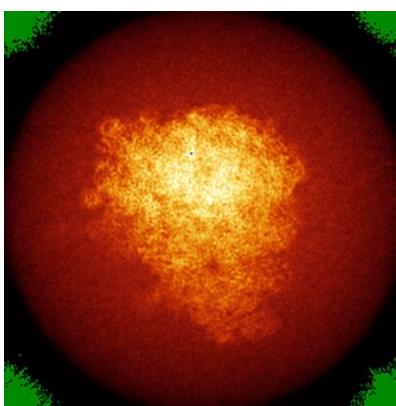
The images above show the largest variance slices of the map in three orthogonal directions.

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

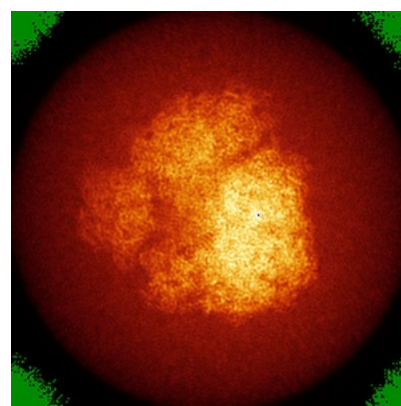
6.4.1 Primary map



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](#)

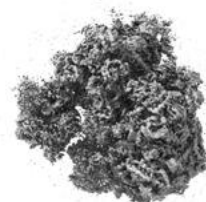
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

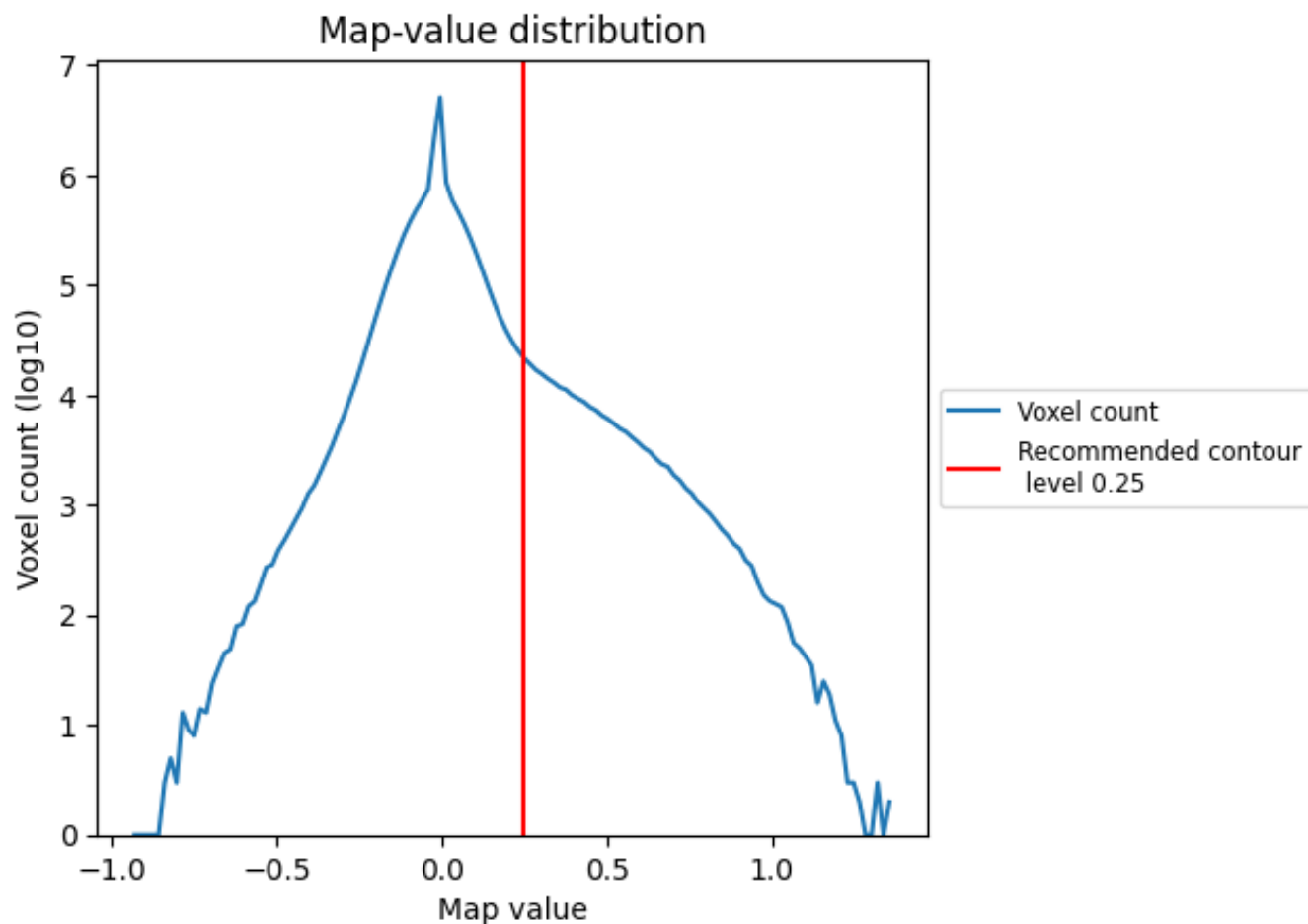
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

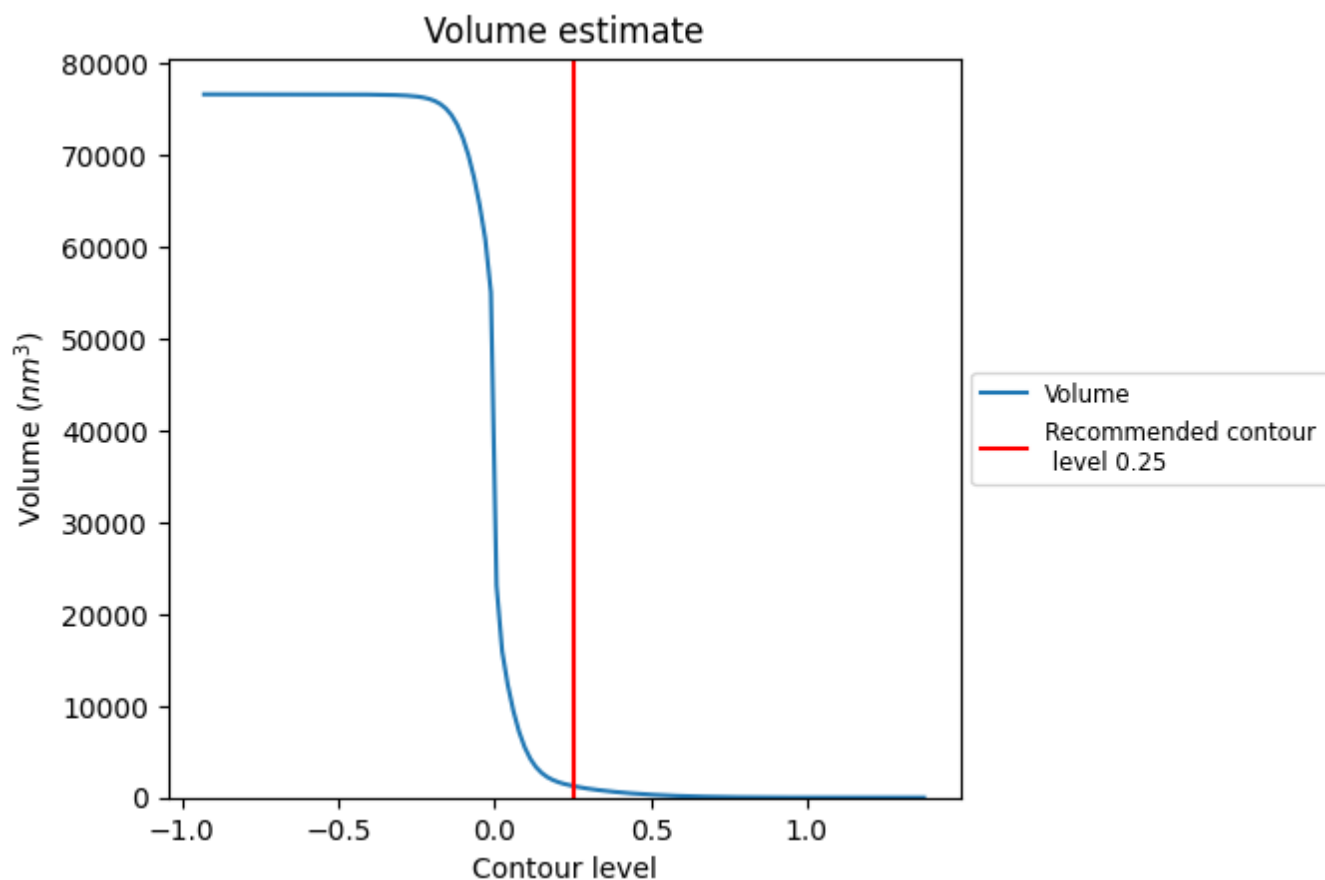
This section contains the results of statistical analysis of the map.

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.

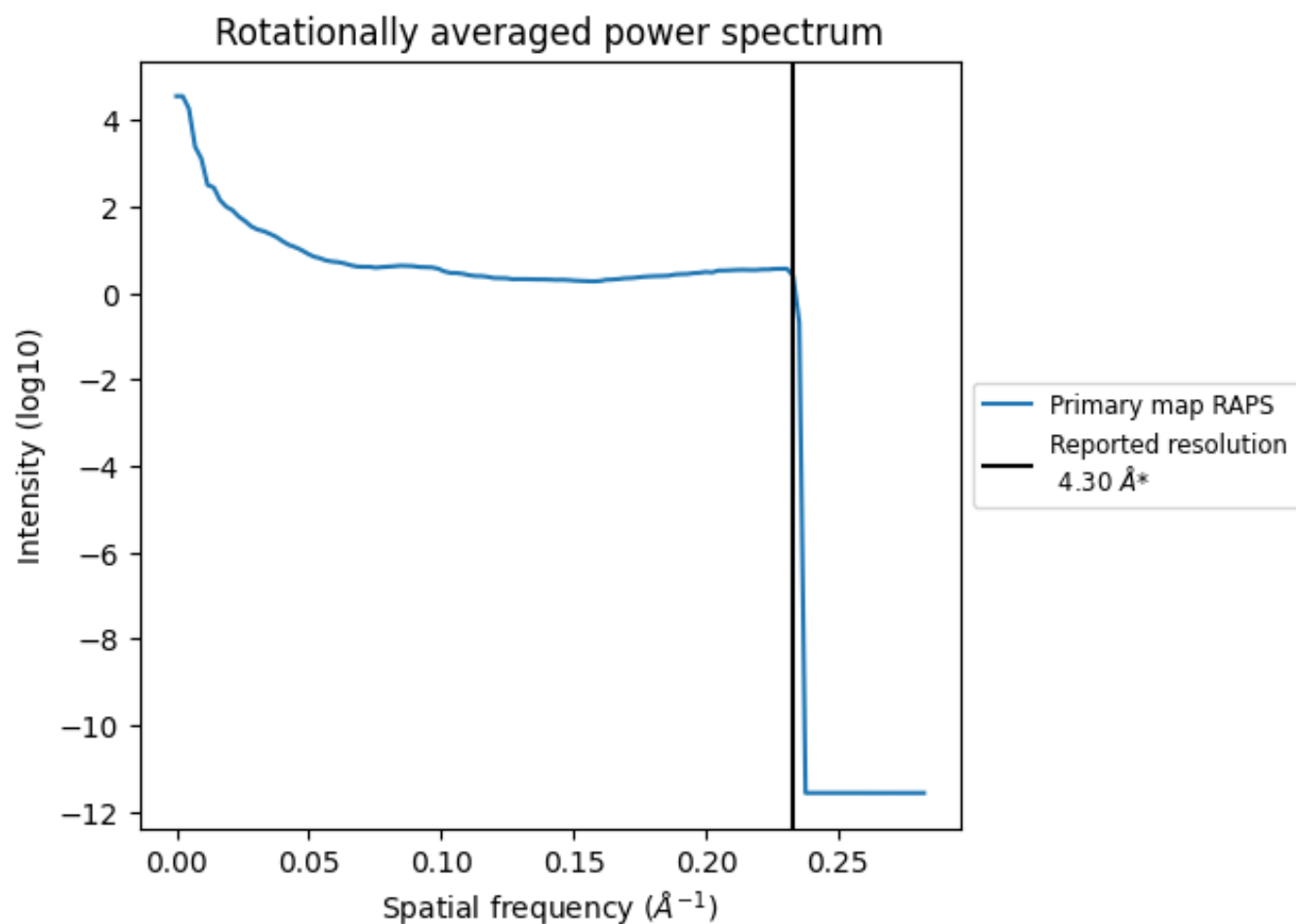
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1268 nm³; this corresponds to an approximate mass of 1145 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 0.233 $\text{\AA}^{-1}$

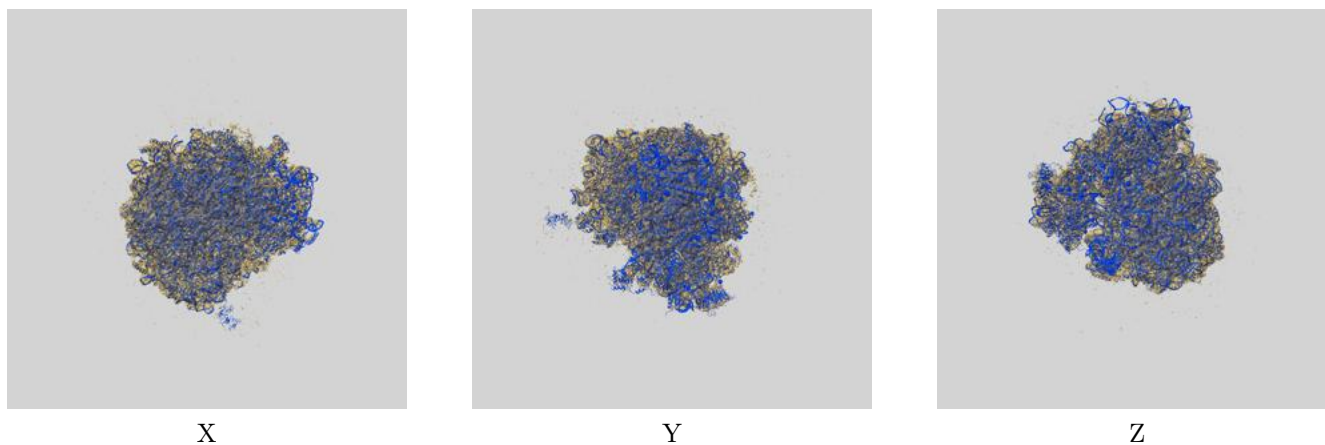
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

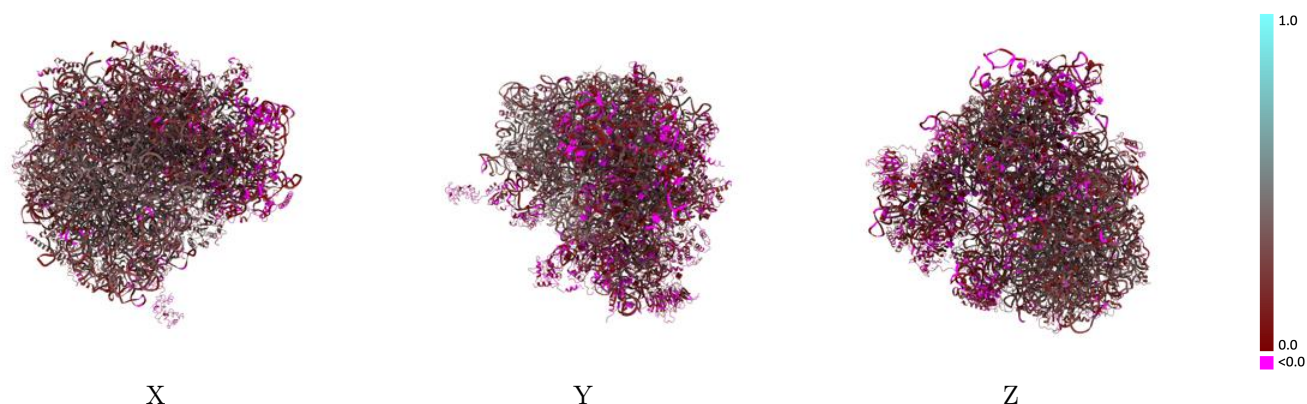
This section contains information regarding the fit between EMDB map EMD-2421 and PDB model 4V8Y. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



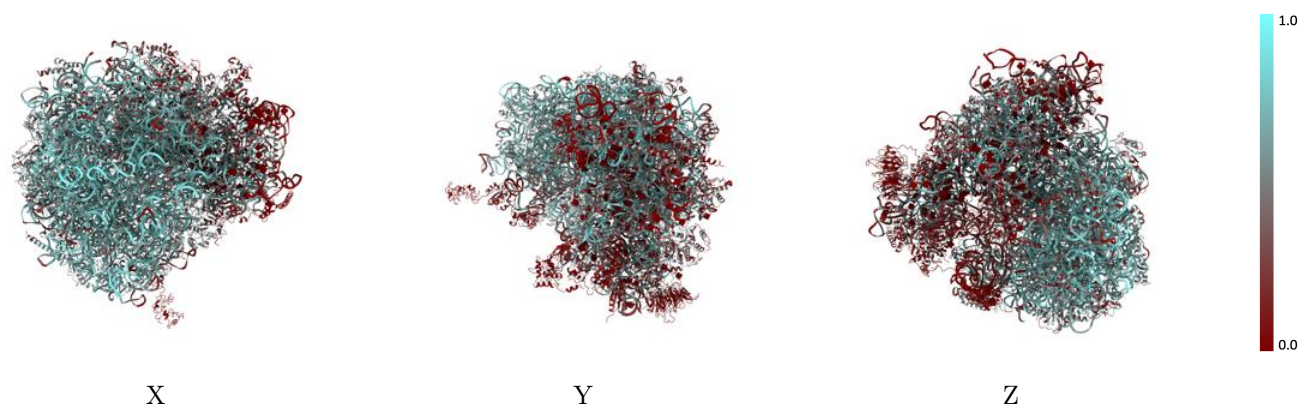
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



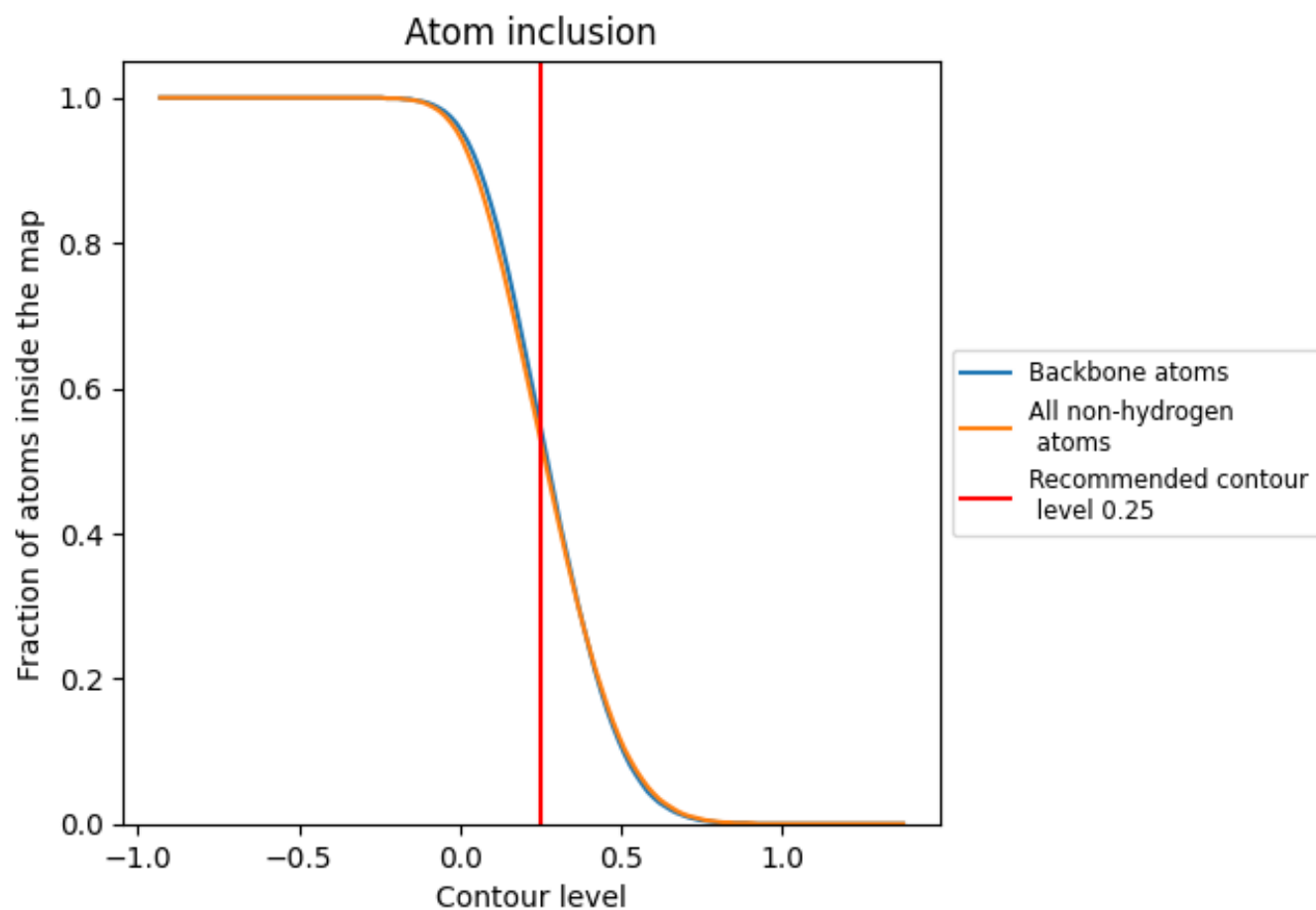
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 53% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5270	 0.2420
A0	 0.2180	 0.1500
A1	 0.3320	 0.2030
A2	 0.1110	 0.0850
A3	 0.3060	 0.1190
A4	 0.3680	 0.2220
A5	 0.0550	 0.0540
A6	 0.1450	 0.1050
A7	 0.0260	 0.0790
AA	 0.3780	 0.1600
AB	 0.1710	 0.1110
AC	 0.4440	 0.2240
AD	 0.1730	 0.1070
AE	 0.4030	 0.1750
AF	 0.1670	 0.1060
AG	 0.2610	 0.0990
AH	 0.3970	 0.2020
AI	 0.3590	 0.1500
AJ	 0.4460	 0.2230
AK	 0.1690	 0.0790
AL	 0.4510	 0.2490
AM	 0.0360	 -0.0000
AN	 0.4670	 0.2480
AO	 0.1450	 0.1020
AP	 0.1740	 0.0870
AQ	 0.2330	 0.1700
AR	 0.2900	 0.1420
AS	 0.1970	 0.1080
AT	 0.2830	 0.1880
AU	 0.1640	 0.1250
AV	 0.3930	 0.1690
AW	 0.5320	 0.2900
AX	 0.5030	 0.3100
AY	 0.3640	 0.1540
AZ	 0.1150	 0.0760



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Chain	Atom inclusion	Q-score
B2	 0.5410	 0.2310
B5	 0.7100	 0.3000
B7	 0.7170	 0.2600
B8	 0.7570	 0.3200
BA	 0.4040	 0.1650
BB	 0.6060	 0.3180
BC	 0.5800	 0.3070
BD	 0.5060	 0.2520
BE	 0.5360	 0.2680
BF	 0.6150	 0.3410
BG	 0.4650	 0.2000
BH	 0.5660	 0.3090
BI	 0.5350	 0.2970
BJ	 0.4740	 0.2450
BK	 0.1010	 0.0740
BL	 0.4900	 0.2450
BM	 0.5740	 0.2720
BN	 0.5280	 0.2690
BO	 0.6200	 0.3580
BP	 0.6110	 0.3320
BQ	 0.5430	 0.2750
BR	 0.3970	 0.1560
BS	 0.6050	 0.3220
BT	 0.5550	 0.3410
BU	 0.3680	 0.1280
BV	 0.5430	 0.3280
BW	 0.2660	 0.1480
BX	 0.4710	 0.2250
BY	 0.5570	 0.2910
BZ	 0.3320	 0.0810
Ba	 0.5480	 0.2710
Bb	 0.5200	 0.2800
Bc	 0.3110	 0.0810
Bd	 0.4900	 0.2340
Be	 0.5940	 0.3510
Bf	 0.6090	 0.3240
Bg	 0.3960	 0.1360
Bh	 0.5220	 0.2380
Bi	 0.4950	 0.2450
Bj	 0.5900	 0.2960
Bk	 0.3260	 0.1190
Bl	 0.4990	 0.2270

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Chain	Atom inclusion	Q-score
Bm	 0.5890	 0.3320
Bn	 0.1280	 0.0630
Bo	 0.5180	 0.3150
Bq	 0.1870	 0.1280
Br	 0.0380	 0.0850
Bs	 0.0040	 0.0850
By	 0.0420	 0.1160
CL	 0.0170	 0.0430
CN	 0.1000	 0.0590
CP	 0.3950	 0.2720
CW	 0.2230	 0.2310