



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 10:41 am GMT

PDB ID : 4V8Y
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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

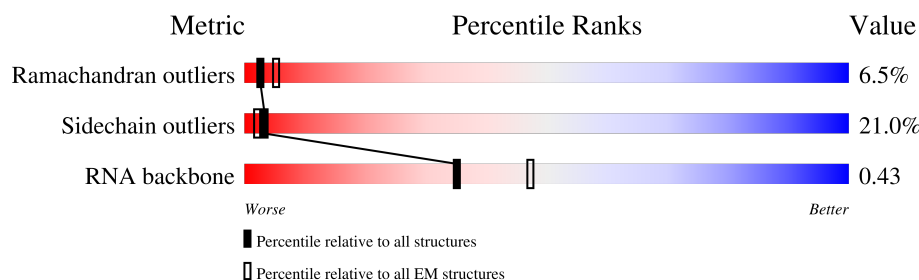
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	A1	82	
3	A2	67	
4	A3	56	
5	A4	63	
6	A5	152	
7	A6	319	
8	A7	273	

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Mol	Chain	Length	Quality of chain
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	
29	AU	121	
30	AV	87	
31	AW	130	
32	AX	145	
33	AY	135	

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Mol	Chain	Length	Quality of chain
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	
54	BT	159	
55	BU	120	
56	BV	136	
57	BW	155	
58	BX	141	

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Mol	Chain	Length	Quality of chain
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	
79	By	229	
79	CL	229	
80	B2	1800	
81	B5	3396	
82	B7	121	

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Mol	Chain	Length	Quality of chain
83	B8	158	<div><div><div></div><div></div><div></div></div><div>49%41%10%</div></div>
84	CN	87	<div><div><div></div><div></div><div></div></div><div>99%36%53%11%</div></div>
85	CP	339	<div><div><div></div><div></div><div></div></div><div>50%83%15%</div></div>
86	CW	76	<div><div><div></div><div></div><div></div></div><div>87%46%34%16%</div></div>

2 Entry composition [i](#)

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		

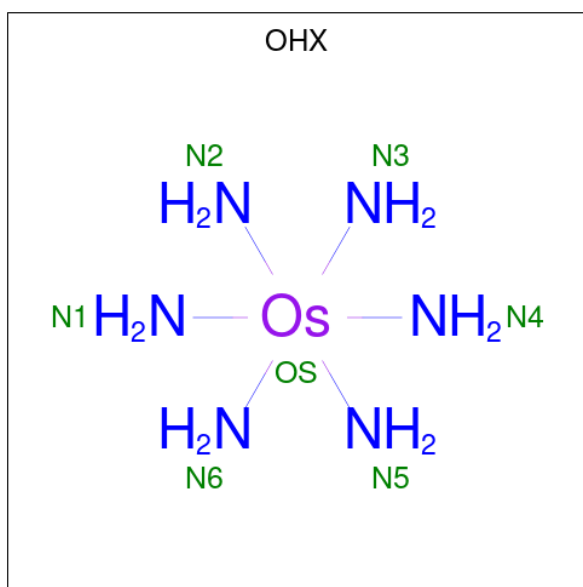
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: 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 (three-letter code: 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
			14	12	2	
89	AI	1	Total	N	Os	0
			14	12	2	
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
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	

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WORLDWIDE
PDB
PROTEIN DATA BANK

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[illegible]

[illegible]

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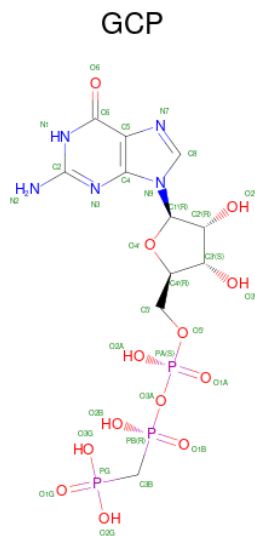
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Mol	Chain	Residues	Atoms			AltConf
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B2	1	Total	N	Os	0
			1288	1104	184	
89	B5	1	Total	N	Os	0
			21	18	3	
89	B5	1	Total	N	Os	0
			21	18	3	
89	B5	1	Total	N	Os	0
			21	18	3	

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

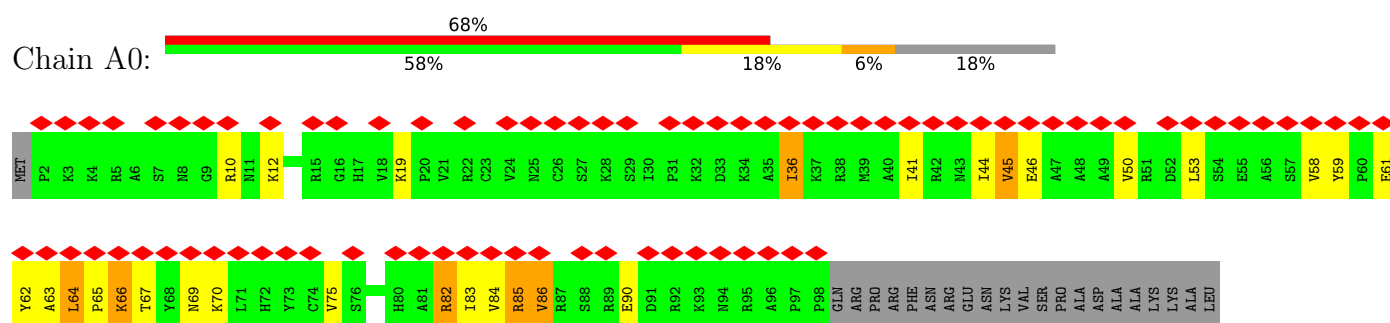


Mol	Chain	Residues	Atoms					AltConf
90	CP	1	Total	C	N	O	P	0
			32	11	5	13	3	

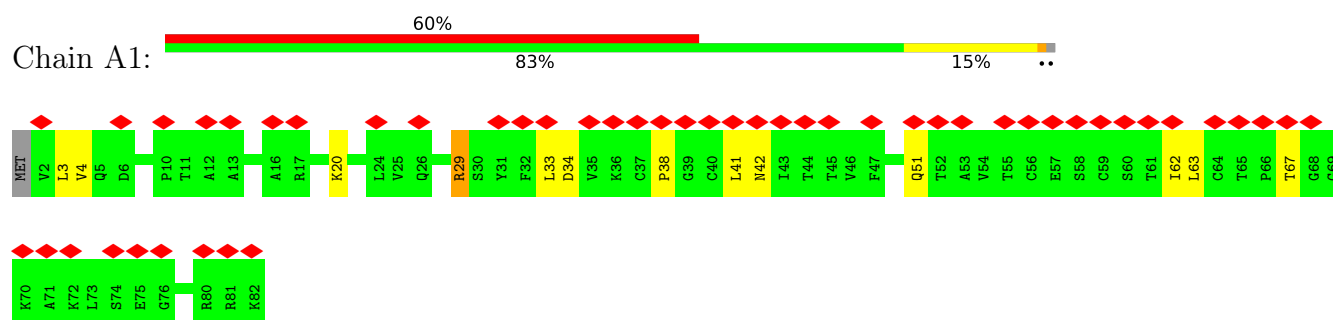
3 Residue-property plots

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.

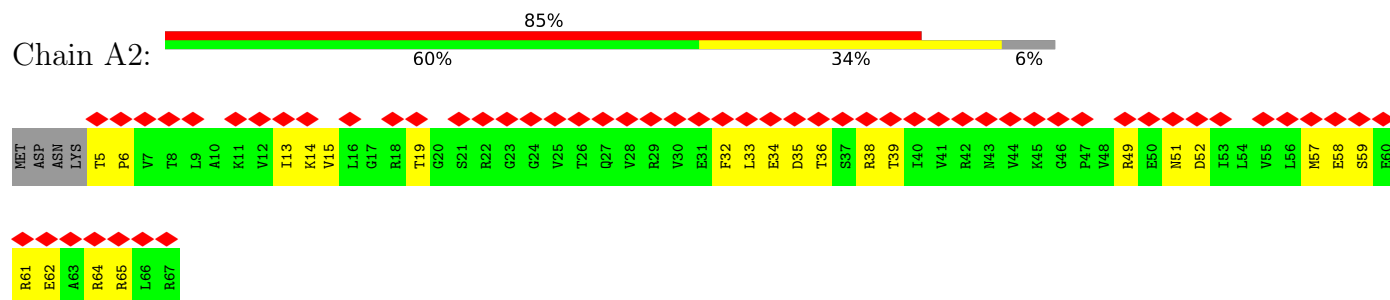
• Molecule 1: 40S RIBOSOMAL PROTEIN S26-A



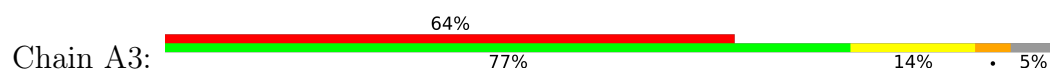
• Molecule 2: 40S RIBOSOMAL PROTEIN S27-A

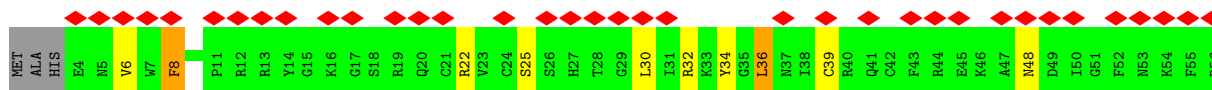


• Molecule 3: 40S RIBOSOMAL PROTEIN S28-A

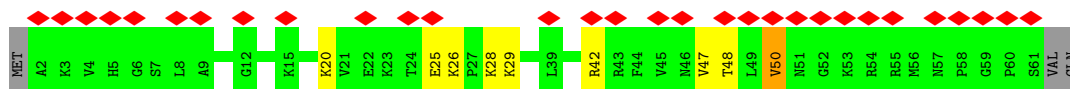
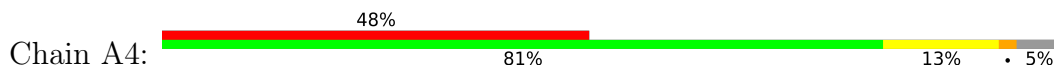


• Molecule 4: 40S RIBOSOMAL PROTEIN S29-A

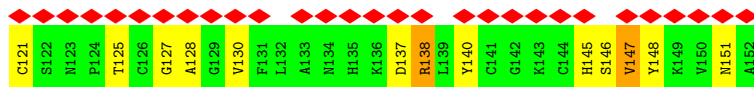
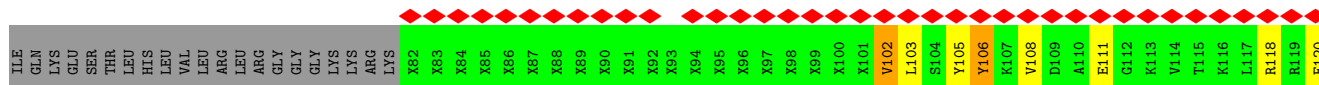
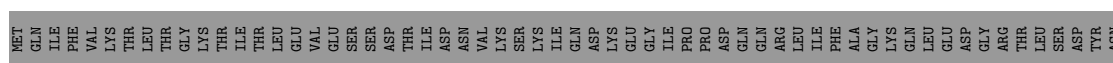
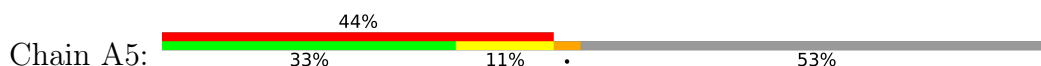




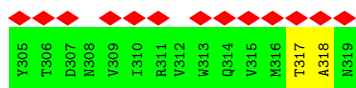
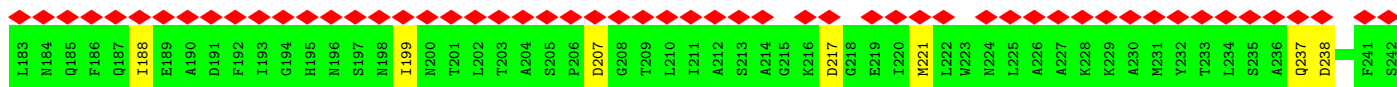
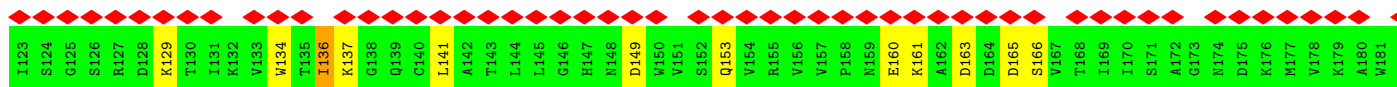
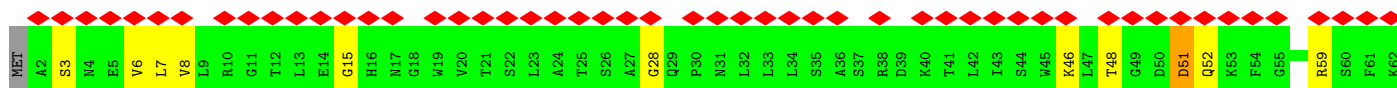
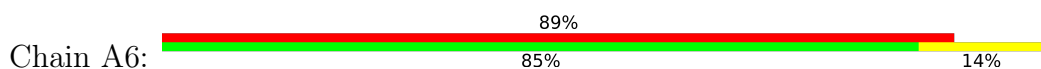
• Molecule 5: 40S RIBOSOMAL PROTEIN S30-A

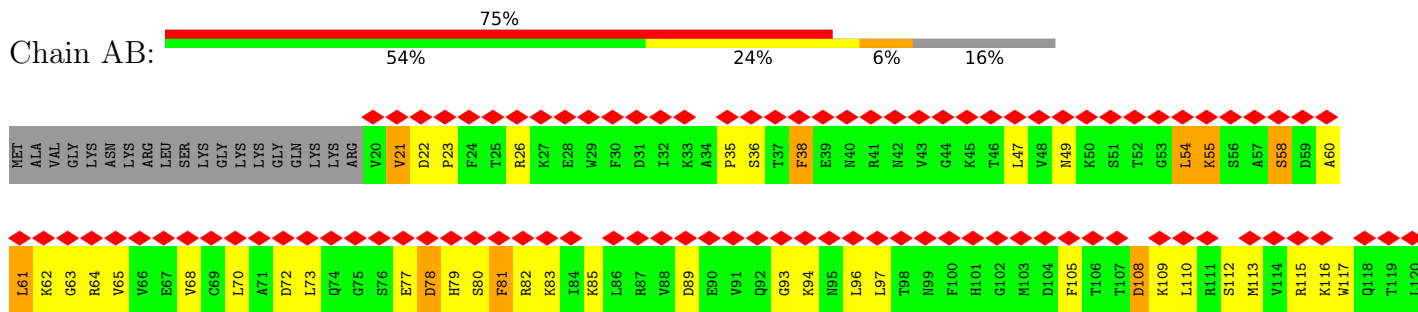


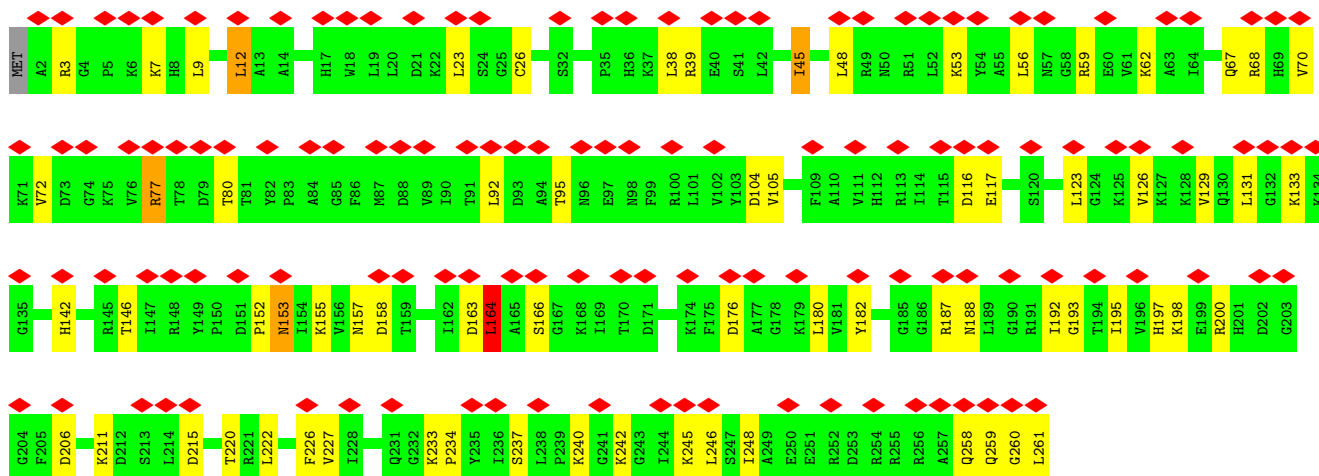
• Molecule 6: UBIQUITIN-40S RIBOSOMAL PROTEIN S31



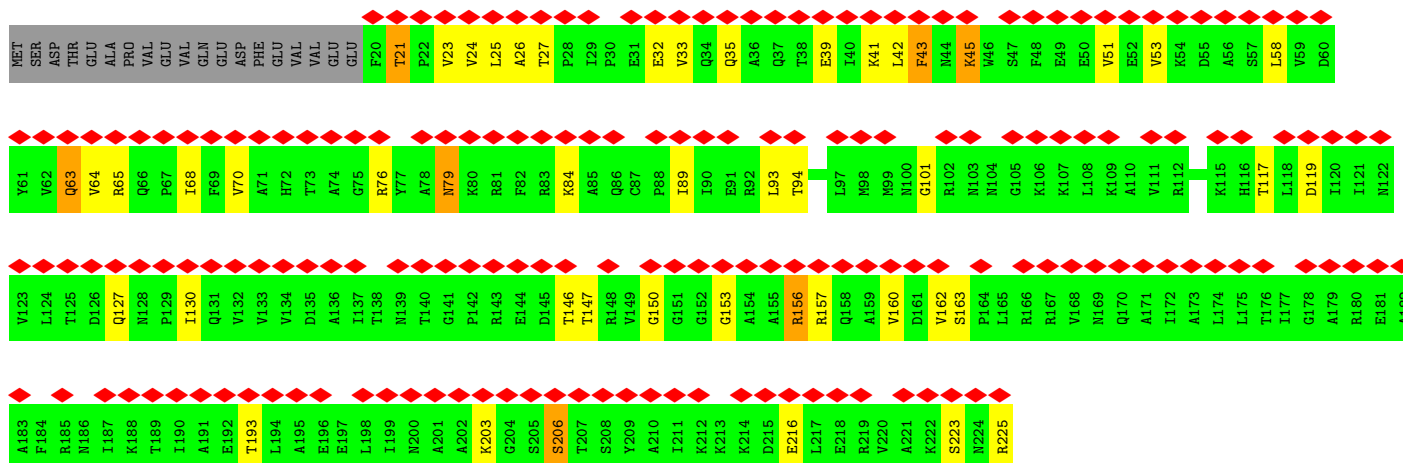
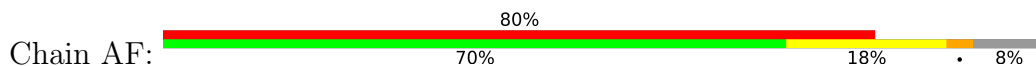
• Molecule 7: GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-LIKE PROTEIN



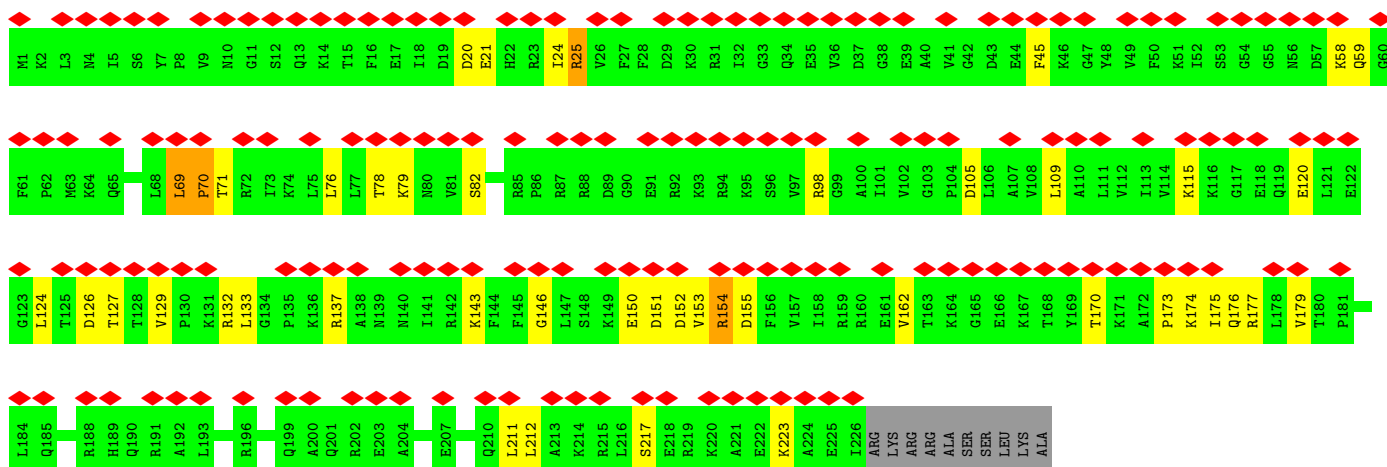
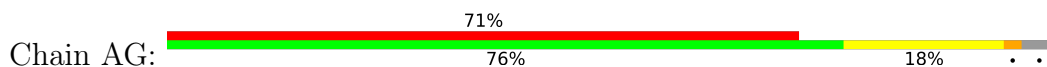


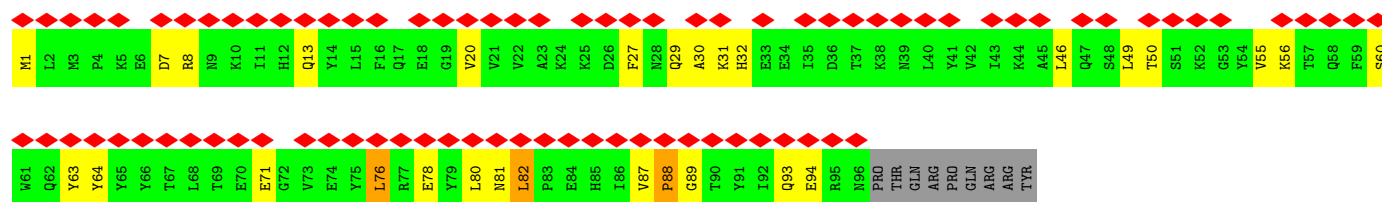


• Molecule 14: 40S RIBOSOMAL PROTEIN S5



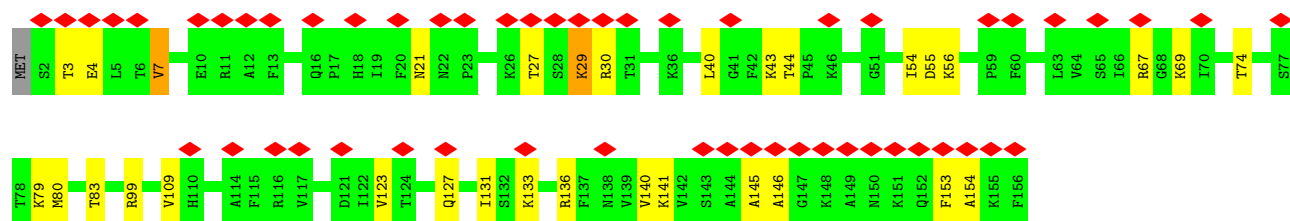
• Molecule 15: 40S RIBOSOMAL PROTEIN S6-A





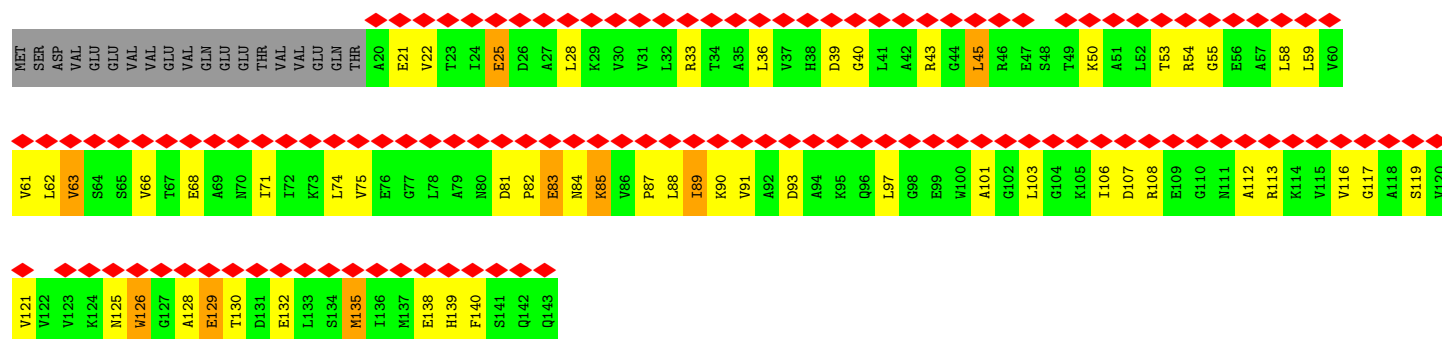
• Molecule 20: 40S RIBOSOMAL PROTEIN S11-A

Chain AL: 35% 79% 19% ..



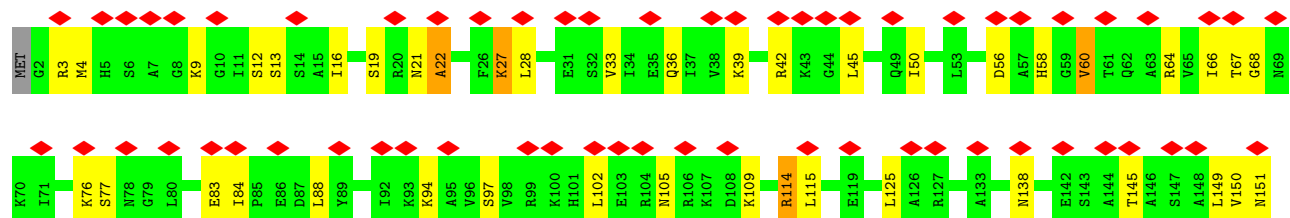
• Molecule 21: 40S RIBOSOMAL PROTEIN S12

Chain AM: 85% 47% 34% 6% 13%



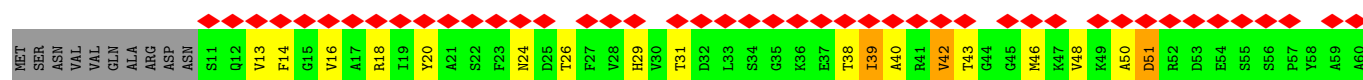
• Molecule 22: 40S RIBOSOMAL PROTEIN S13

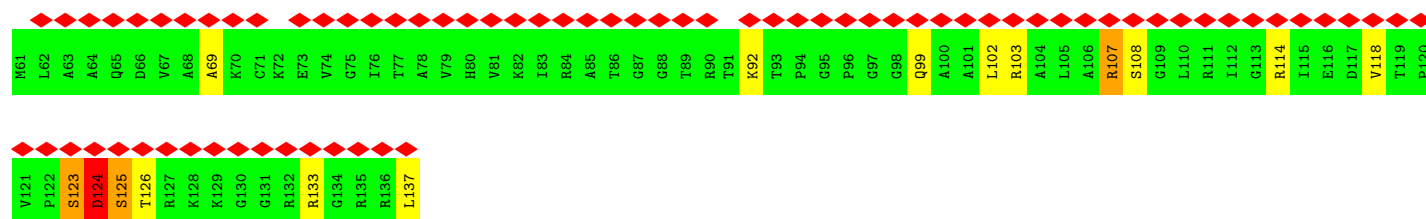
Chain AN: 40% 72% 25% ..



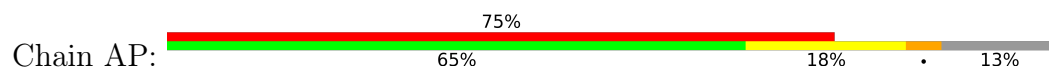
• Molecule 23: 40S RIBOSOMAL PROTEIN S14-A

Chain AO: 87% 69% 19% 7%

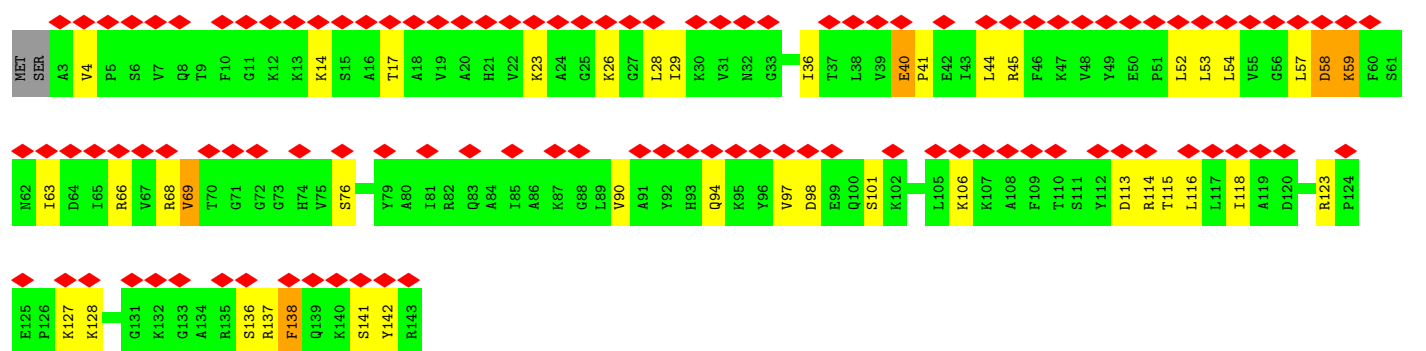
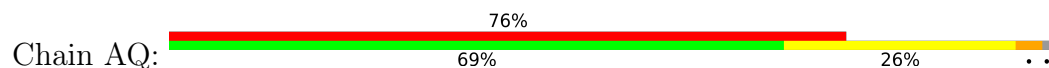




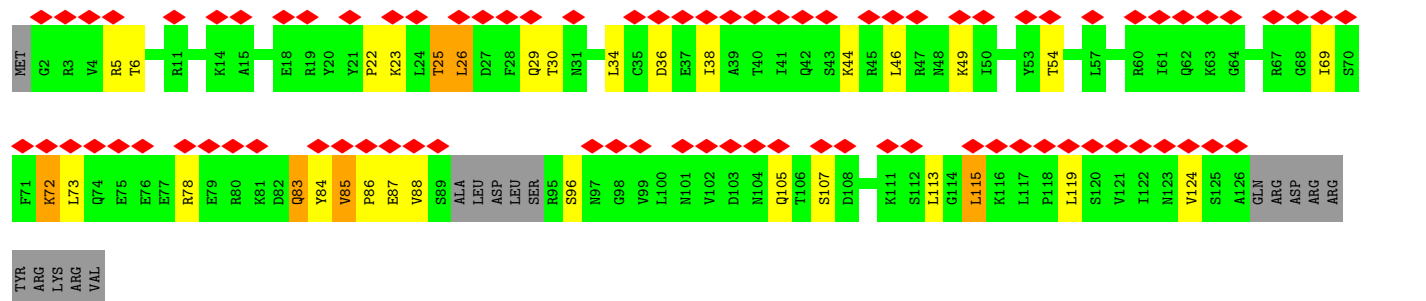
• Molecule 24: 40S RIBOSOMAL PROTEIN S15



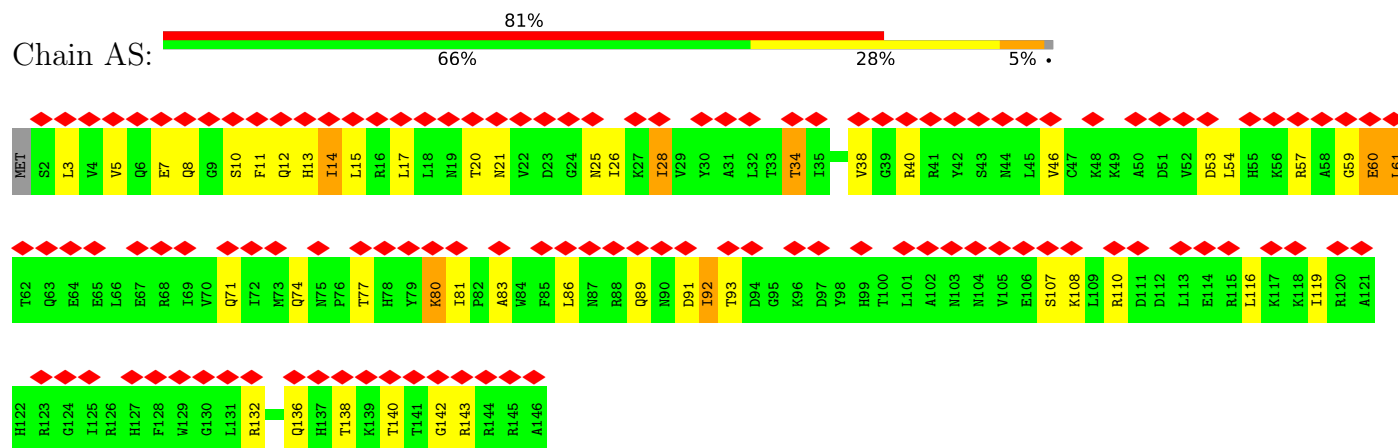
• Molecule 25: 40S RIBOSOMAL PROTEIN S16-A



• Molecule 26: 40S RIBOSOMAL PROTEIN S17-A



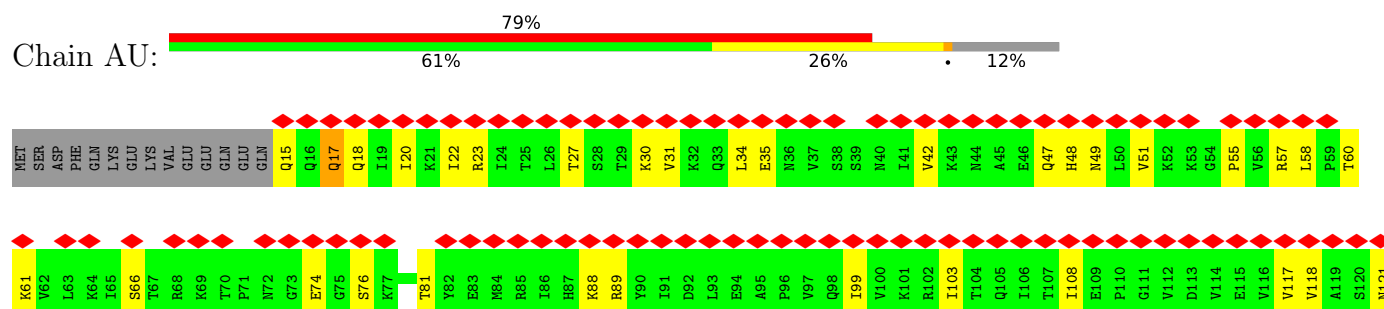
- Molecule 27: 40S RIBOSOMAL PROTEIN S18-A



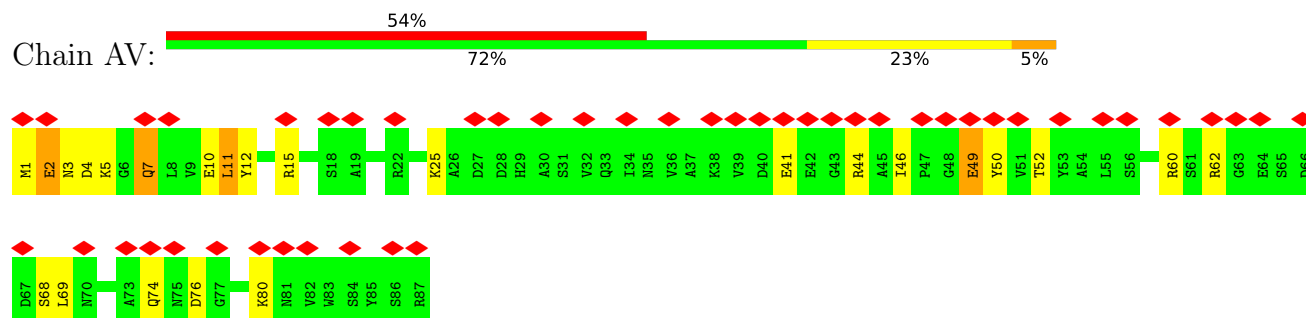
- Molecule 28: 40S RIBOSOMAL PROTEIN S19-A



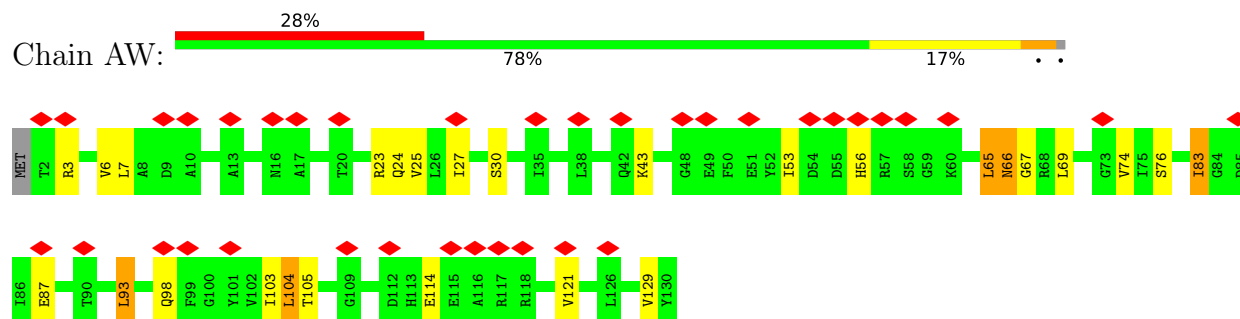
- Molecule 29: 40S RIBOSOMAL PROTEIN S20



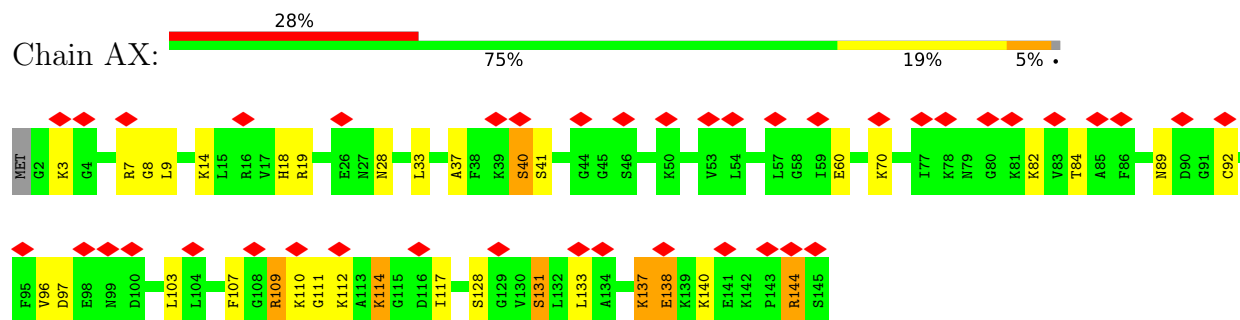
- Molecule 30: 40S RIBOSOMAL PROTEIN S21-A



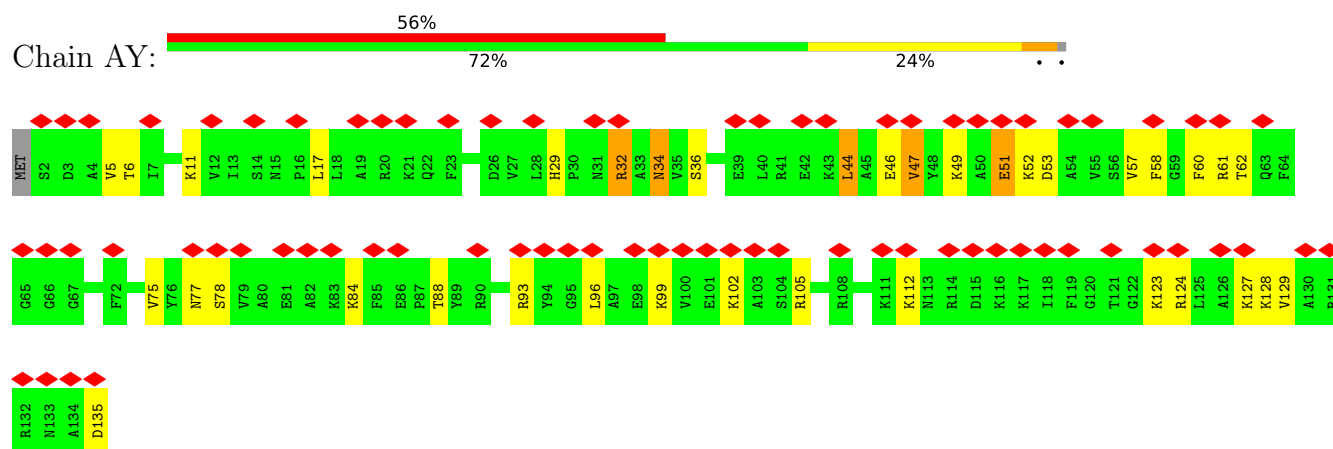
- Molecule 31: 40S RIBOSOMAL PROTEIN S22-A



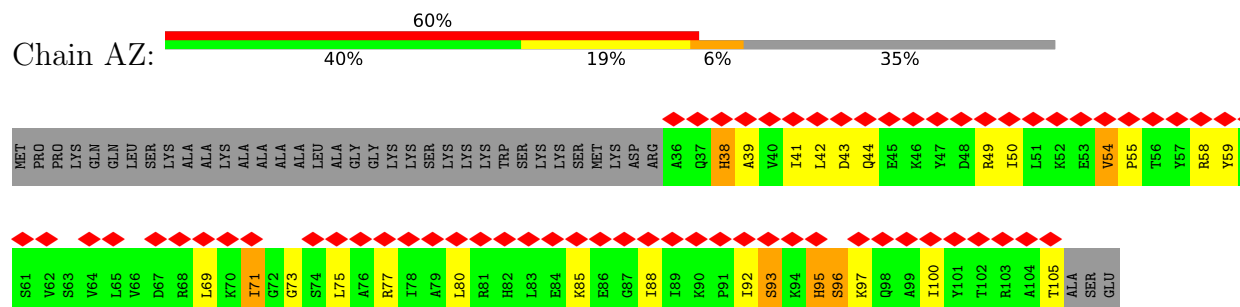
- Molecule 32: 40S RIBOSOMAL PROTEIN S23-A



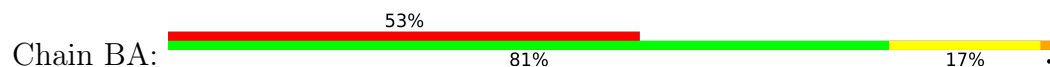
- Molecule 33: 40S RIBOSOMAL PROTEIN S24-A

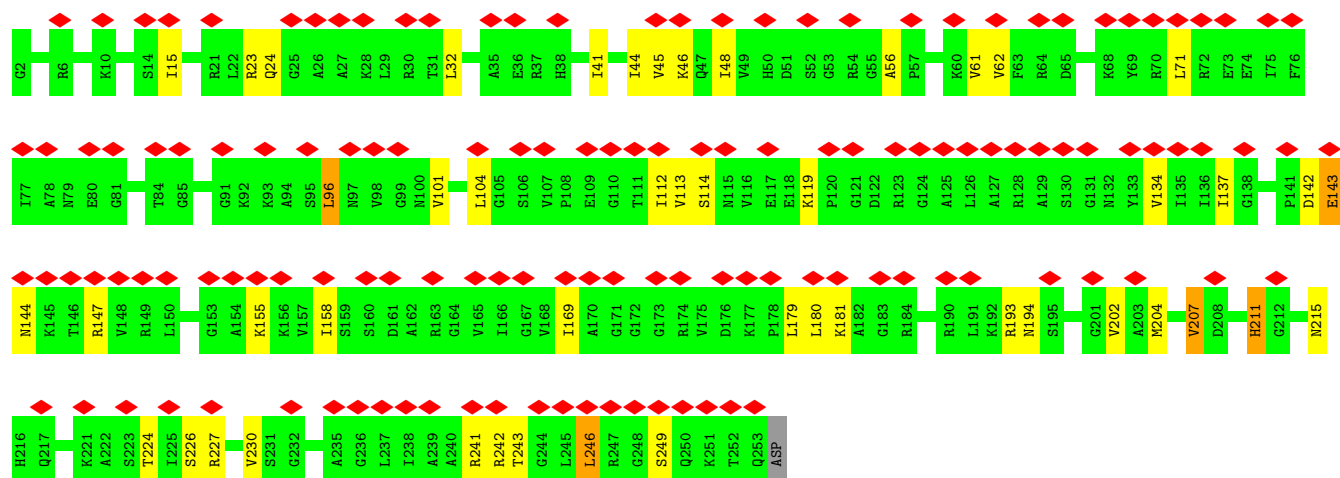


- Molecule 34: 40S RIBOSOMAL PROTEIN S25-A

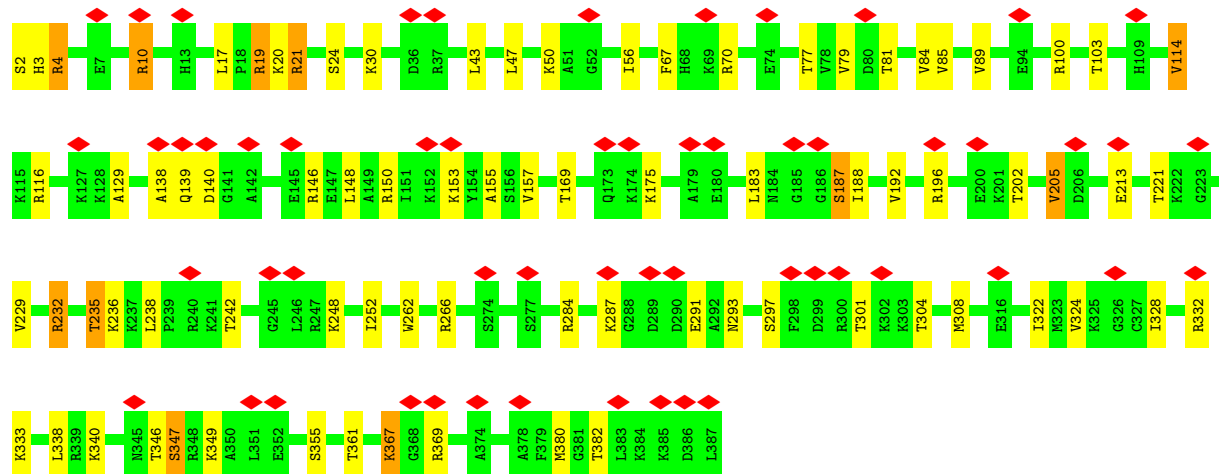
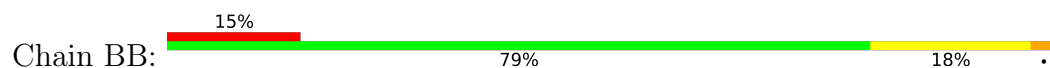


- Molecule 35: 60S RIBOSOMAL PROTEIN L2-B

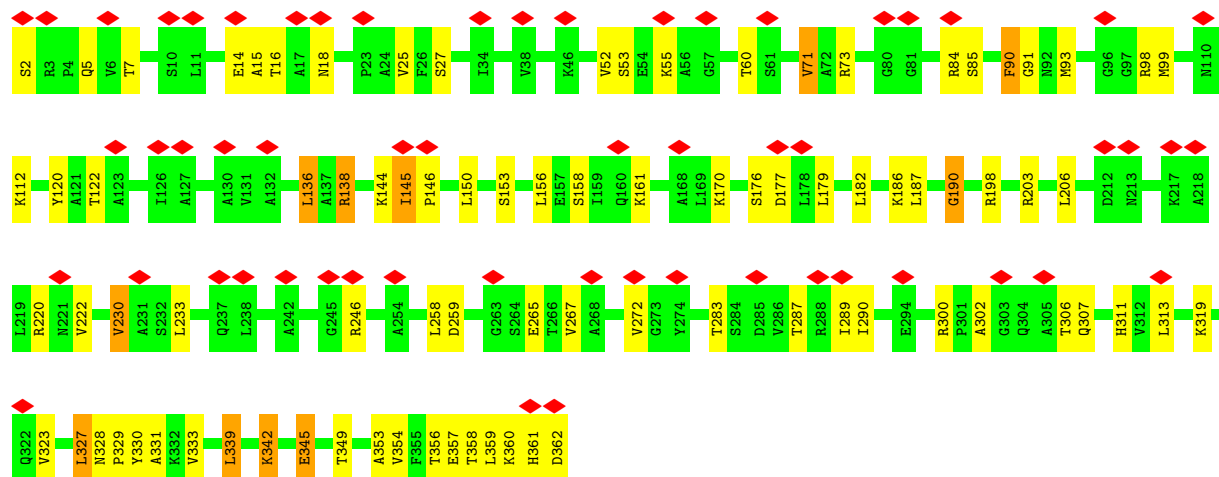
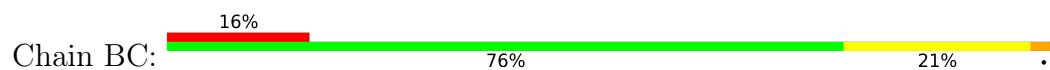




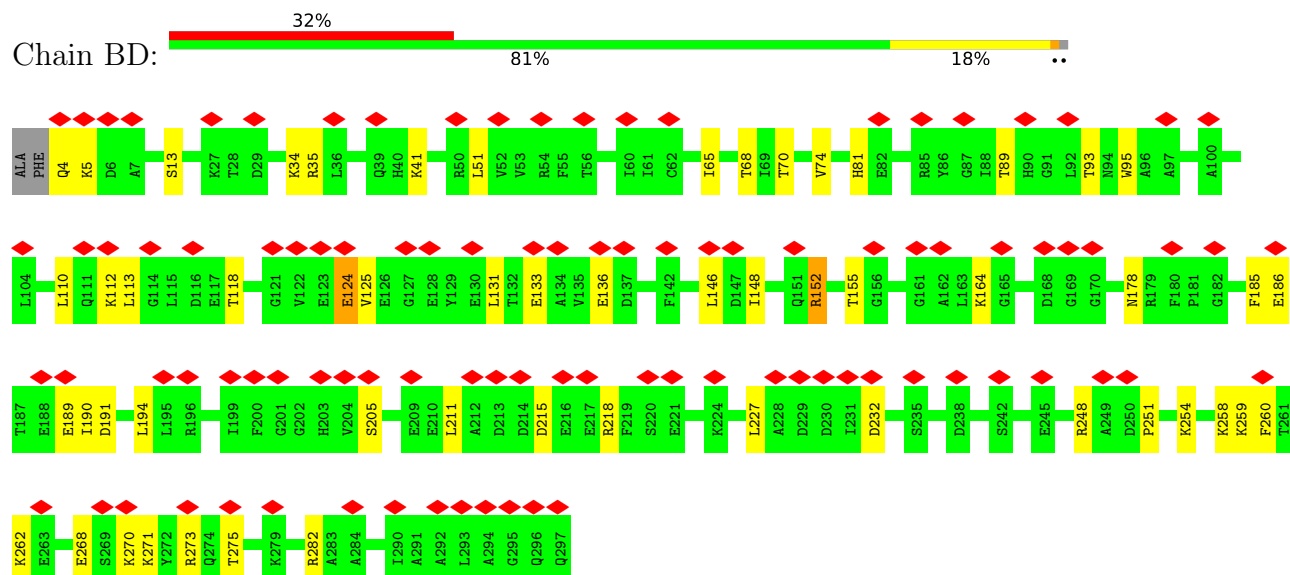
• Molecule 36: 60S RIBOSOMAL PROTEIN L3



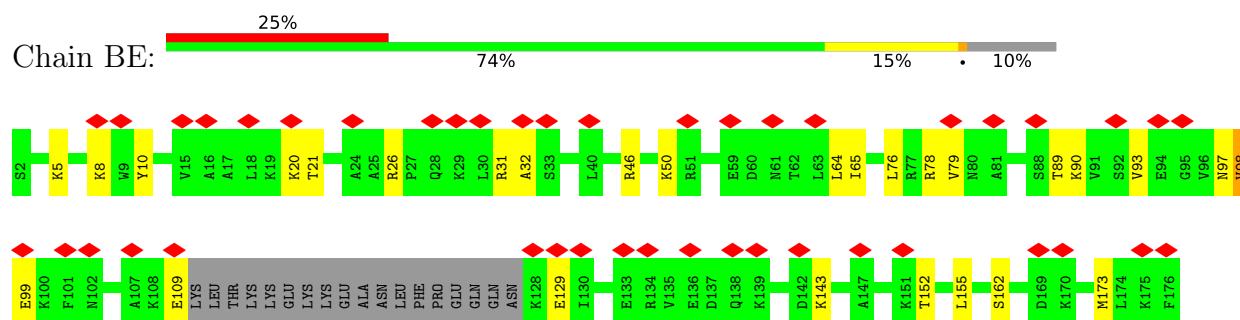
• Molecule 37: 60S RIBOSOMAL PROTEIN L4-A



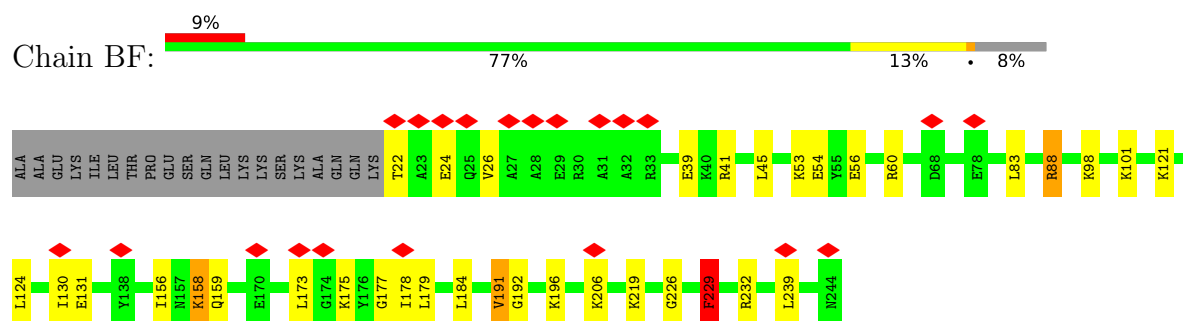
- Molecule 38: 60S RIBOSOMAL PROTEIN L5



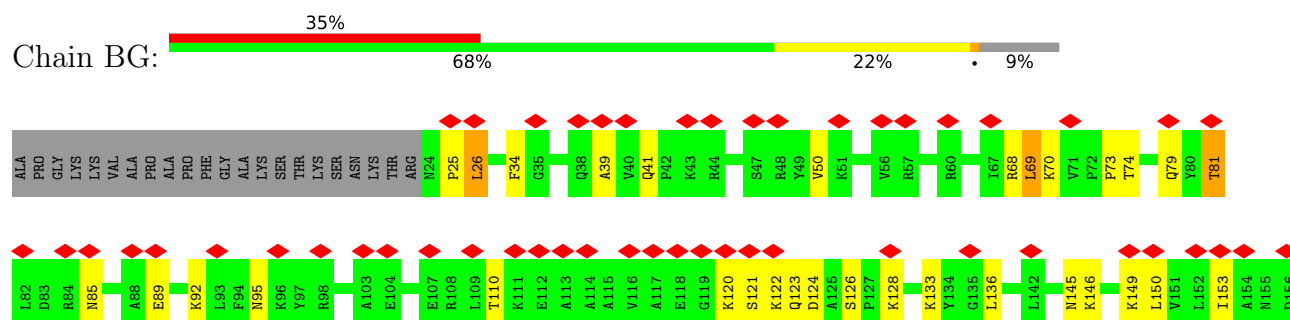
- Molecule 39: 60S RIBOSOMAL PROTEIN L6-A

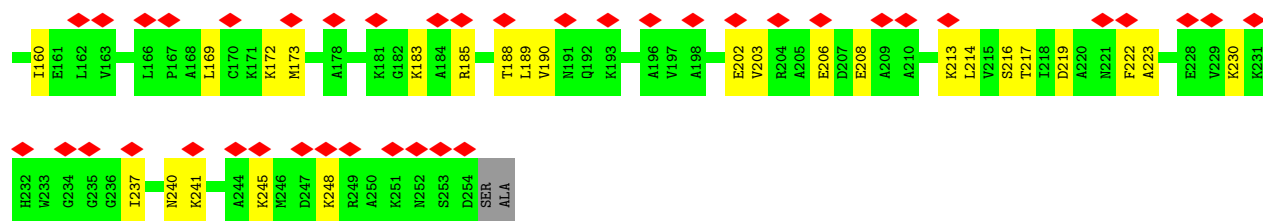


- Molecule 40: 60S RIBOSOMAL PROTEIN L7-A

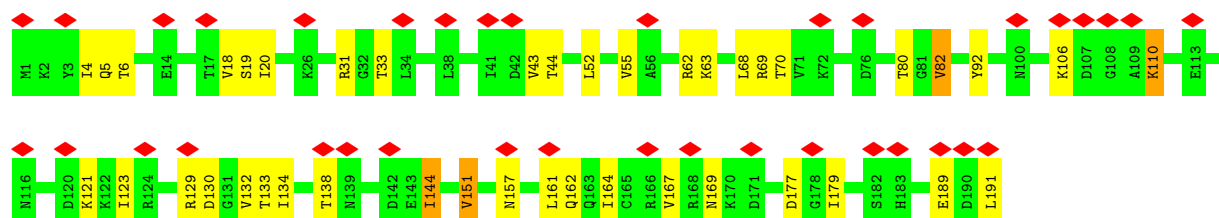
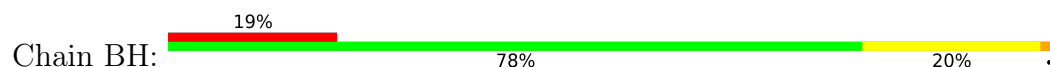


- Molecule 41: 60S RIBOSOMAL PROTEIN L8-A

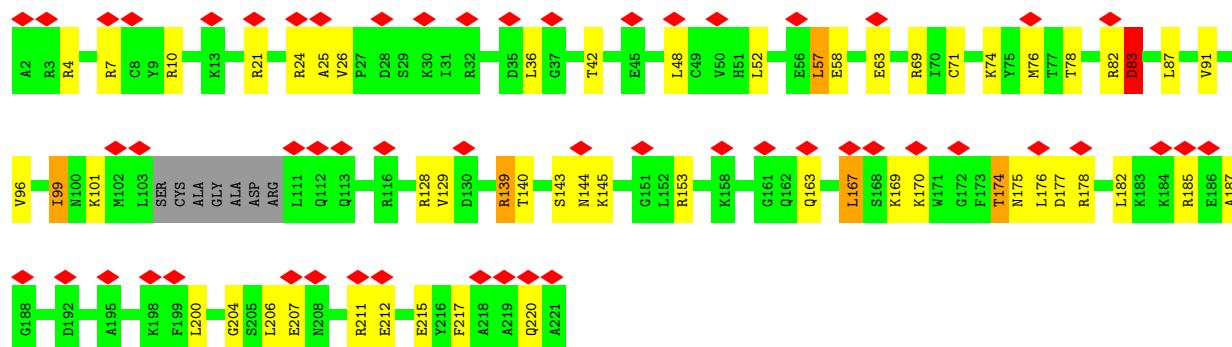
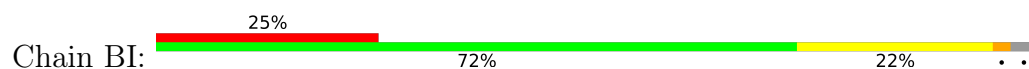




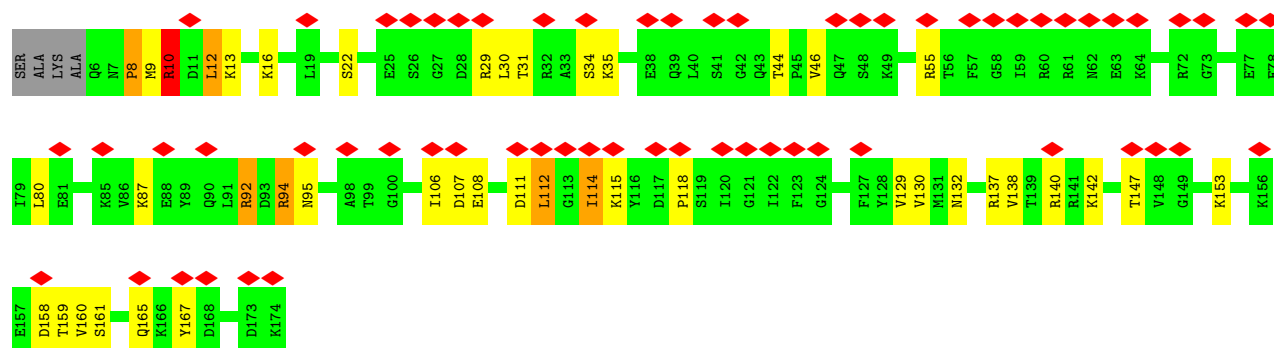
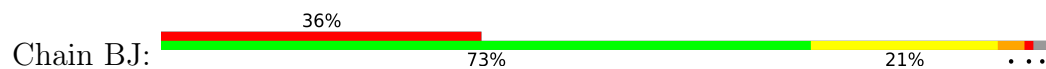
• Molecule 42: 60S RIBOSOMAL PROTEIN L9-A




• Molecule 43: 60S RIBOSOMAL PROTEIN L10

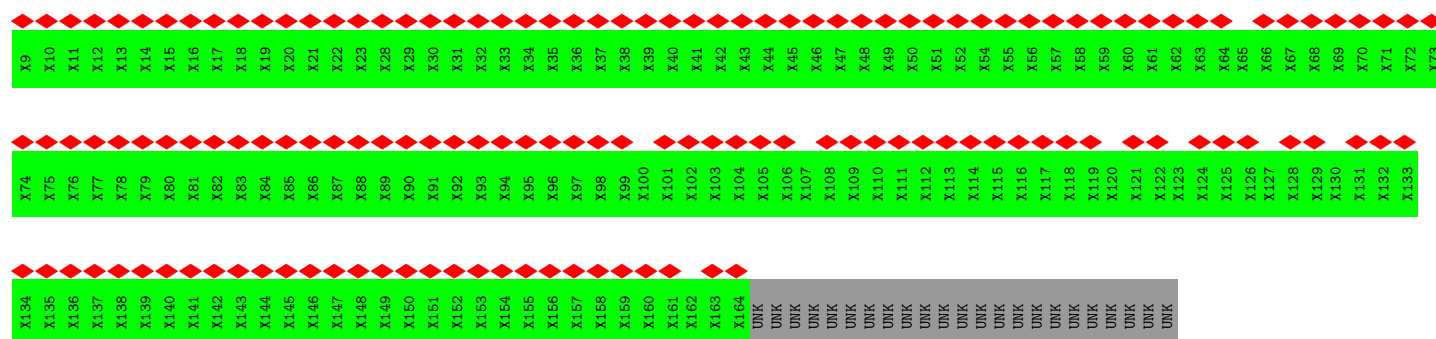


• Molecule 44: 60S RIBOSOMAL PROTEIN L11-A




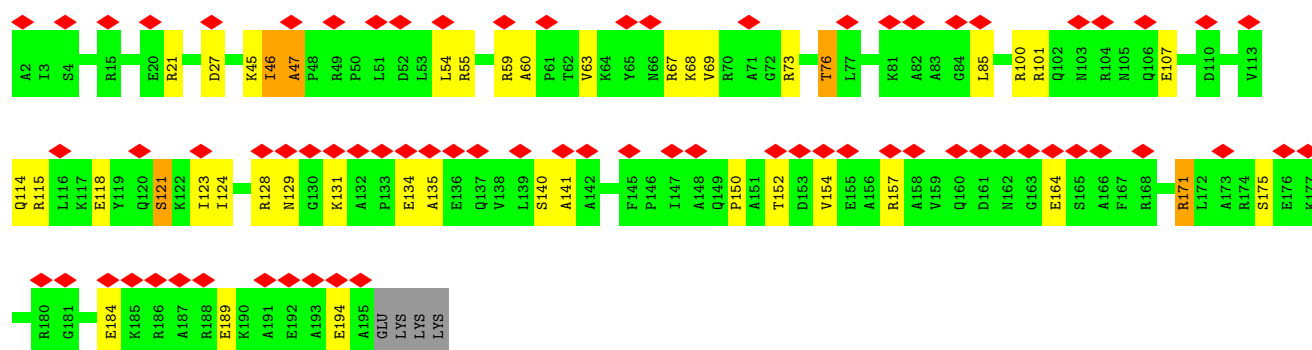
• Molecule 45: 60S RIBOSOMAL PROTEIN L11-A

Chain BK: 




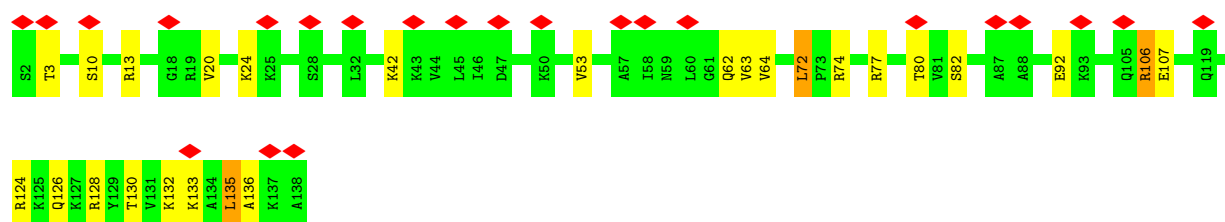
• Molecule 46: 60S RIBOSOMAL PROTEIN L13-A

Chain BL: 




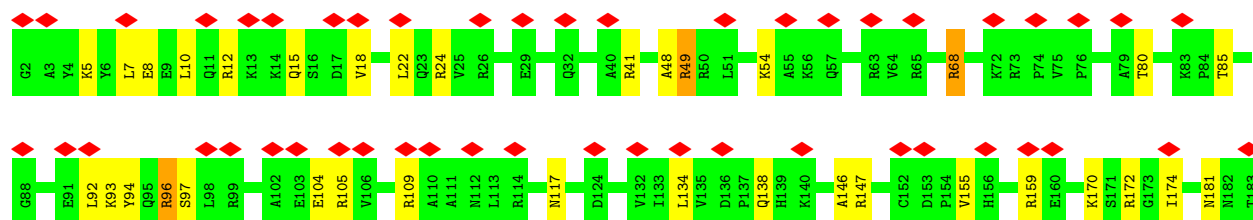
• Molecule 47: 60S RIBOSOMAL PROTEIN L14-B

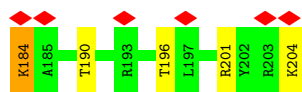
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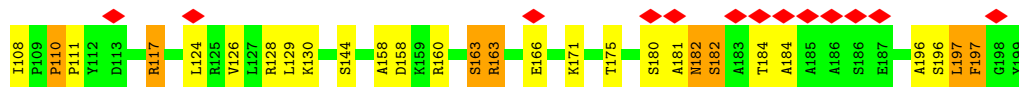
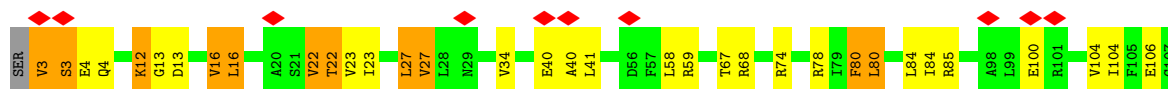
• Molecule 48: 60S RIBOSOMAL PROTEIN L15-A

Chain BN: 

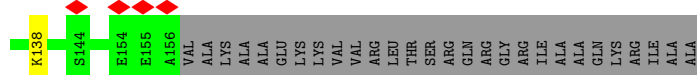
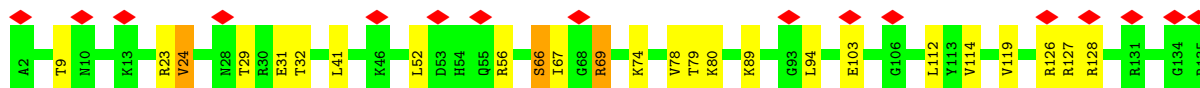
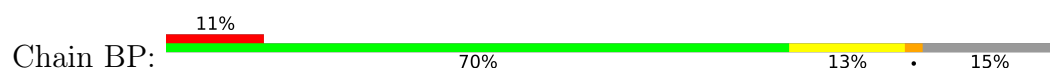




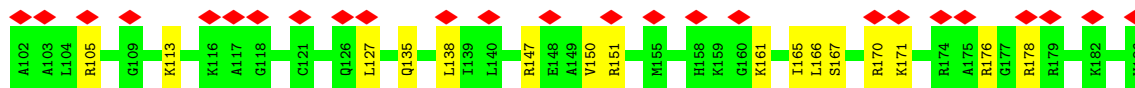
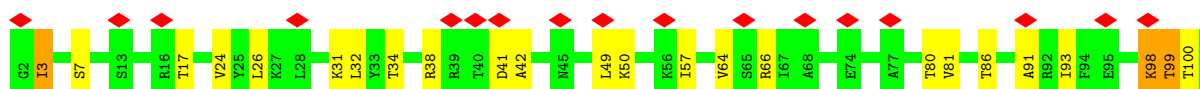
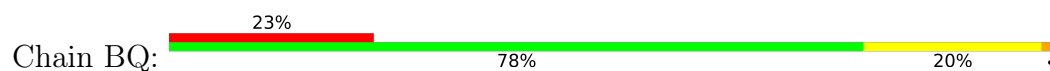
• Molecule 49: 60S RIBOSOMAL PROTEIN L16-A



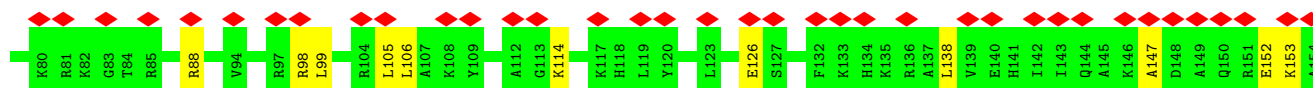
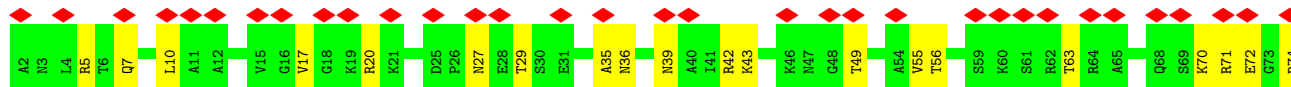
• Molecule 50: 60S RIBOSOMAL PROTEIN L17-A

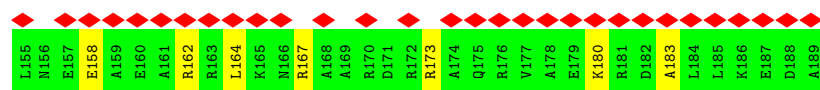


• Molecule 51: 60S RIBOSOMAL PROTEIN L18-A

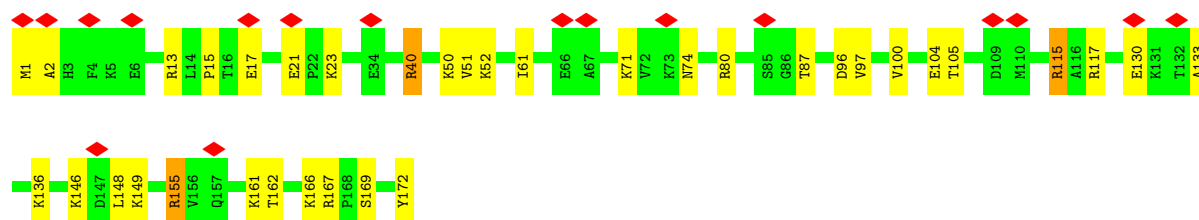
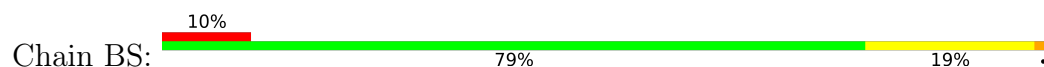


• Molecule 52: 60S RIBOSOMAL PROTEIN L19-B

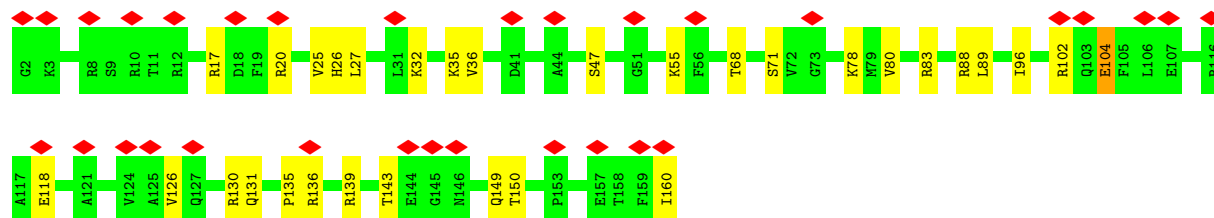
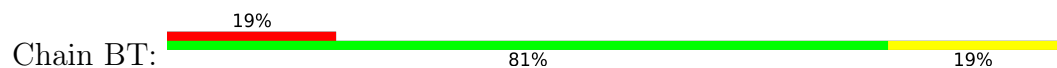




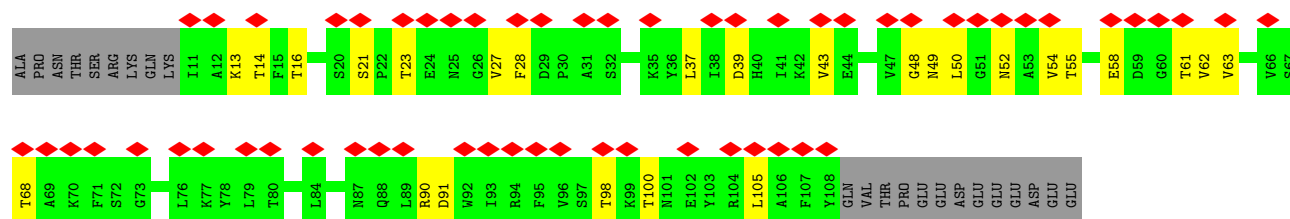
• Molecule 53: 60S RIBOSOMAL PROTEIN L20-B



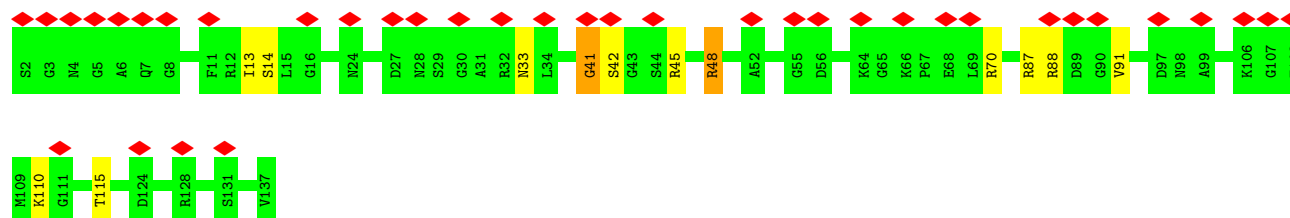
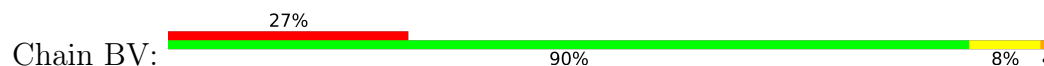
• Molecule 54: 60S RIBOSOMAL PROTEIN L21-A



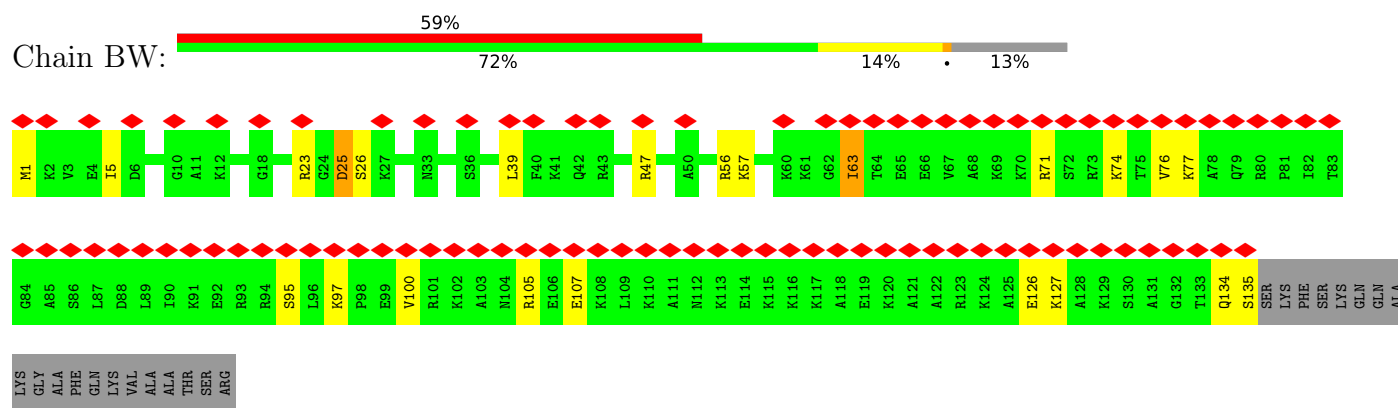
• Molecule 55: 60S RIBOSOMAL PROTEIN L22-A



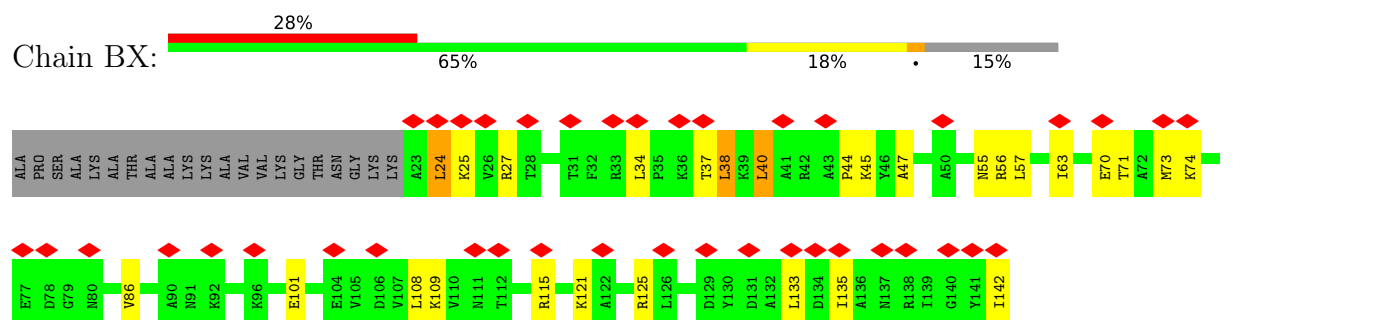
• Molecule 56: 60S RIBOSOMAL PROTEIN L23-A



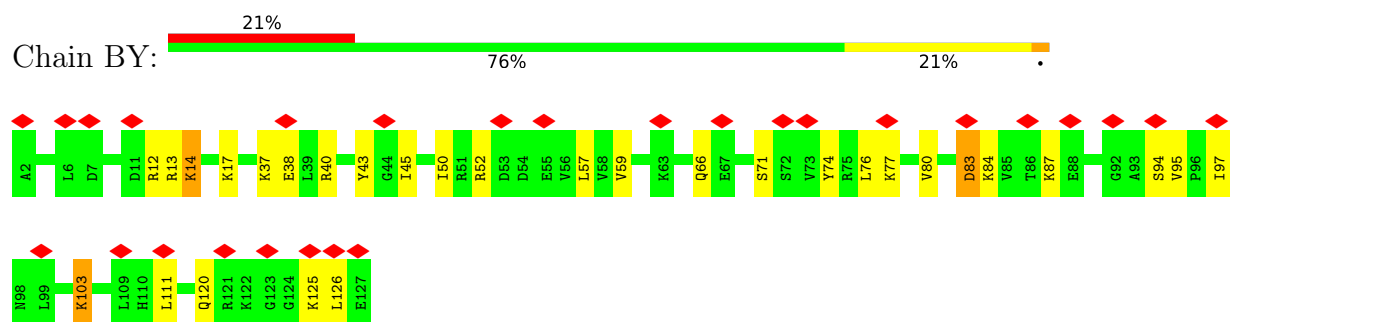
• Molecule 57: 60S RIBOSOMAL PROTEIN L24-A



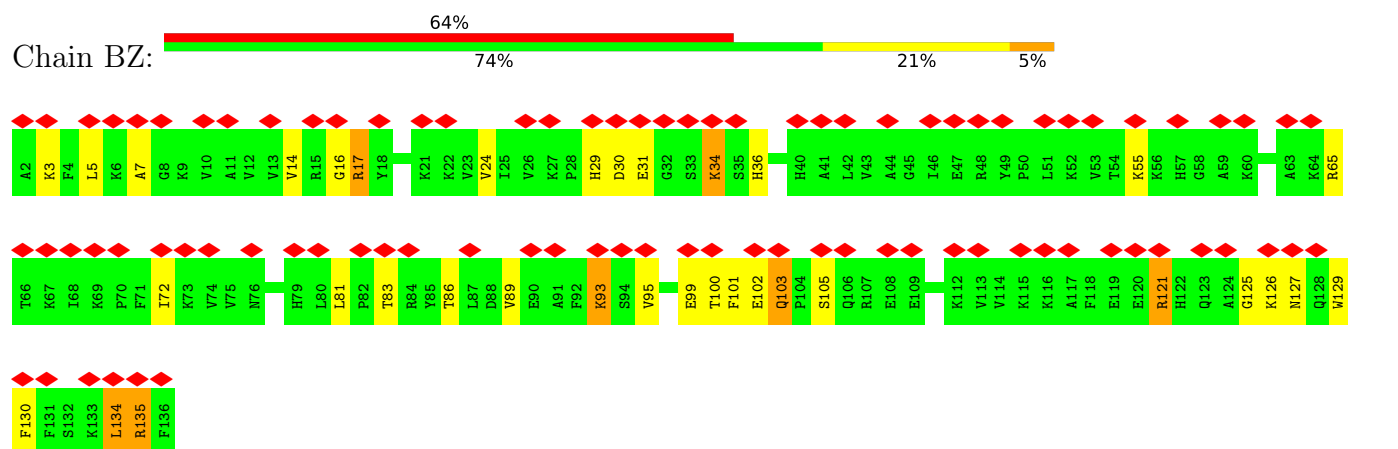
• Molecule 58: 60S RIBOSOMAL PROTEIN L25



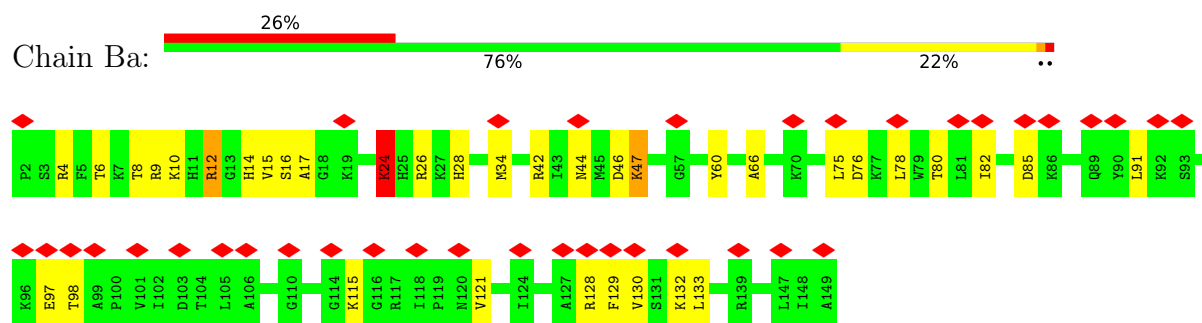
• Molecule 59: 60S RIBOSOMAL PROTEIN L26-A



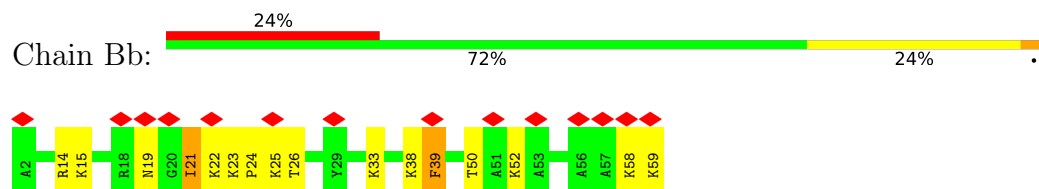
• Molecule 60: 60S RIBOSOMAL PROTEIN L27-A



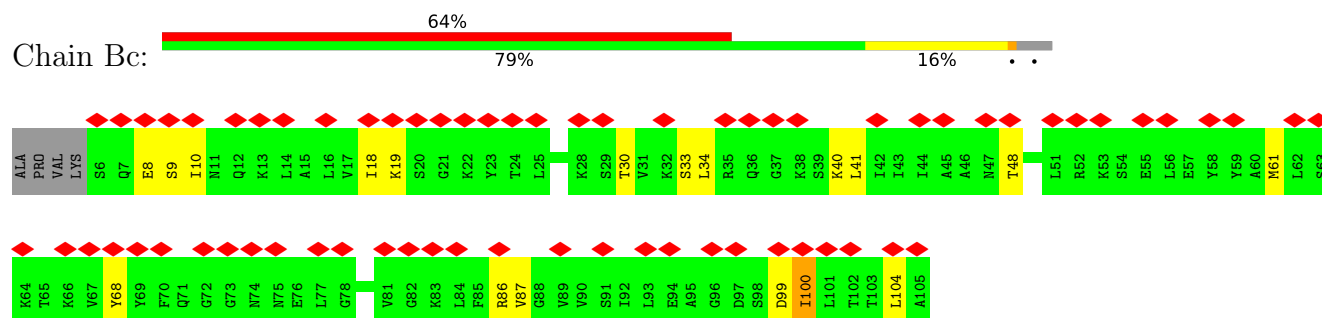
• Molecule 61: 60S RIBOSOMAL PROTEIN L28



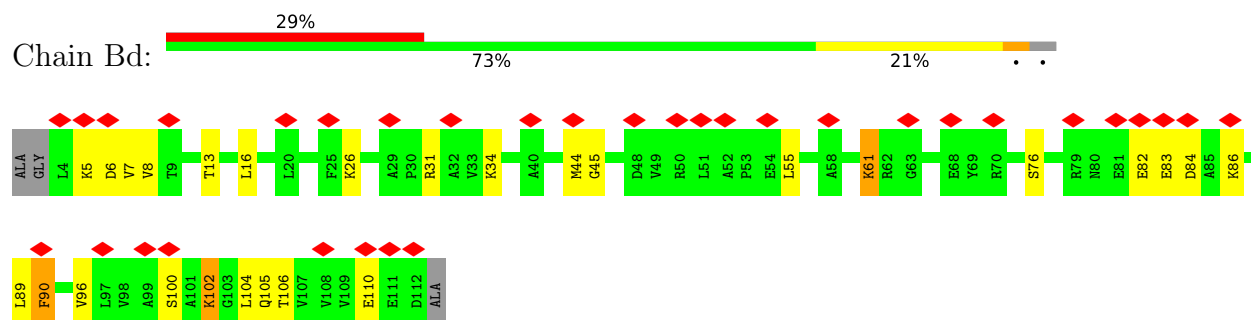
• Molecule 62: 60S RIBOSOMAL PROTEIN L29



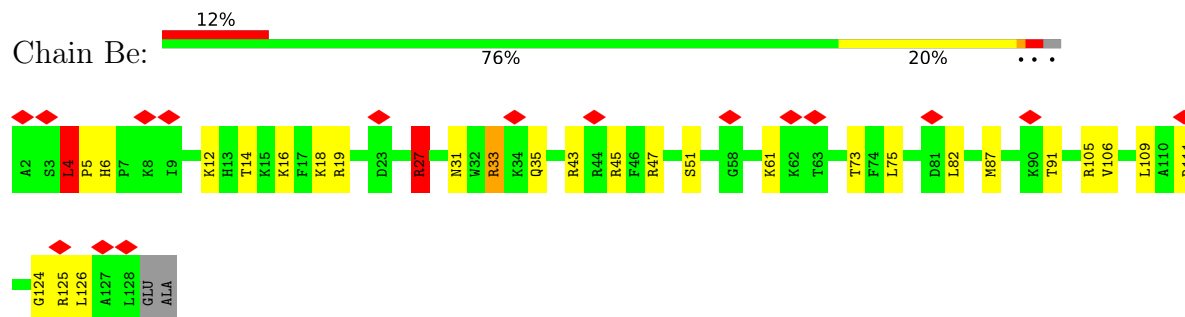
• Molecule 63: 60S RIBOSOMAL PROTEIN L30




• Molecule 64: 60S RIBOSOMAL PROTEIN L31-A



• Molecule 65: 60S RIBOSOMAL PROTEIN L32




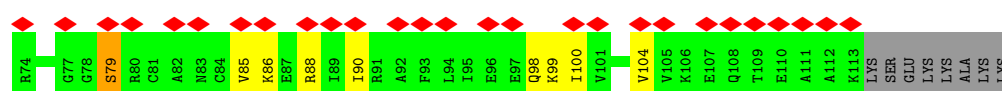
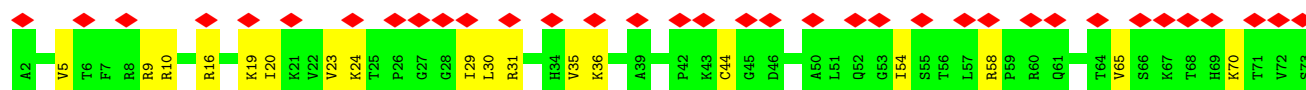
- Molecule 66: 60S RIBOSOMAL PROTEIN L33-A

Chain Bf: 




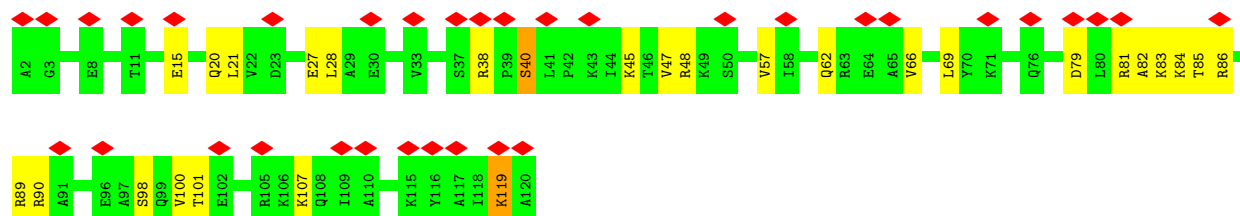
- Molecule 67: 60S RIBOSOMAL PROTEIN L34-A

Chain Bg: 




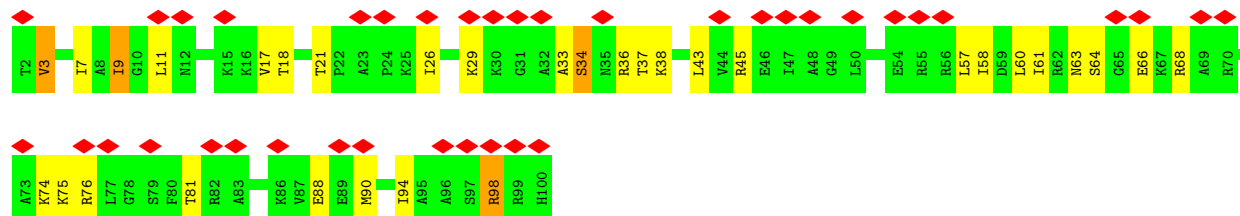
- Molecule 68: 60S RIBOSOMAL PROTEIN L35-B

Chain Bh: 




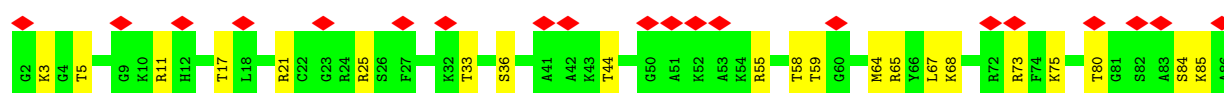
- Molecule 69: 60S RIBOSOMAL PROTEIN L36-A

Chain Bi: 



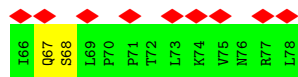
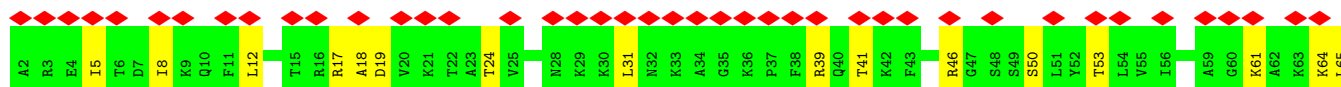
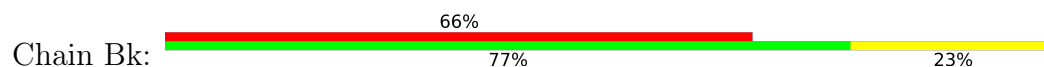
- Molecule 70: 60S RIBOSOMAL PROTEIN L37-A

Chain Bj: 

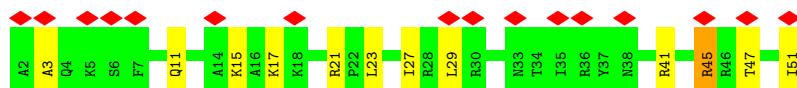
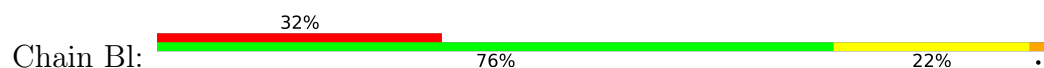




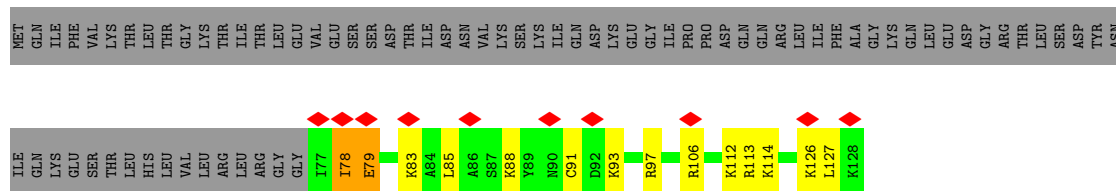
• Molecule 71: 60S RIBOSOMAL PROTEIN L38



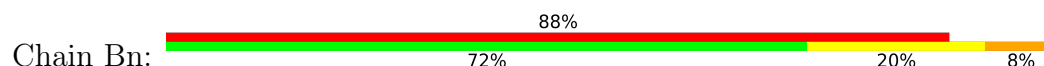
• Molecule 72: 60S RIBOSOMAL PROTEIN L39



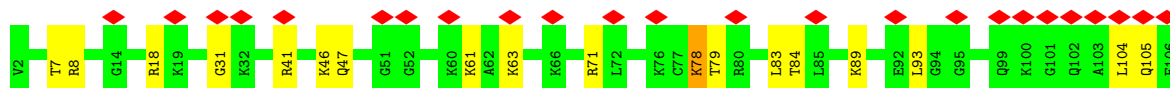
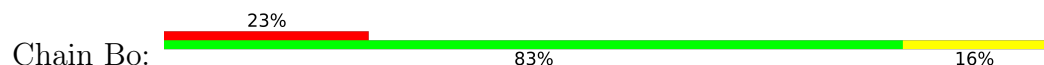
• Molecule 73: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



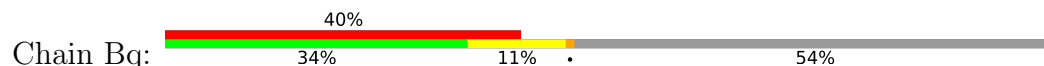
• Molecule 74: 60S RIBOSOMAL PROTEIN L41-B

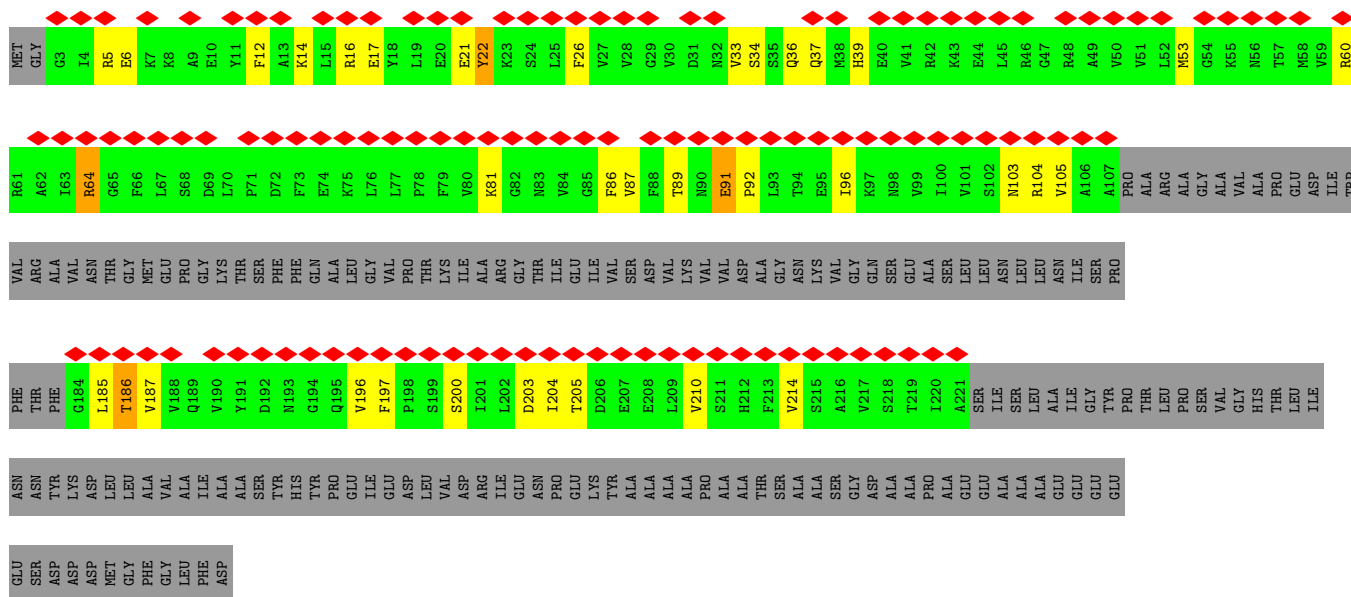


• Molecule 75: 60S RIBOSOMAL PROTEIN L42-A

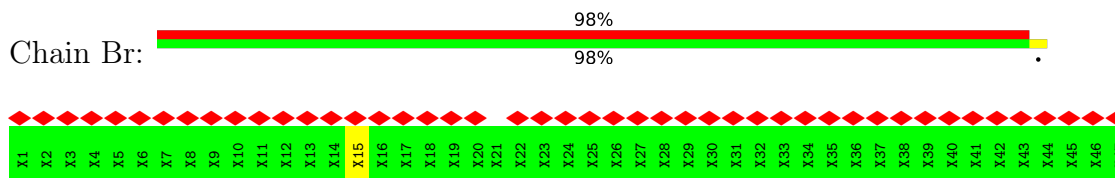


• Molecule 76: 60S ACIDIC RIBOSOMAL PROTEIN P0

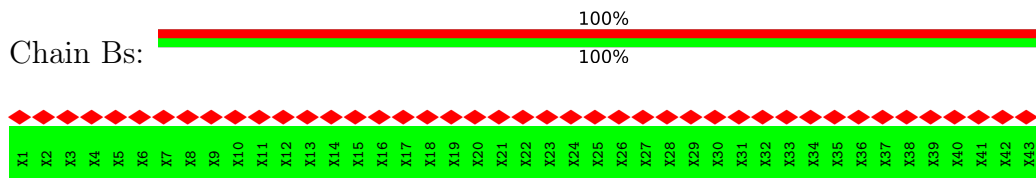




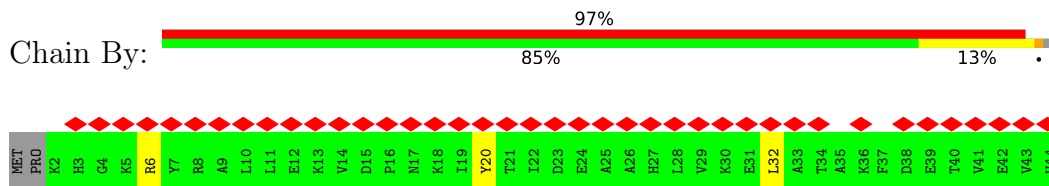
• Molecule 77: 60S ACIDIC RIBOSOMAL PROTEIN P1



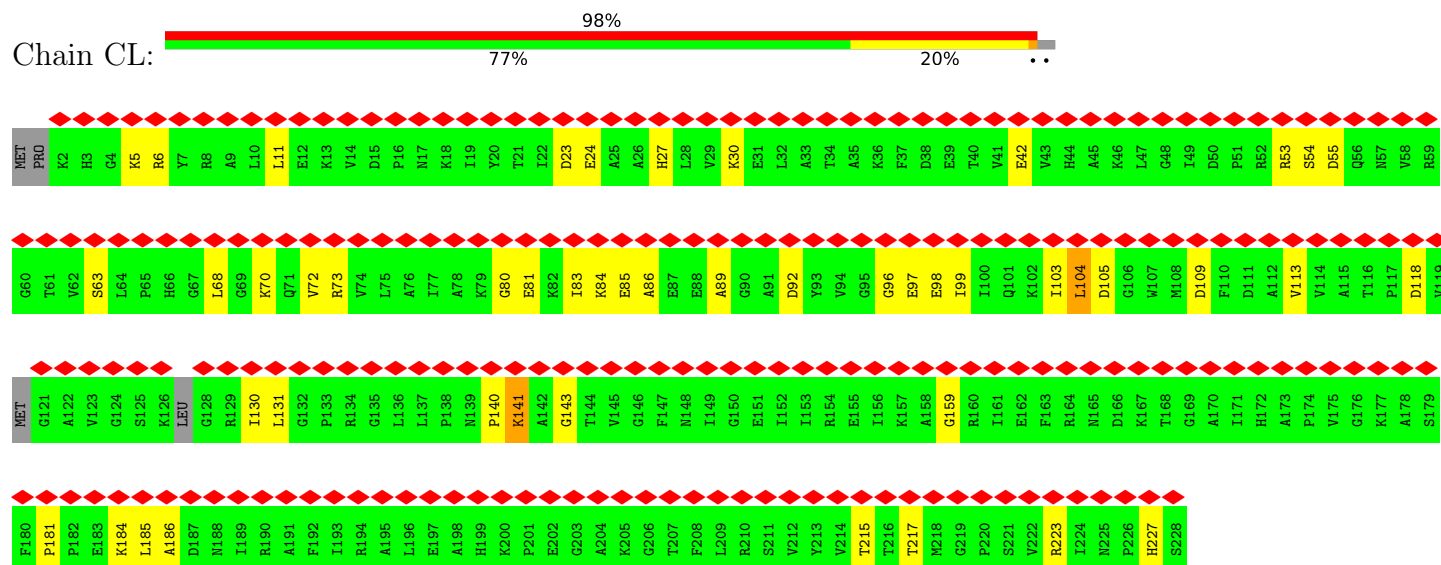
• Molecule 78: 60S ACIDIC RIBOSOMAL PROTEIN P2



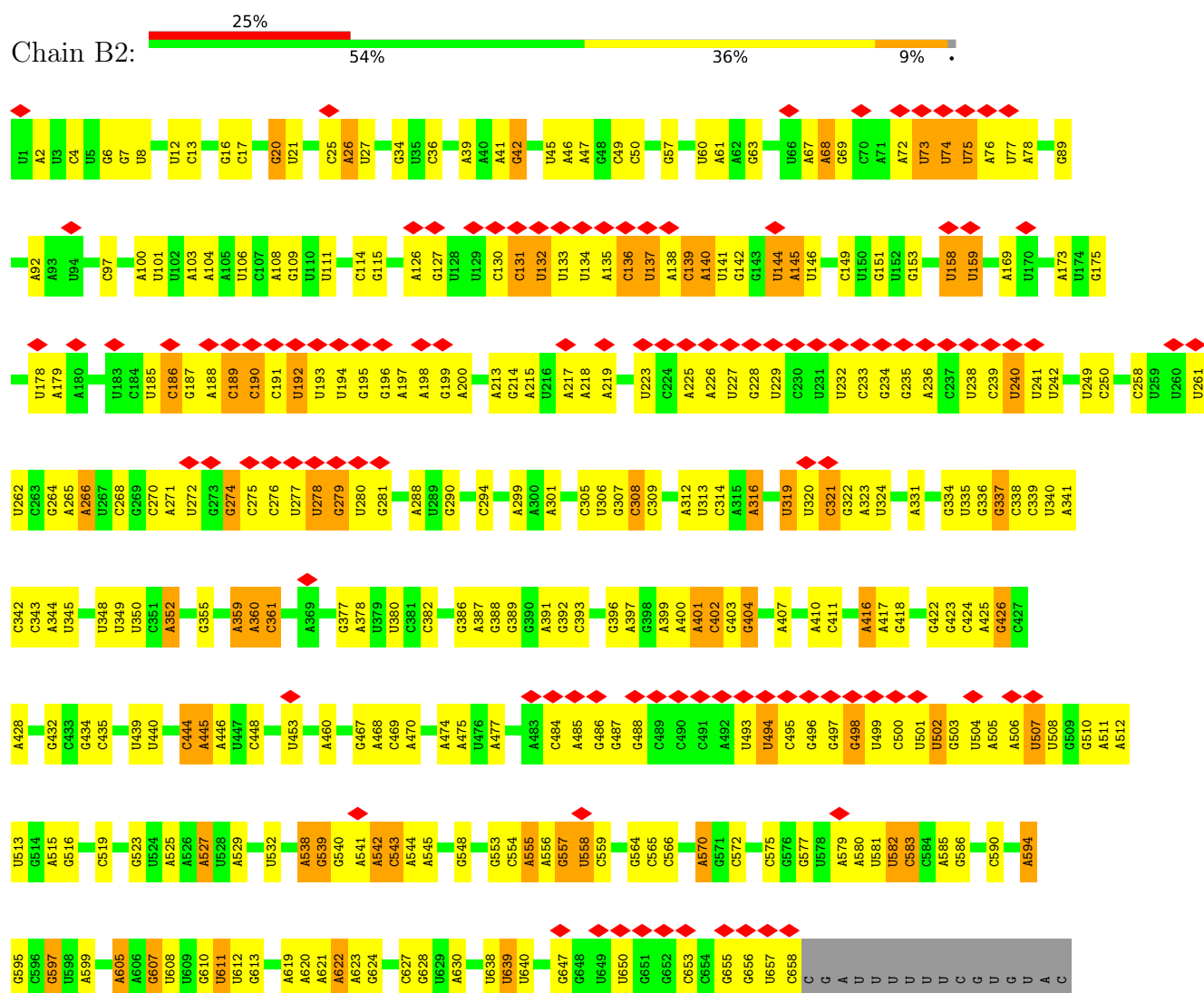
• Molecule 79: 50S RIBOSOMAL PROTEIN L1



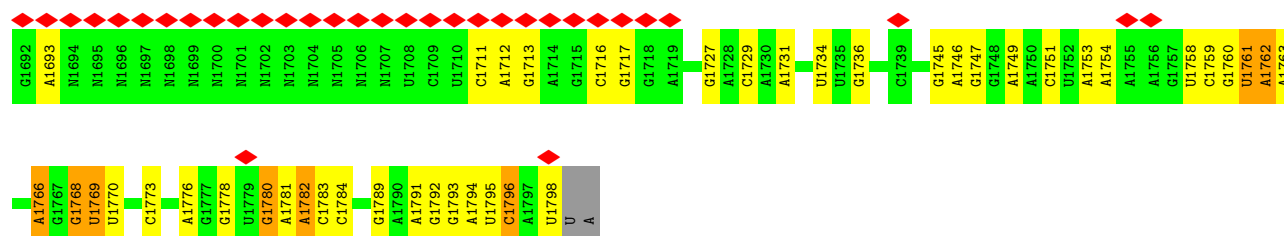
• Molecule 79: 50S RIBOSOMAL PROTEIN L1



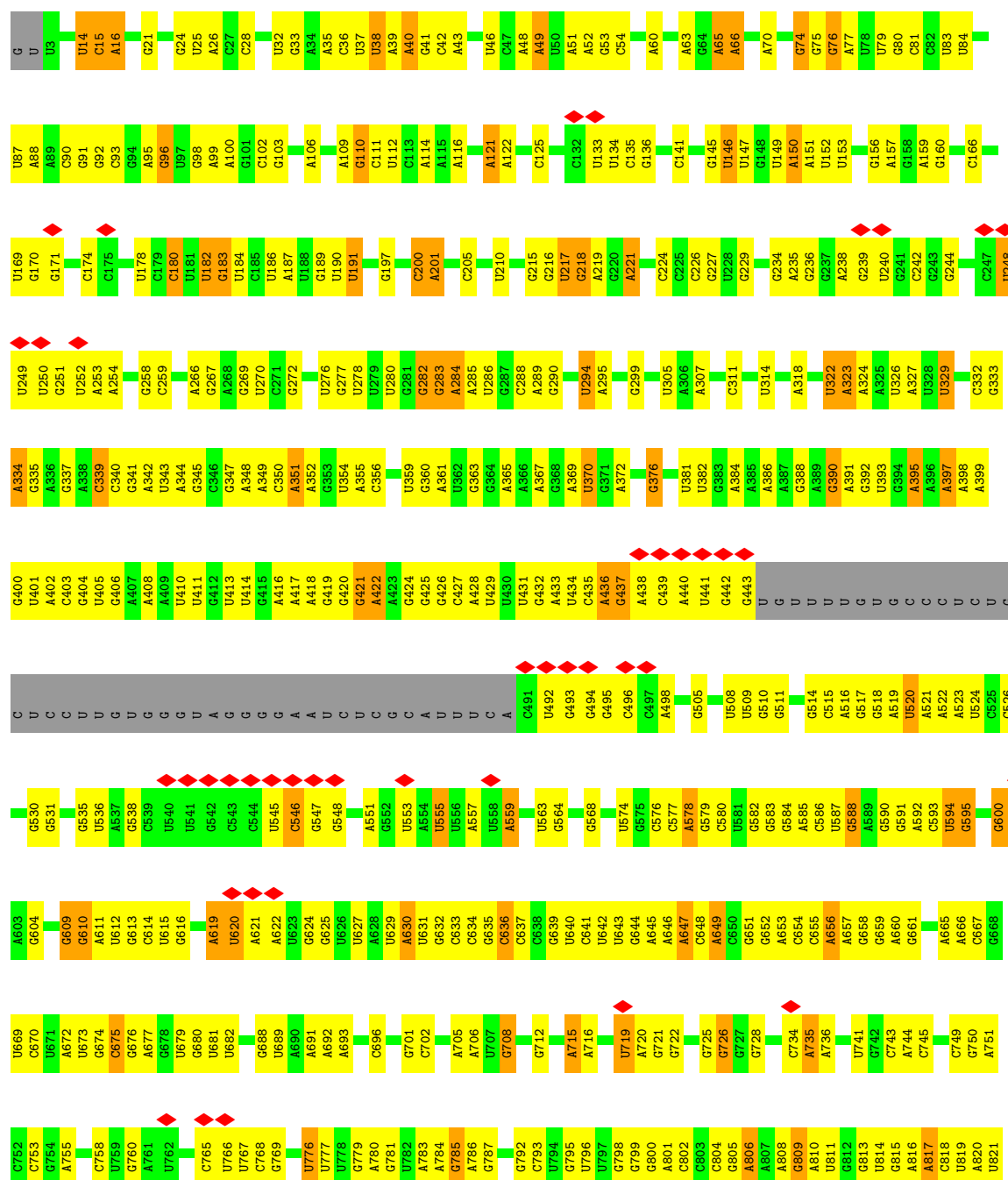
• Molecule 80: 18S RIBOSOMAL RNA





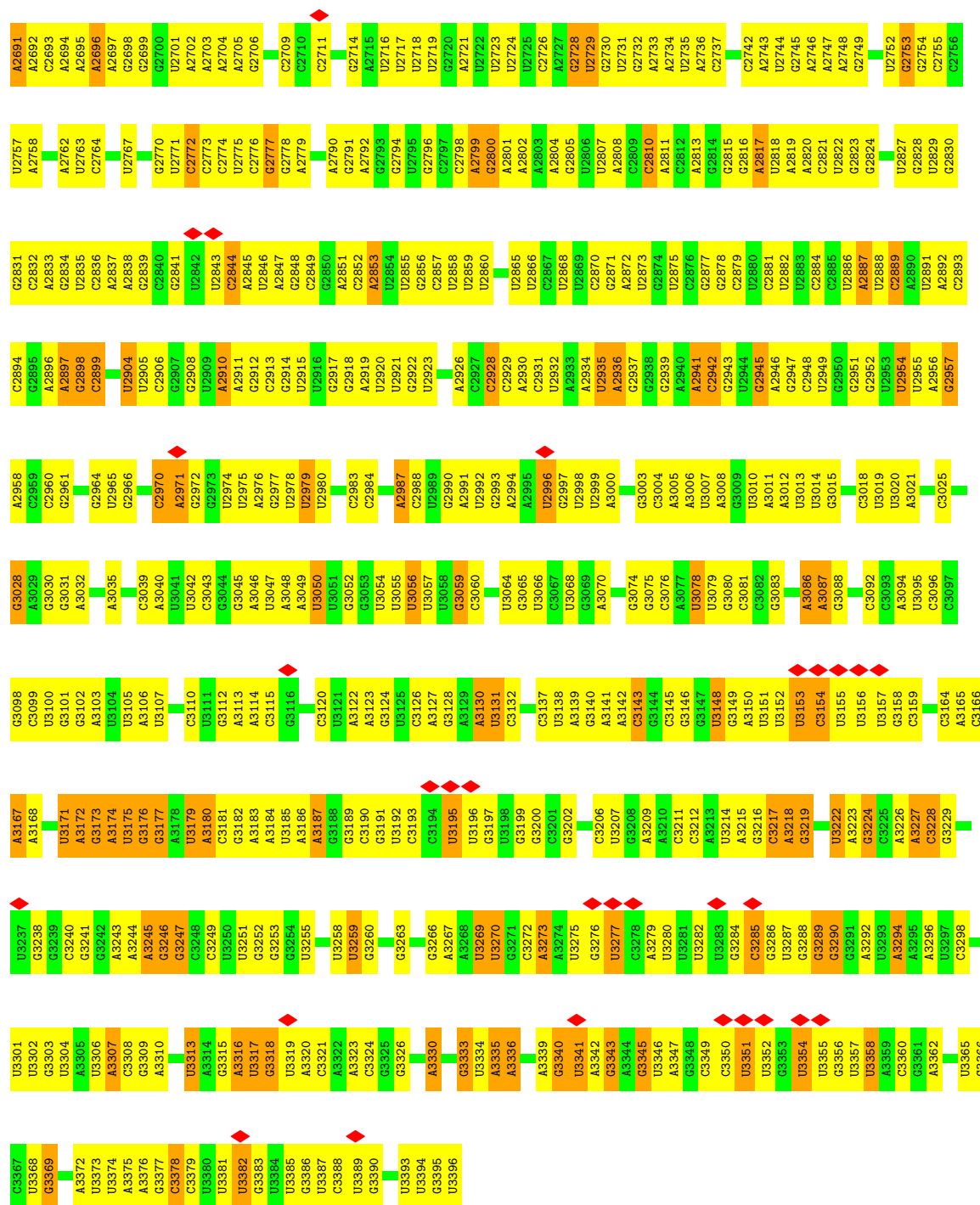


• Molecule 81: 25S RIBOSOMAL RNA



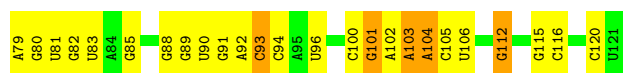


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A2626	U2550	U2423	A2363	G2294	C2163	C	G	A1886	A1813	C1725
U2629	U2551	A2424	C2364	U2237	A2164	U	C	A1887	C1726	
C2630	C2552	U2425	C2365	G2237	G2165	A	C	U1888	G1733	
U2631	A2553	G2426	C2366	G2238	A2166	C	U	G1889	U1816	
C2632	U2554	U2427	A2367	G2239	A2167	A	U	U1890	G1736	
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C2635	U2557	A2430	C2370	A2243	U2170	U	C	U1893	U1819	
A2636	U2558	U2431	G2371	A2244	G2171	U	U	U1894	U1740	
C2637	U2559	U2432	A2372	C2245	G2172	A	A	A1895	A1741	
C2638	U2560	U2433	C2373	G2246	U2173	U	G	A1896	G1744	
G2639	A2562	U2434	G2374	G2247	U2174	C	A	G1897		
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A2642	U2565	U2437	G2377	G2250	U2177	U	C	U1902	A1750	
C2643	U2566	A2438	G2378	G2251	U2178	U	C	U1903	G1751	
A2644	C2567	U2439	U2379	G2252	U2179	U	C	C1904	U1752	
C2645	U2568	A2440	U2380	G2253	C2179	U	C	G1905	G1753	
A2646	C2569	U2441	G2381	U2254	G2180	U	C	G1906	U1754	
C2647	U2570	A2442	C2382	A2255	C2181	U	C	C1907	G1758	
U2648	U2571	U2443	A2383	A2256	A2182	U	C	A1908	C1759	
C2649	C2572	C2444	G2384	C2257	U2184	U	C	A1909	A1760	
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C2651	U2574	A	G2386	U2259	A2188	U	C	U1912	C1761	
U2652	U2575	U	A2387	A2260	U2189	A	C	U1913	C1762	
C2653	U2576	G	U2388	U2261	U2190	U	C	G1914	U1764	
U2654	U2577	A	C2389	G2262	U2191	U	C	C1917	U1765	
C2655	U2578	G	A2390	C2263	C2192	U	C	C1918	G1766	
U2656	U2579	U	G2391	U2264	U2193	U	C	A1921	C1767	
A2657	U2580	U	C2392	U2265	C2197	U	C	U1925	G1770	
C2658	U2581	G	G2393	C2266	A2198	U	C	C1926	G1771	
U2659	U2582	U	U2394	U2267	G2201	U	C	G1927	U1772	
A2660	U2583	A	A2395	U2268	C2202	U	C	U1928	C1773	
C2661	U2584	G	G2396	U2269	U2203	U	C	G1929	G1778	
U2662	U2585	U	A2397	A2270	C2204	U	C	U1931	C1779	
C2663	U2586	A	C2398	G2271	U2205	U	C	A1932	G1780	
U2664	U2587	U	A2399	G2272	U2206	U	C	U1937	U1783	
C2665	U2588	U	G2400	G2273	U2207	U	C	U1938	G1786	
U2666	U2589	A	A2401	U2276	U2209	U	C	G1939	A1787	
C2667	U2590	U	U2402	C2277	G2210	U	C	G1940	C1788	
A2668	U2591	G	G2403	C2278	U2211	U	C	C1941	C1791	
U2669	U2592	U	A2404	C2279	U2212	U	C	U1942	C1792	
C2670	U2593	A	C2405	C2280	A2213	U	C	G1953	C1793	
U2671	U2594	G	U2406	A2281	A2214	U	C	U	A1797	
C2672	U2595	U	G2407	U2282	A2215	U	C	G	A1804	
U2673	U2596	U	U2408	G2283	G2216	U	C	U	C1805	
C2674	U2597	A	G2409	C2284	U2217	U	C	U	G1808	
U2675	U2598	G	U2410	C2285		U	C	A	A1810	
C2676	U2599	U	U2411	A2286	A2222	U	C	U		
U2677	U2600	A	U2412	U2287	A2223	U	C	U		
A2678	U2601	G	G2413	C2288		U	C	U		
U2679	U2602	U	C2414	U2289	A2228	U	C	U		
C2680	U2603	A	C2415	C2290	A2229	U	C	U		
U2681	U2604	U	U2416	A2291	U2292	U	C	U		
C2682	U2605	G	U2417	U2292	C2293	U	C	U		
U2683	U2606	U	G2418	U2294	U2298	U	C	U		
C2684	U2607	C	C2419	U2299		U	C	U		
U2685	U2608	G	C2420	U2298		U	C	U		
C2686	U2609	U		U2298		U	C	U		
U2687	U2610	A		U2298		U	C	U		
C2688	U2611	G		U2298		U	C	U		
U2689	U2612	U		U2298		U	C	U		
A2690	U2613	C		U2298		U	C	U		
C2691	U2614	G		U2298		U	C	U		
U2692	U2615	U		U2298		U	C	U		
C2693	U2616	C		U2298		U	C	U		
U2694	U2617	U		U2298		U	C	U		
C2695	U2618	G		U2298		U	C	U		
U2696	U2619	U		U2298		U	C	U		
C2697	U2620	A		U2298		U	C	U		
U2698	U2621	G		U2298		U	C	U		



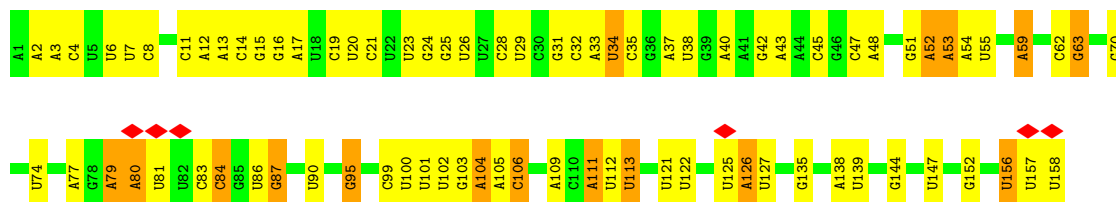
• Molecule 82: 5S RIBOSOMAL RNA





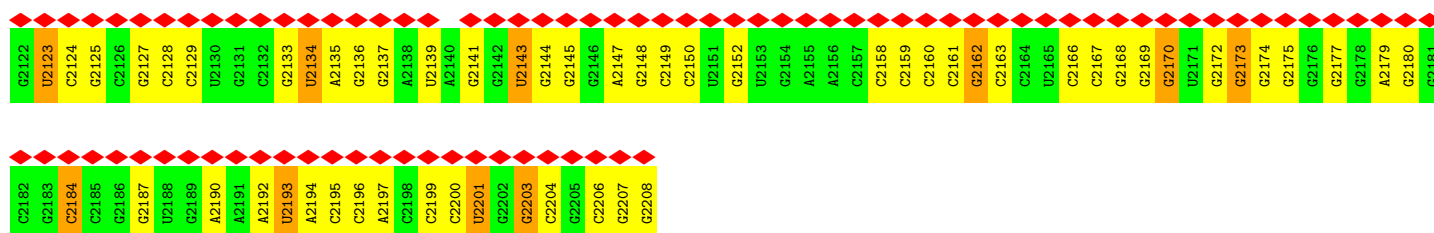
• Molecule 83: 5.8S RIBOSOMAL RNA

Chain B8: 49% 41% 10%



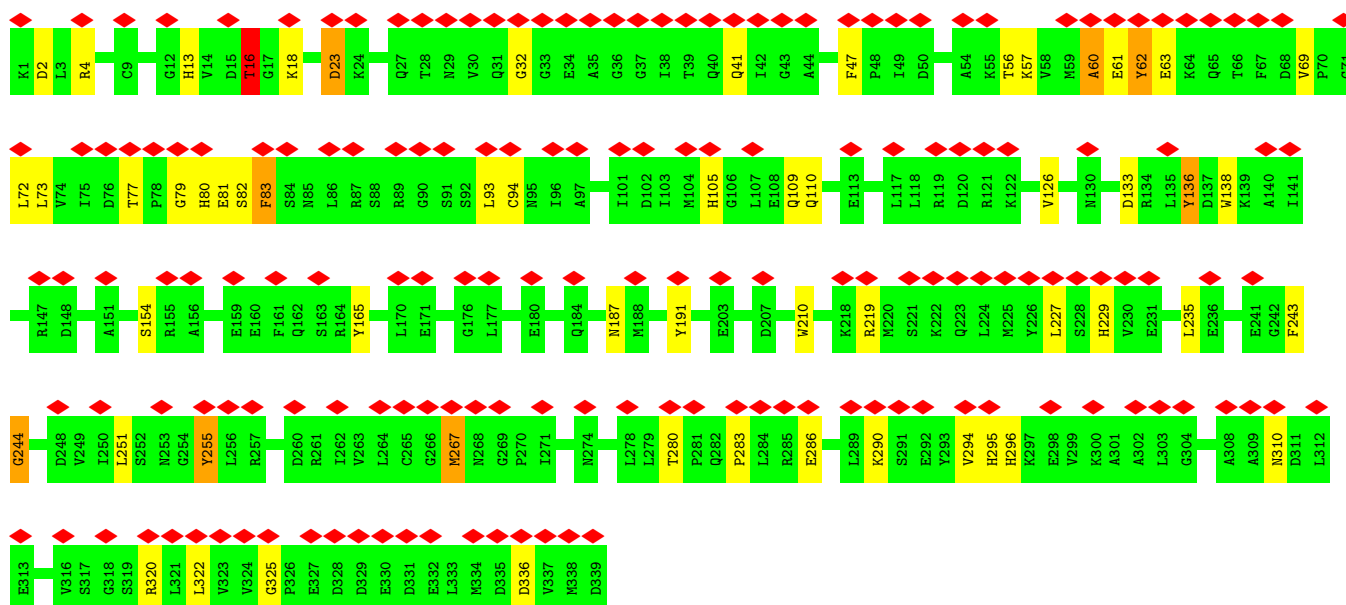
• Molecule 84: EUKARYOTIC RIBOSOMAL L1_RRNA

Chain CN: 36% 99% 53% 11%



• Molecule 85: EUKARYOTIC TRANSLATION INITIATION FACTOR 5B

Chain CP: 50% 83% 15%



• Molecule 86: EUKARYOTIC RIBOSOMAL P_E TRNA

Chain CW: 46% 87% 34% 16%



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 (\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 (\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: HSO, OHX, MG, ZN, GCP

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	0.54	0/782	0.77	0/1047
2	A1	0.53	0/620	0.81	1/838 (0.1%)
3	A2	0.43	0/499	0.72	0/670
4	A3	0.70	0/452	0.94	1/600 (0.2%)
5	A4	0.50	0/483	0.71	0/643
6	A5	0.53	0/404	0.99	1/542 (0.2%)
7	A6	0.49	0/2490	0.70	0/3389
8	A7	0.86	2/925 (0.2%)	0.87	2/1240 (0.2%)
9	AA	0.54	0/1617	0.80	0/2215
10	AB	0.45	0/1735	0.81	0/2335
11	AC	0.60	0/1665	0.77	0/2263
12	AD	0.59	0/1759	0.74	0/2368
13	AE	0.57	0/2109	0.86	1/2839 (0.0%)
14	AF	0.49	0/1629	0.72	0/2202
15	AG	0.55	0/1823	0.75	0/2439
16	AH	0.52	0/1506	0.77	0/2028
17	AI	0.68	0/1514	0.89	3/2021 (0.1%)
18	AJ	0.59	0/1519	0.81	0/2035
19	AK	0.55	0/789	0.83	3/1067 (0.3%)
20	AL	0.70	0/1239	0.81	0/1673
21	AM	0.49	0/898	0.76	0/1220
22	AN	0.61	0/1215	0.83	3/1638 (0.2%)
23	AO	0.48	0/901	0.82	1/1217 (0.1%)
24	AP	0.60	0/998	0.86	3/1341 (0.2%)
25	AQ	0.56	0/1125	0.85	3/1510 (0.2%)
26	AR	0.54	0/935	0.81	0/1254
27	AS	0.59	0/1211	0.80	0/1628
28	AT	0.57	0/1130	0.81	0/1517
29	AU	0.55	0/865	0.76	0/1169
30	AV	0.52	0/693	0.75	0/935
31	AW	0.65	0/1038	0.86	3/1395 (0.2%)
32	AX	0.72	0/1139	0.91	2/1518 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AY	0.56	0/1087	0.77	1/1449 (0.1%)
34	AZ	0.50	0/571	0.85	1/768 (0.1%)
35	BA	0.87	1/1946 (0.1%)	1.05	4/2614 (0.2%)
36	BB	1.02	4/3146 (0.1%)	1.11	13/4228 (0.3%)
37	BC	0.87	0/2800	1.07	11/3790 (0.3%)
38	BD	0.89	1/2408 (0.0%)	0.96	3/3248 (0.1%)
39	BE	0.90	1/1269 (0.1%)	1.00	3/1705 (0.2%)
40	BF	0.99	1/1828 (0.1%)	1.04	6/2461 (0.2%)
41	BG	0.64	0/1795	0.81	1/2429 (0.0%)
42	BH	0.97	2/1539 (0.1%)	1.01	1/2073 (0.0%)
43	BI	0.92	1/1758 (0.1%)	1.08	12/2358 (0.5%)
44	BJ	0.81	1/1374 (0.1%)	0.99	4/1842 (0.2%)
46	BL	0.82	0/1573	1.04	6/2113 (0.3%)
47	BM	0.96	0/1074	1.01	4/1446 (0.3%)
48	BN	0.83	1/1757 (0.1%)	1.00	6/2354 (0.3%)
49	BO	0.98	11/3159 (0.3%)	1.02	25/4205 (0.6%)
50	BP	1.05	1/1250 (0.1%)	1.09	5/1683 (0.3%)
51	BQ	0.89	1/1465 (0.1%)	1.12	9/1965 (0.5%)
52	BR	0.78	1/1538 (0.1%)	0.87	2/2050 (0.1%)
53	BS	1.02	0/1481	1.09	7/1990 (0.4%)
54	BT	1.01	2/1300 (0.2%)	1.01	1/1743 (0.1%)
55	BU	0.56	0/794	0.77	0/1076
56	BV	0.98	0/1018	1.09	4/1369 (0.3%)
57	BW	0.80	0/1052	0.90	2/1398 (0.1%)
58	BX	0.72	0/974	0.86	0/1314
59	BY	0.79	1/1004 (0.1%)	0.98	2/1341 (0.1%)
60	BZ	0.55	0/1118	0.83	2/1497 (0.1%)
61	Ba	0.95	2/1204 (0.2%)	1.14	9/1612 (0.6%)
62	Bb	0.91	0/473	1.14	1/629 (0.2%)
63	Bc	0.61	0/775	0.77	0/1040
64	Bd	0.94	2/897 (0.2%)	0.95	1/1205 (0.1%)
65	Be	1.03	0/1041	1.27	12/1394 (0.9%)
66	Bf	1.12	0/868	1.09	3/1168 (0.3%)
67	Bg	0.72	0/890	0.92	0/1189
68	Bh	0.67	0/974	0.80	0/1297
69	Bi	0.67	0/777	0.85	0/1033
70	Bj	0.87	0/696	1.04	3/923 (0.3%)
71	Bk	0.50	0/614	0.70	0/822
72	Bl	0.90	0/443	1.02	1/588 (0.2%)
73	Bm	1.08	2/423 (0.5%)	1.13	1/562 (0.2%)
74	Bn	0.90	0/234	1.15	1/300 (0.3%)
75	Bo	0.83	0/860	0.89	1/1136 (0.1%)
76	Bq	1.07	0/1092	1.31	4/1474 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
79	By	0.98	0/1749	1.24	8/2355 (0.3%)
79	CL	0.80	2/1749 (0.1%)	1.02	4/2355 (0.2%)
80	B2	0.92	33/42128 (0.1%)	1.49	828/65642 (1.3%)
81	B5	1.49	661/75336 (0.9%)	1.92	3722/117449 (3.2%)
82	B7	1.38	12/2883 (0.4%)	1.80	119/4491 (2.6%)
83	B8	1.16	4/3746 (0.1%)	1.70	128/5832 (2.2%)
84	CN	0.76	7/2097 (0.3%)	1.20	23/3273 (0.7%)
85	CP	2.24	8/2623 (0.3%)	1.38	24/3532 (0.7%)
86	CW	1.86	27/1761 (1.5%)	2.72	212/2743 (7.7%)
All	All	1.13	792/226118 (0.4%)	1.51	5267/331349 (1.6%)

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 792 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	CP	63	GLU	N-CA	69.03	2.84	1.46
85	CP	210	TRP	CD2-CE3	34.76	1.92	1.40
85	CP	210	TRP	CD2-CE2	33.01	1.80	1.41
85	CP	210	TRP	CE2-CZ2	31.95	1.94	1.39
85	CP	210	TRP	CE3-CZ3	26.33	1.83	1.38

The worst 5 of 5267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B5	1152	G	N3-C4-C5	33.59	145.40	128.60
81	B5	1256	G	P-O3'-C3'	32.78	159.04	119.70
81	B5	1152	G	N3-C4-N9	-31.65	107.01	126.00
81	B5	1152	G	N3-C2-N2	-26.89	101.08	119.90
81	B5	1152	G	C2-N3-C4	-23.94	99.93	111.90

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	2	22
3	A2	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	1	13
4	A3	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	3	26
5	A4	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	3	29
6	A5	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0	1
7	A6	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	3	25
8	A7	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	1	12
9	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0	5
10	AB	212/255 (83%)	132 (62%)	42 (20%)	38 (18%)	0	2
11	AC	215/254 (85%)	187 (87%)	16 (7%)	12 (6%)	2	21
12	AD	221/240 (92%)	180 (81%)	27 (12%)	14 (6%)	1	19
13	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1	13
14	AF	204/225 (91%)	155 (76%)	30 (15%)	19 (9%)	0	12
15	AG	224/236 (95%)	190 (85%)	23 (10%)	11 (5%)	2	23
16	AH	182/190 (96%)	128 (70%)	27 (15%)	27 (15%)	0	3
17	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	1	13
18	AJ	183/197 (93%)	153 (84%)	18 (10%)	12 (7%)	1	18
19	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	0	8
20	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	1	20
21	AM	122/143 (85%)	66 (54%)	23 (19%)	33 (27%)	0	1
22	AN	148/151 (98%)	125 (84%)	15 (10%)	8 (5%)	2	22
23	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	0	6
24	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	0	5
25	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0	9
27	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	0	10
28	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	1	13
29	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	2	23
30	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	6
31	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	6	36
32	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0	5
33	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	0	10
34	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0	3
35	BA	250/253 (99%)	213 (85%)	30 (12%)	7 (3%)	5	33
36	BB	384/386 (100%)	341 (89%)	34 (9%)	9 (2%)	6	37
37	BC	359/361 (99%)	306 (85%)	32 (9%)	21 (6%)	1	20
38	BD	292/296 (99%)	267 (91%)	19 (6%)	6 (2%)	7	39
39	BE	153/175 (87%)	134 (88%)	15 (10%)	4 (3%)	5	35
40	BF	221/243 (91%)	201 (91%)	16 (7%)	4 (2%)	8	42
41	BG	229/255 (90%)	180 (79%)	28 (12%)	21 (9%)	1	12
42	BH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	7	39
43	BI	209/220 (95%)	175 (84%)	22 (10%)	12 (6%)	1	20
44	BJ	167/173 (96%)	135 (81%)	19 (11%)	13 (8%)	1	15
46	BL	192/198 (97%)	161 (84%)	20 (10%)	11 (6%)	1	20
47	BM	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	22	62
48	BN	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	4	32
49	BO	352/218 (162%)	324 (92%)	18 (5%)	10 (3%)	5	33
50	BP	153/183 (84%)	142 (93%)	9 (6%)	2 (1%)	12	48
51	BQ	183/185 (99%)	168 (92%)	9 (5%)	6 (3%)	4	30
52	BR	186/188 (99%)	167 (90%)	16 (9%)	3 (2%)	9	45
53	BS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	65
54	BT	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	12	48
55	BU	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	4	31
56	BV	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	10	46
57	BW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	BX	118/141 (84%)	104 (88%)	6 (5%)	8 (7%)	1	17
59	BY	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	3	26
60	BZ	133/135 (98%)	107 (80%)	13 (10%)	13 (10%)	0	10
61	Ba	146/148 (99%)	123 (84%)	18 (12%)	5 (3%)	3	29
62	Bb	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	12
63	Bc	98/104 (94%)	87 (89%)	8 (8%)	3 (3%)	4	31
64	Bd	107/112 (96%)	88 (82%)	13 (12%)	6 (6%)	2	21
65	Be	125/129 (97%)	110 (88%)	9 (7%)	6 (5%)	2	23
66	Bf	104/106 (98%)	96 (92%)	5 (5%)	3 (3%)	4	32
67	Bg	110/120 (92%)	93 (84%)	13 (12%)	4 (4%)	3	28
68	Bh	117/119 (98%)	99 (85%)	14 (12%)	4 (3%)	3	29
69	Bi	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	16
70	Bj	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	6	36
71	Bk	75/77 (97%)	61 (81%)	10 (13%)	4 (5%)	2	22
72	Bl	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	39
73	Bm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	7	40
74	Bn	23/25 (92%)	22 (96%)	0	1 (4%)	2	25
75	Bo	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	8	41
76	Bq	139/312 (45%)	104 (75%)	14 (10%)	21 (15%)	0	3
79	By	219/229 (96%)	178 (81%)	24 (11%)	17 (8%)	1	15
79	CL	219/229 (96%)	165 (75%)	35 (16%)	19 (9%)	1	13
85	CP	331/339 (98%)	276 (83%)	32 (10%)	23 (7%)	1	17
All	All	12051/13155 (92%)	10001 (83%)	1275 (11%)	775 (6%)	2	19

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%)	65 (78%)	18 (22%)	1	6
2	A1	70/71 (99%)	62 (89%)	8 (11%)	5	24
3	A2	56/60 (93%)	38 (68%)	18 (32%)	0	2
4	A3	47/49 (96%)	38 (81%)	9 (19%)	1	9
5	A4	51/54 (94%)	43 (84%)	8 (16%)	2	16
6	A5	43/116 (37%)	32 (74%)	11 (26%)	0	4
7	A6	259/262 (99%)	221 (85%)	38 (15%)	3	17
8	A7	97/195 (50%)	74 (76%)	23 (24%)	1	5
9	AA	164/210 (78%)	122 (74%)	42 (26%)	0	4
10	AB	191/224 (85%)	137 (72%)	54 (28%)	0	3
11	AC	176/205 (86%)	130 (74%)	46 (26%)	0	4
12	AD	182/195 (93%)	138 (76%)	44 (24%)	0	5
13	AE	221/222 (100%)	166 (75%)	55 (25%)	0	4
14	AF	173/191 (91%)	137 (79%)	36 (21%)	1	7
15	AG	188/201 (94%)	149 (79%)	39 (21%)	1	7
16	AH	165/170 (97%)	124 (75%)	41 (25%)	0	4
17	AI	150/161 (93%)	118 (79%)	32 (21%)	1	7
18	AJ	158/166 (95%)	117 (74%)	41 (26%)	0	4
19	AK	77/98 (79%)	58 (75%)	19 (25%)	0	4
20	AL	129/137 (94%)	105 (81%)	24 (19%)	1	10
21	AM	88/119 (74%)	55 (62%)	33 (38%)	0	0
22	AN	127/128 (99%)	91 (72%)	36 (28%)	0	3
23	AO	81/105 (77%)	57 (70%)	24 (30%)	0	2
24	AP	101/118 (86%)	82 (81%)	19 (19%)	1	10
25	AQ	117/119 (98%)	83 (71%)	34 (29%)	0	3
26	AR	94/124 (76%)	70 (74%)	24 (26%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	71 (71%)	29 (29%)	0	3
30	AV	74/74 (100%)	56 (76%)	18 (24%)	0	4
31	AW	110/111 (99%)	84 (76%)	26 (24%)	1	5
32	AX	119/120 (99%)	97 (82%)	22 (18%)	1	11
33	AY	112/113 (99%)	84 (75%)	28 (25%)	0	4
34	AZ	61/89 (68%)	43 (70%)	18 (30%)	0	2
35	BA	192/195 (98%)	153 (80%)	39 (20%)	1	8
36	BB	320/322 (99%)	250 (78%)	70 (22%)	1	6
37	BC	288/288 (100%)	223 (77%)	65 (23%)	1	6
38	BD	243/244 (100%)	196 (81%)	47 (19%)	1	9
39	BE	135/152 (89%)	115 (85%)	20 (15%)	3	17
40	BF	187/204 (92%)	158 (84%)	29 (16%)	2	16
41	BG	177/207 (86%)	138 (78%)	39 (22%)	1	6
42	BH	171/171 (100%)	132 (77%)	39 (23%)	1	6
43	BI	179/186 (96%)	142 (79%)	37 (21%)	1	7
44	BJ	147/149 (99%)	114 (78%)	33 (22%)	1	6
46	BL	154/158 (98%)	124 (80%)	30 (20%)	1	9
47	BM	108/108 (100%)	84 (78%)	24 (22%)	1	6
48	BN	175/175 (100%)	143 (82%)	32 (18%)	1	11
49	BO	323/178 (182%)	267 (83%)	56 (17%)	2	13
50	BP	125/145 (86%)	103 (82%)	22 (18%)	2	12
51	BQ	150/150 (100%)	123 (82%)	27 (18%)	1	11
52	BR	153/153 (100%)	121 (79%)	32 (21%)	1	7
53	BS	156/156 (100%)	123 (79%)	33 (21%)	1	7
54	BT	136/136 (100%)	109 (80%)	27 (20%)	1	8
55	BU	85/106 (80%)	62 (73%)	23 (27%)	0	3
56	BV	104/104 (100%)	96 (92%)	8 (8%)	13	39
57	BW	100/129 (78%)	85 (85%)	15 (15%)	3	17
58	BX	104/117 (89%)	81 (78%)	23 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	BY	109/109 (100%)	85 (78%)	24 (22%)	1	6
60	BZ	115/115 (100%)	89 (77%)	26 (23%)	1	6
61	Ba	118/118 (100%)	95 (80%)	23 (20%)	1	9
62	Bb	46/46 (100%)	35 (76%)	11 (24%)	0	5
63	Bc	84/87 (97%)	68 (81%)	16 (19%)	1	9
64	Bd	94/96 (98%)	73 (78%)	21 (22%)	1	6
65	Be	109/110 (99%)	89 (82%)	20 (18%)	1	11
66	Bf	90/90 (100%)	79 (88%)	11 (12%)	5	23
67	Bg	95/102 (93%)	71 (75%)	24 (25%)	0	4
68	Bh	103/104 (99%)	77 (75%)	26 (25%)	0	4
69	Bi	80/81 (99%)	51 (64%)	29 (36%)	0	1
70	Bj	70/70 (100%)	53 (76%)	17 (24%)	0	4
71	Bk	67/68 (98%)	53 (79%)	14 (21%)	1	7
72	Bl	45/45 (100%)	34 (76%)	11 (24%)	0	4
73	Bm	47/116 (40%)	34 (72%)	13 (28%)	0	3
74	Bn	23/23 (100%)	16 (70%)	7 (30%)	0	2
75	Bo	90/90 (100%)	74 (82%)	16 (18%)	2	12
76	Bq	105/254 (41%)	94 (90%)	11 (10%)	7	27
79	By	177/181 (98%)	171 (97%)	6 (3%)	37	61
79	CL	177/181 (98%)	153 (86%)	24 (14%)	3	20
85	CP	290/290 (100%)	275 (95%)	15 (5%)	23	50
All	All	10153/10976 (92%)	8029 (79%)	2124 (21%)	3	7

5 of 2124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
63	Bc	48	THR
66	Bf	81	VAL
63	Bc	40	LYS
79	By	107	TRP
27	AS	5	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
48	BN	90	ASN
67	Bg	33	GLN
51	BQ	158	HIS
60	BZ	57	HIS
72	Bl	19	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
80	B2	1764/1800 (98%)	545 (30%)	86 (4%)
81	B5	3140/3396 (92%)	741 (23%)	131 (4%)
82	B7	120/121 (99%)	18 (15%)	0
83	B8	157/158 (99%)	32 (20%)	3 (1%)
84	CN	86/87 (98%)	41 (47%)	8 (9%)
86	CW	73/76 (96%)	26 (35%)	7 (9%)
All	All	5340/5638 (94%)	1403 (26%)	235 (4%)

5 of 1403 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 ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	HSO	CP	105	85	6,10,10	2.30	2 (33%)	4,12,12	1.84	2 (50%)
85	HSO	CP	295	85	6,10,10	2.10	1 (16%)	4,12,12	1.46	1 (25%)
85	HSO	CP	80	85	6,10,10	2.37	2 (33%)	4,12,12	1.35	0
85	HSO	CP	296	85	6,10,10	2.30	2 (33%)	4,12,12	2.25	2 (50%)
85	HSO	CP	13	85	6,10,10	2.17	1 (16%)	4,12,12	1.46	1 (25%)
85	HSO	CP	229	85	6,10,10	2.01	1 (16%)	4,12,12	1.69	1 (25%)

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
85	HSO	CP	105	85	-	3/6/6/6	0/1/1/1
85	HSO	CP	295	85	-	2/6/6/6	0/1/1/1
85	HSO	CP	80	85	-	4/6/6/6	0/1/1/1
85	HSO	CP	296	85	-	2/6/6/6	0/1/1/1
85	HSO	CP	13	85	-	5/6/6/6	0/1/1/1
85	HSO	CP	229	85	-	2/6/6/6	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	CP	296	HSO	O-C	-4.65	1.22	1.42
85	CP	295	HSO	O-C	-4.63	1.22	1.42
85	CP	13	HSO	O-C	-4.60	1.23	1.42
85	CP	80	HSO	O-C	-4.59	1.23	1.42
85	CP	105	HSO	O-C	-4.59	1.23	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	CP	296	HSO	CB-CA-C	-3.71	105.49	112.21
85	CP	105	HSO	CB-CA-C	-2.64	107.44	112.21
85	CP	229	HSO	O-C-CA	2.63	121.91	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	CP	13	HSO	O-C-CA	2.43	121.14	111.52
85	CP	296	HSO	O-C-CA	2.39	120.95	111.52

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	CP	13	HSO	N-CA-CB-CG
85	CP	13	HSO	O-C-CA-CB
85	CP	13	HSO	CA-CB-CG-ND1
85	CP	13	HSO	CA-CB-CG-CD2
85	CP	80	HSO	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1917	-	0,6,6	-	-	-		
89	OHX	B2	1962	-	0,6,6	-	-	-		
89	OHX	AI	302	-	0,6,6	-	-	-		
89	OHX	B2	1973	-	0,6,6	-	-	-		
89	OHX	B2	2061	-	0,6,6	-	-	-		
89	OHX	B2	1999	-	0,6,6	-	-	-		
89	OHX	B2	2050	88	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	2012	-	0,6,6	-	-	-		
89	OHX	B2	1922	-	0,6,6	-	-	-		
89	OHX	B2	1929	-	0,6,6	-	-	-		
89	OHX	B2	1948	-	0,6,6	-	-	-		
89	OHX	B2	2016	-	0,6,6	-	-	-		
89	OHX	B2	2066	-	0,6,6	-	-	-		
89	OHX	B2	1951	-	0,6,6	-	-	-		
89	OHX	B2	1982	-	0,6,6	-	-	-		
89	OHX	B2	2065	-	0,6,6	-	-	-		
89	OHX	B2	1991	-	0,6,6	-	-	-		
89	OHX	B2	2039	-	0,6,6	-	-	-		
89	OHX	B2	2076	-	0,6,6	-	-	-		
89	OHX	B2	2034	-	0,6,6	-	-	-		
89	OHX	B2	1911	-	0,6,6	-	-	-		
89	OHX	B2	1968	-	0,6,6	-	-	-		
89	OHX	B2	2011	-	0,6,6	-	-	-		
89	OHX	B2	2036	-	0,6,6	-	-	-		
89	OHX	B2	1901	-	0,6,6	-	-	-		
89	OHX	B2	2054	-	0,6,6	-	-	-		
89	OHX	B2	1925	-	0,6,6	-	-	-		
89	OHX	B2	2047	-	0,6,6	-	-	-		
89	OHX	B2	2023	-	0,6,6	-	-	-		
89	OHX	B2	1965	-	0,6,6	-	-	-		
89	OHX	B2	2025	-	0,6,6	-	-	-		
89	OHX	B2	2077	-	0,6,6	-	-	-		
89	OHX	B2	1927	-	0,6,6	-	-	-		
89	OHX	B2	1967	-	0,6,6	-	-	-		
89	OHX	B2	1970	-	0,6,6	-	-	-		
89	OHX	B2	2018	-	0,6,6	-	-	-		
89	OHX	B2	1987	-	0,6,6	-	-	-		
89	OHX	B2	2020	-	0,6,6	-	-	-		
89	OHX	B2	2063	-	0,6,6	-	-	-		
89	OHX	B2	1985	-	0,6,6	-	-	-		
89	OHX	B2	1997	-	0,6,6	-	-	-		
89	OHX	B2	1945	-	0,6,6	-	-	-		
89	OHX	B2	1950	-	0,6,6	-	-	-		
89	OHX	B2	2049	-	0,6,6	-	-	-		
89	OHX	AI	301	-	0,6,6	-	-	-		
89	OHX	B2	2004	-	0,6,6	-	-	-		
89	OHX	B2	1943	-	0,6,6	-	-	-		
89	OHX	B2	2060	-	0,6,6	-	-	-		
89	OHX	B2	1918	89	0,6,6	-	-	-		
89	OHX	B2	1977	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	1920	-	0,6,6	-	-	-		
89	OHX	B2	1981	-	0,6,6	-	-	-		
89	OHX	B2	1931	-	0,6,6	-	-	-		
89	OHX	B2	1912	-	0,6,6	-	-	-		
89	OHX	B2	1952	-	0,6,6	-	-	-		
89	OHX	B2	1902	-	0,6,6	-	-	-		
89	OHX	B2	2007	-	0,6,6	-	-	-		
89	OHX	B2	1989	-	0,6,6	-	-	-		
89	OHX	B2	1949	-	0,6,6	-	-	-		
89	OHX	B2	2030	-	0,6,6	-	-	-		
89	OHX	B2	1937	-	0,6,6	-	-	-		
89	OHX	B2	1960	-	0,6,6	-	-	-		
89	OHX	B2	2001	-	0,6,6	-	-	-		
89	OHX	B2	2056	-	0,6,6	-	-	-		
89	OHX	B2	1919	-	0,6,6	-	-	-		
89	OHX	A3	102	-	0,6,6	-	-	-		
89	OHX	B2	2022	-	0,6,6	-	-	-		
89	OHX	B2	1947	-	0,6,6	-	-	-		
89	OHX	B2	2059	-	0,6,6	-	-	-		
89	OHX	B2	2064	88,89	0,6,6	-	-	-		
89	OHX	B2	1909	89	0,6,6	-	-	-		
89	OHX	B2	1942	-	0,6,6	-	-	-		
89	OHX	B2	2021	-	0,6,6	-	-	-		
89	OHX	B2	2033	-	0,6,6	-	-	-		
89	OHX	B2	2062	-	0,6,6	-	-	-		
89	OHX	AP	201	-	0,6,6	-	-	-		
89	OHX	B2	1938	-	0,6,6	-	-	-		
89	OHX	B2	1966	-	0,6,6	-	-	-		
89	OHX	B2	1928	-	0,6,6	-	-	-		
89	OHX	B2	1905	-	0,6,6	-	-	-		
89	OHX	B2	1924	-	0,6,6	-	-	-		
89	OHX	B2	2017	-	0,6,6	-	-	-		
89	OHX	B2	2032	-	0,6,6	-	-	-		
90	GCP	CP	401	-	27,34,34	2.12	6 (22%)	34,54,54	2.52	9 (26%)
89	OHX	AL	201	-	0,6,6	-	-	-		
89	OHX	B2	2067	-	0,6,6	-	-	-		
89	OHX	B2	2082	-	0,6,6	-	-	-		
89	OHX	B2	1956	-	0,6,6	-	-	-		
89	OHX	B2	2005	-	0,6,6	-	-	-		
89	OHX	B2	2075	-	0,6,6	-	-	-		
89	OHX	B2	1955	-	0,6,6	-	-	-		
89	OHX	B2	1972	-	0,6,6	-	-	-		
89	OHX	B2	1958	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	AC	301	-	0,6,6	-	-	-		
89	OHX	B2	2029	-	0,6,6	-	-	-		
89	OHX	B2	2081	-	0,6,6	-	-	-		
89	OHX	B2	2024	-	0,6,6	-	-	-		
89	OHX	B2	1914	-	0,6,6	-	-	-		
89	OHX	B2	1992	-	0,6,6	-	-	-		
89	OHX	B2	1935	-	0,6,6	-	-	-		
89	OHX	B2	1904	-	0,6,6	-	-	-		
89	OHX	B2	1971	-	0,6,6	-	-	-		
89	OHX	B2	1975	-	0,6,6	-	-	-		
89	OHX	B2	2044	-	0,6,6	-	-	-		
89	OHX	B2	1906	88	0,6,6	-	-	-		
89	OHX	B2	1953	-	0,6,6	-	-	-		
89	OHX	B2	2009	-	0,6,6	-	-	-		
89	OHX	B2	1933	-	0,6,6	-	-	-		
89	OHX	B2	2069	-	0,6,6	-	-	-		
89	OHX	B2	1923	-	0,6,6	-	-	-		
89	OHX	B2	1961	-	0,6,6	-	-	-		
89	OHX	B2	1978	-	0,6,6	-	-	-		
89	OHX	B2	1963	-	0,6,6	-	-	-		
89	OHX	B2	2053	-	0,6,6	-	-	-		
89	OHX	B2	2015	-	0,6,6	-	-	-		
89	OHX	B2	2057	-	0,6,6	-	-	-		
89	OHX	B2	2084	-	0,6,6	-	-	-		
89	OHX	B2	1957	-	0,6,6	-	-	-		
89	OHX	B2	1996	-	0,6,6	-	-	-		
89	OHX	B2	2045	-	0,6,6	-	-	-		
89	OHX	B2	1980	-	0,6,6	-	-	-		
89	OHX	B2	2031	89	0,6,6	-	-	-		
89	OHX	B2	1939	-	0,6,6	-	-	-		
89	OHX	B2	1908	-	0,6,6	-	-	-		
89	OHX	B2	1959	-	0,6,6	-	-	-		
89	OHX	B2	2071	80	0,6,6	-	-	-		
89	OHX	B2	1926	-	0,6,6	-	-	-		
89	OHX	B2	2046	-	0,6,6	-	-	-		
89	OHX	B2	1946	-	0,6,6	-	-	-		
89	OHX	B2	2051	-	0,6,6	-	-	-		
89	OHX	B2	1995	-	0,6,6	-	-	-		
89	OHX	B2	2078	-	0,6,6	-	-	-		
89	OHX	B2	2010	-	0,6,6	-	-	-		
89	OHX	B2	2073	-	0,6,6	-	-	-		
89	OHX	B2	1983	-	0,6,6	-	-	-		
89	OHX	B2	2013	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	1969	-	0,6,6	-	-	-		
89	OHX	B2	1936	-	0,6,6	-	-	-		
89	OHX	B2	2038	-	0,6,6	-	-	-		
89	OHX	B2	1944	-	0,6,6	-	-	-		
89	OHX	B2	1954	-	0,6,6	-	-	-		
89	OHX	B2	1990	-	0,6,6	-	-	-		
89	OHX	B2	2083	-	0,6,6	-	-	-		
89	OHX	B2	1907	-	0,6,6	-	-	-		
89	OHX	B2	2035	-	0,6,6	-	-	-		
89	OHX	B2	1993	-	0,6,6	-	-	-		
89	OHX	B2	1903	-	0,6,6	-	-	-		
89	OHX	B2	1934	-	0,6,6	-	-	-		
89	OHX	B2	1932	-	0,6,6	-	-	-		
89	OHX	B2	2080	-	0,6,6	-	-	-		
89	OHX	B2	1910	-	0,6,6	-	-	-		
89	OHX	B2	2074	-	0,6,6	-	-	-		
89	OHX	B2	2019	-	0,6,6	-	-	-		
89	OHX	B2	1988	-	0,6,6	-	-	-		
89	OHX	B2	2008	-	0,6,6	-	-	-		
89	OHX	B2	2040	-	0,6,6	-	-	-		
89	OHX	B2	2042	-	0,6,6	-	-	-		
89	OHX	B2	2041	-	0,6,6	-	-	-		
89	OHX	B2	2002	-	0,6,6	-	-	-		
89	OHX	B2	2048	-	0,6,6	-	-	-		
89	OHX	B2	2055	-	0,6,6	-	-	-		
89	OHX	B2	2003	-	0,6,6	-	-	-		
89	OHX	B5	3401	-	0,6,6	-	-	-		
89	OHX	B2	2026	-	0,6,6	-	-	-		
89	OHX	B2	2079	-	0,6,6	-	-	-		
89	OHX	B2	2043	-	0,6,6	-	-	-		
89	OHX	B2	2058	-	0,6,6	-	-	-		
89	OHX	B2	2072	-	0,6,6	-	-	-		
89	OHX	B2	1974	-	0,6,6	-	-	-		
89	OHX	B2	1916	-	0,6,6	-	-	-		
89	OHX	B2	1940	-	0,6,6	-	-	-		
89	OHX	B2	1930	-	0,6,6	-	-	-		
89	OHX	B2	1986	-	0,6,6	-	-	-		
89	OHX	B2	2068	-	0,6,6	-	-	-		
89	OHX	B5	3403	-	0,6,6	-	-	-		
89	OHX	B2	1921	-	0,6,6	-	-	-		
89	OHX	Bn	101	-	0,6,6	-	-	-		
89	OHX	BR	201	-	0,6,6	-	-	-		
89	OHX	A6	401	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	OHX	B2	2014	-	0,6,6	-	-	-		
89	OHX	B2	1979	-	0,6,6	-	-	-		
89	OHX	AN	201	-	0,6,6	-	-	-		
89	OHX	B2	2052	-	0,6,6	-	-	-		
89	OHX	B2	1964	-	0,6,6	-	-	-		
89	OHX	B2	1941	-	0,6,6	-	-	-		
89	OHX	B2	2027	-	0,6,6	-	-	-		
89	OHX	B2	2028	-	0,6,6	-	-	-		
89	OHX	B2	2070	-	0,6,6	-	-	-		
89	OHX	B5	3402	-	0,6,6	-	-	-		
89	OHX	B2	1915	-	0,6,6	-	-	-		
89	OHX	B2	1976	-	0,6,6	-	-	-		
89	OHX	B2	2037	-	0,6,6	-	-	-		
89	OHX	B2	1994	-	0,6,6	-	-	-		
89	OHX	B2	1998	-	0,6,6	-	-	-		
89	OHX	B2	2006	-	0,6,6	-	-	-		
89	OHX	B2	1913	-	0,6,6	-	-	-		
89	OHX	B2	2000	-	0,6,6	-	-	-		
89	OHX	B2	1984	-	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	-	-	1/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	CP	401	GCP	C2'-C1'	-6.48	1.43	1.53
90	CP	401	GCP	C6-N1	5.32	1.42	1.33
90	CP	401	GCP	C4-N3	2.81	1.40	1.35
90	CP	401	GCP	C8-N7	-2.35	1.30	1.34
90	CP	401	GCP	PB-O3A	-2.31	1.55	1.58

The worst 5 of 9 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	C5-C6-N1	-7.05	113.79	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	CP	401	GCP	C2-N1-C6	5.19	124.18	115.93
90	CP	401	GCP	N3-C2-N1	-3.57	122.46	127.22
90	CP	401	GCP	C4-C5-C6	-2.97	117.96	120.80

There are no chirality outliers.

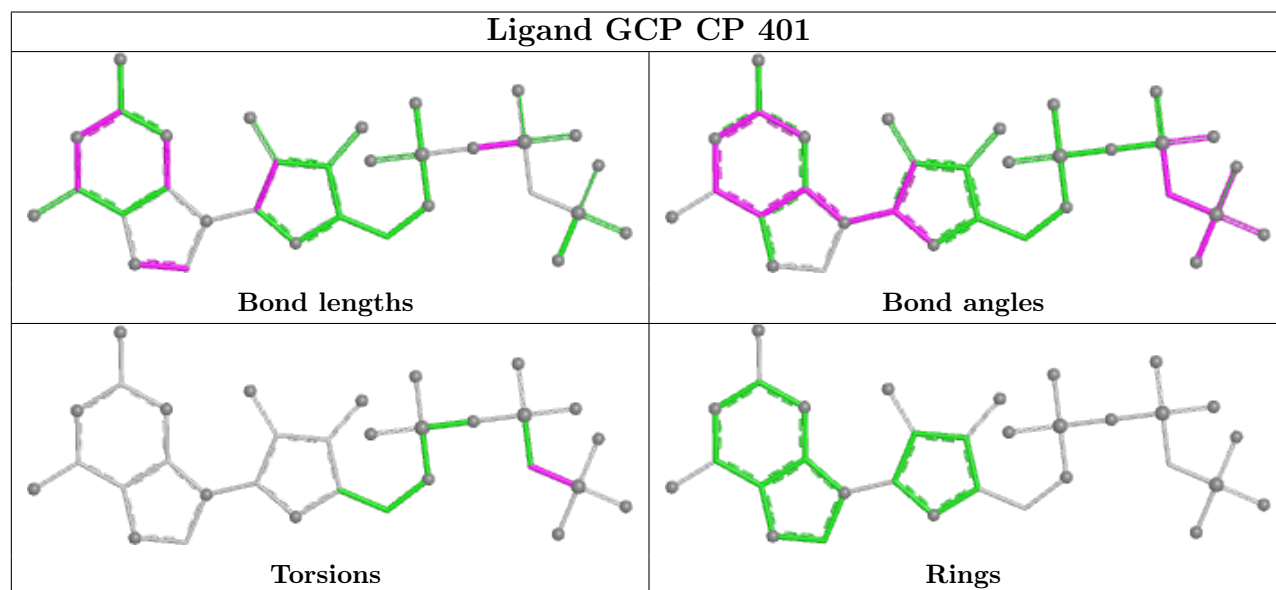
All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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
1	BK	23:UNK	C	28:UNK	N	8.84
1	B5	1285:G	O3'	1286:A	P	6.77

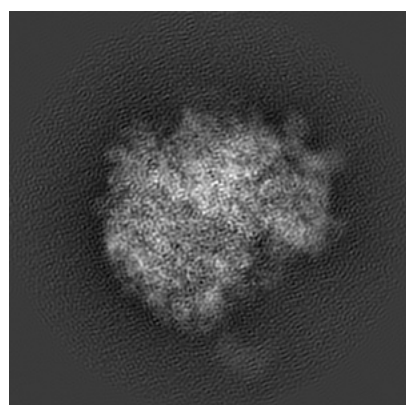
6 Map visualisation [i](#)

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.

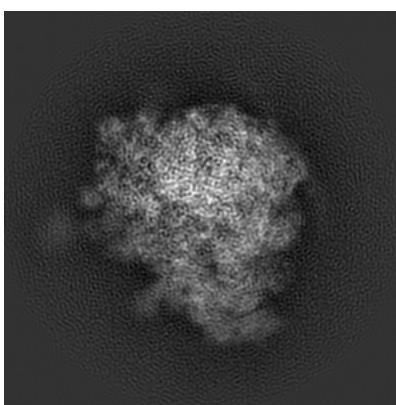
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

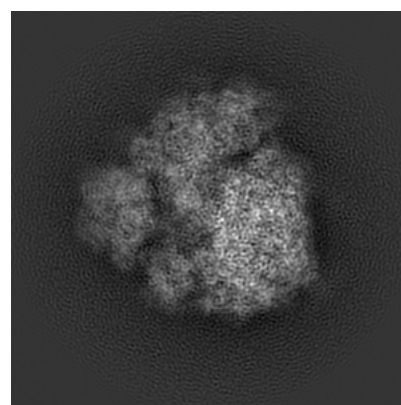
6.1.1 Primary map



X



Y

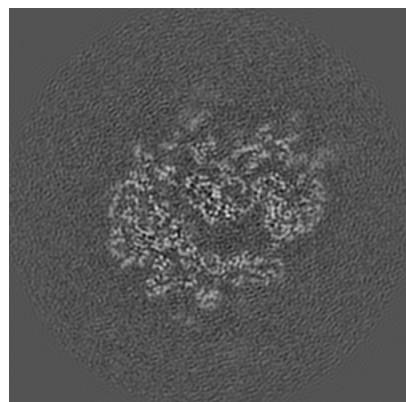


Z

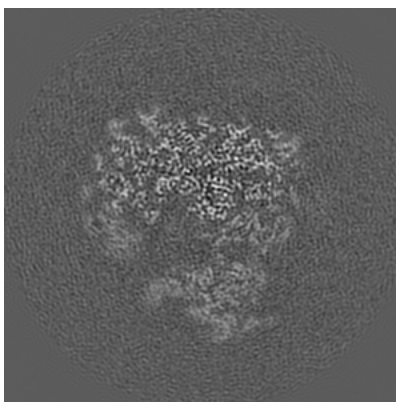
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

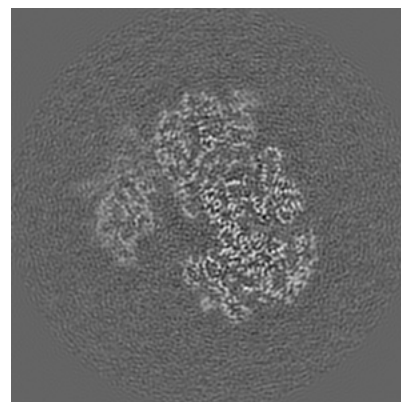
6.2.1 Primary map



X Index: 120



Y Index: 120

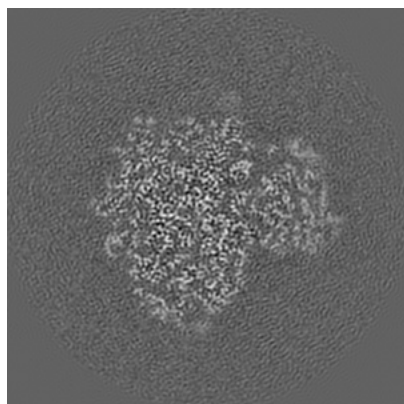


Z Index: 120

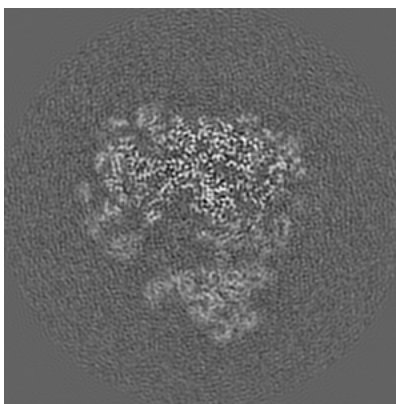
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

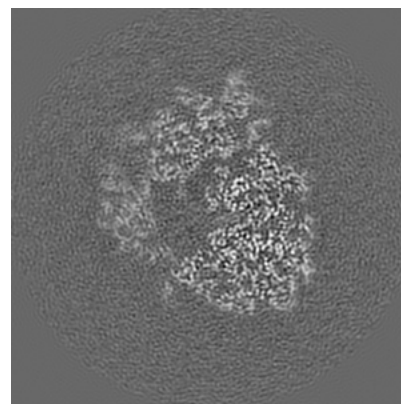
6.3.1 Primary map



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 surface views [i](#)

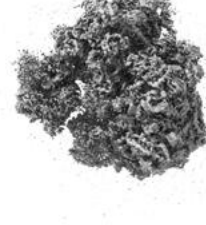
6.4.1 Primary map



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.

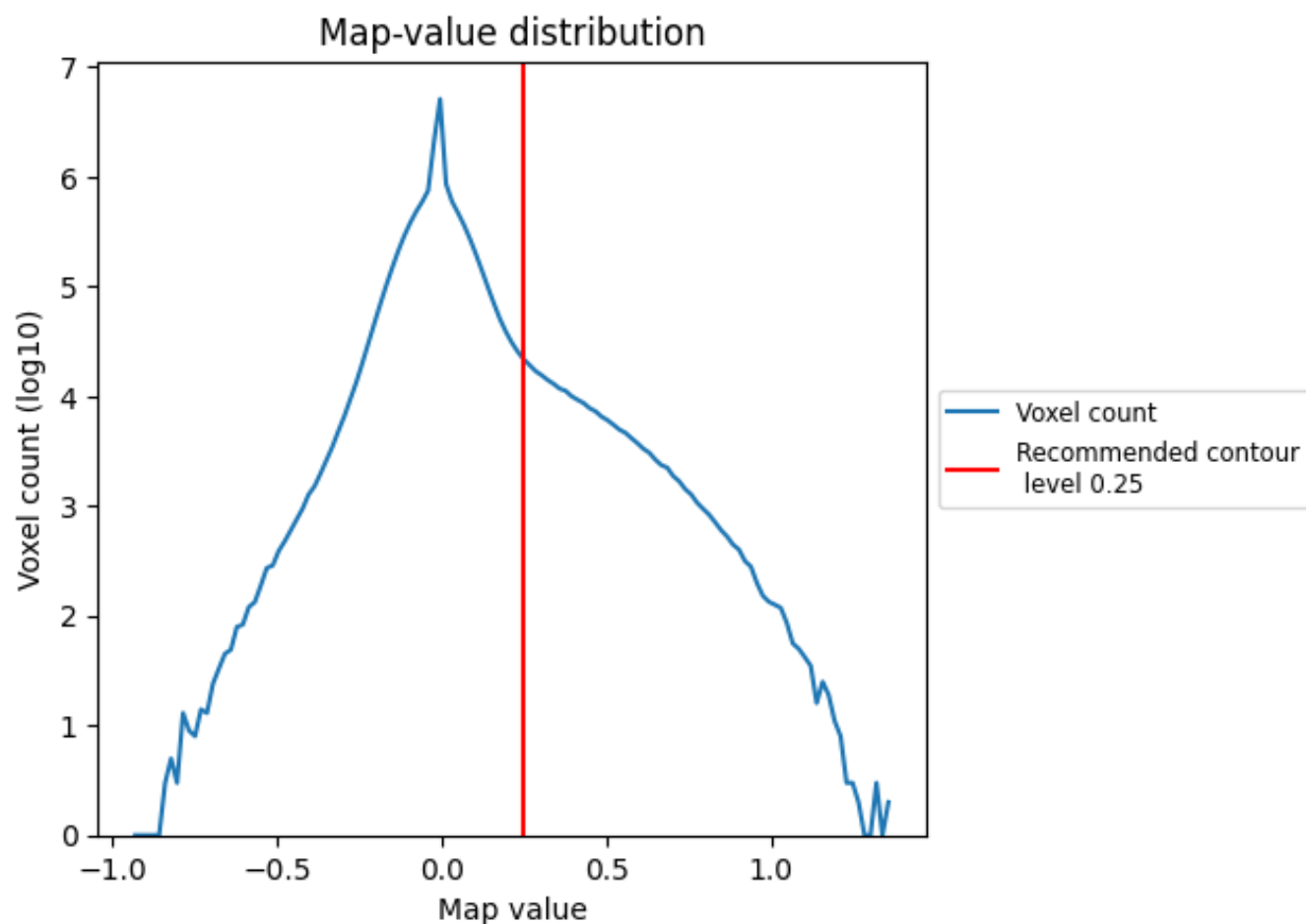
6.5 Mask visualisation

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

7 Map analysis [i](#)

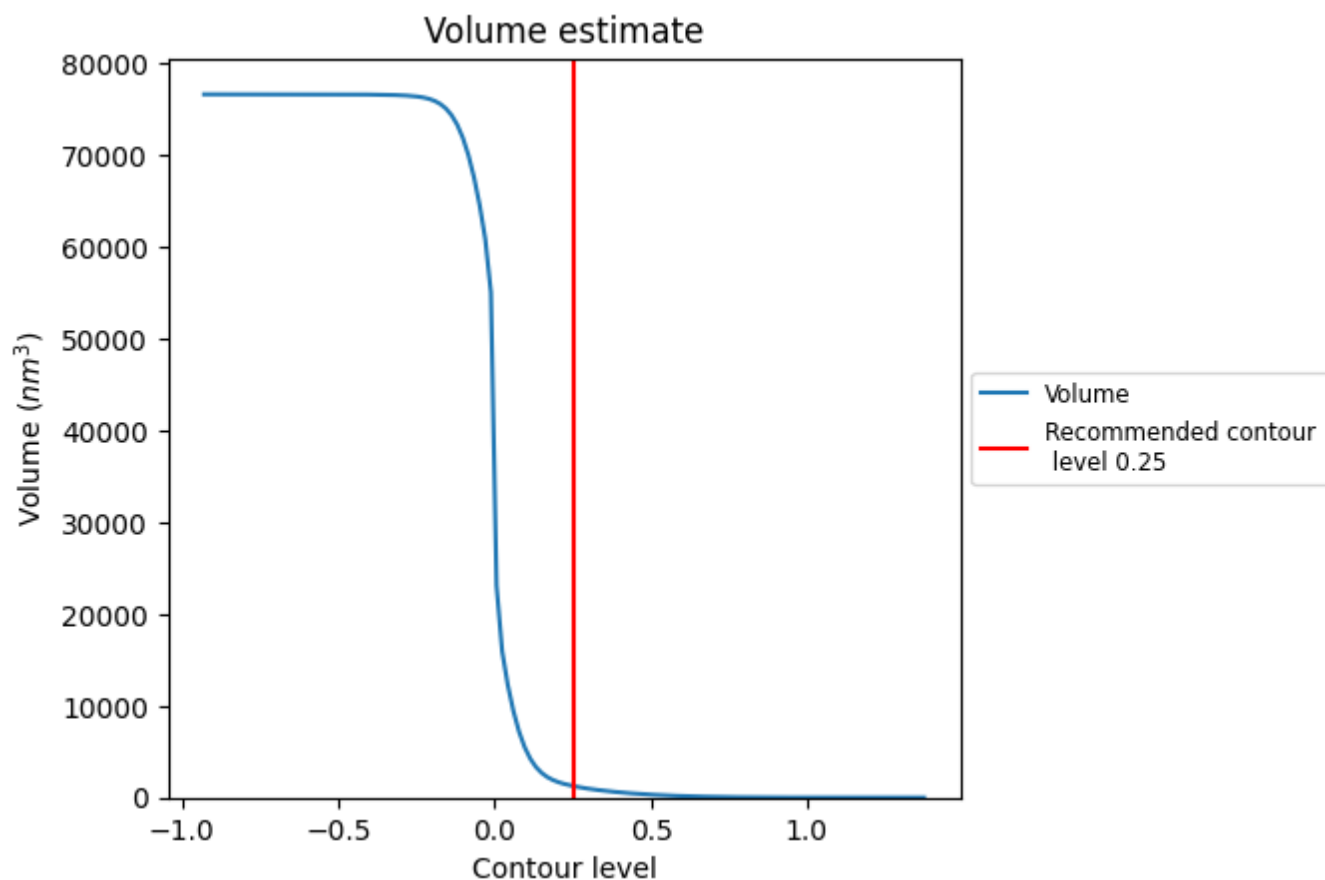
This section contains the results of statistical analysis of the map.

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.

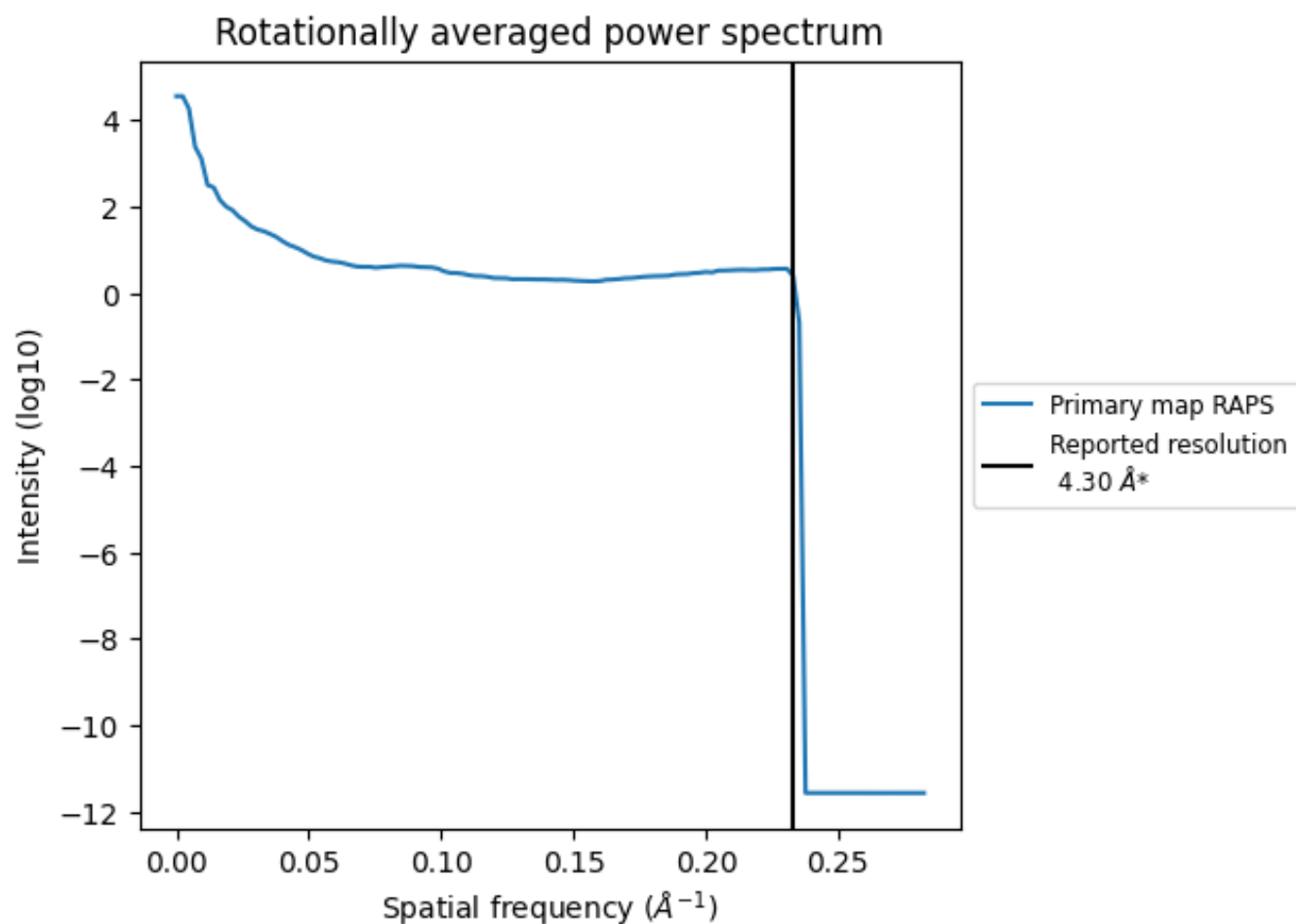
7.2 Volume estimate [i](#)



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 \AA^{-1}

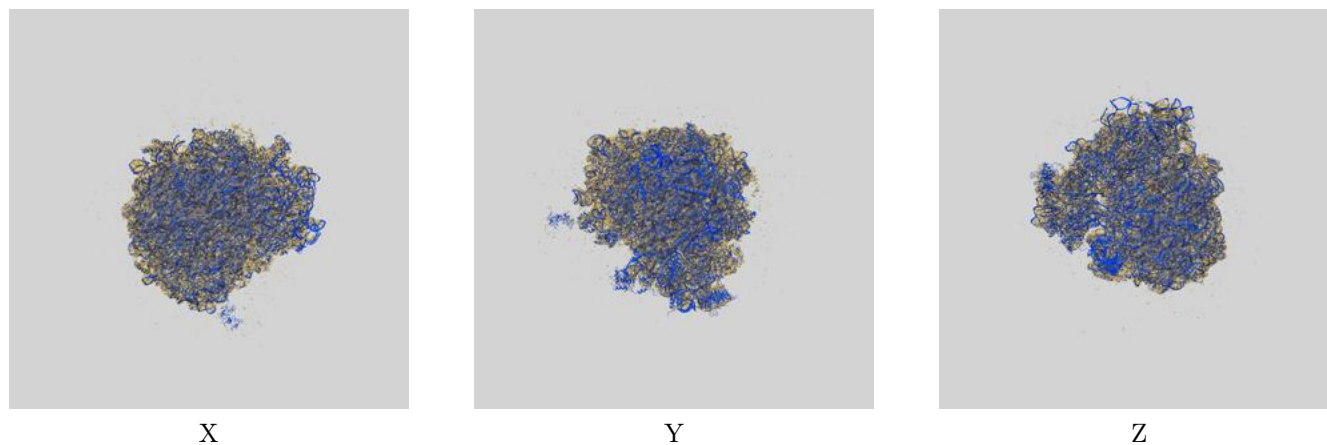
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

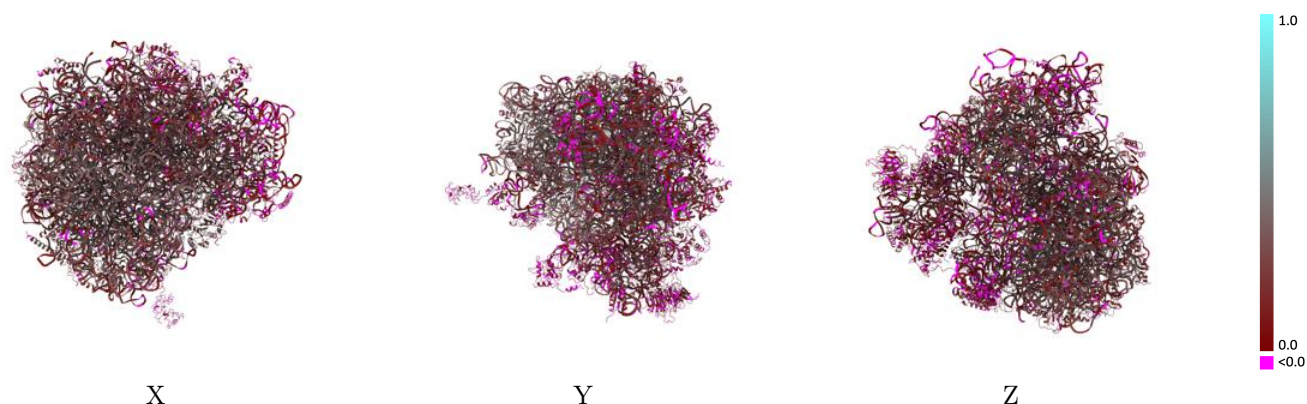
This section contains information regarding the fit between EMDB map EMD-2421 and PDB model 4V8Y. Per-residue inclusion information can be found in [section 3](#) on [page 34](#).

9.1 Map-model overlay [i](#)



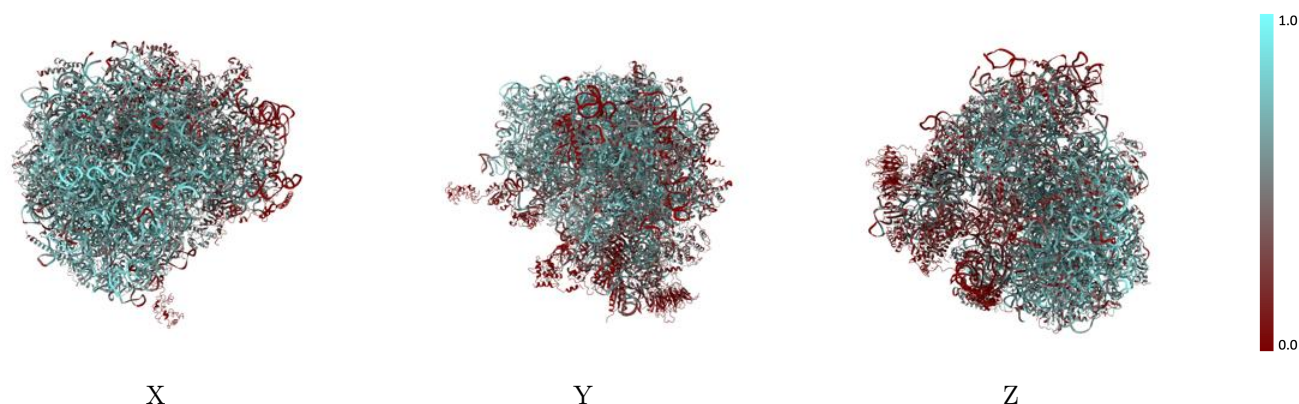
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



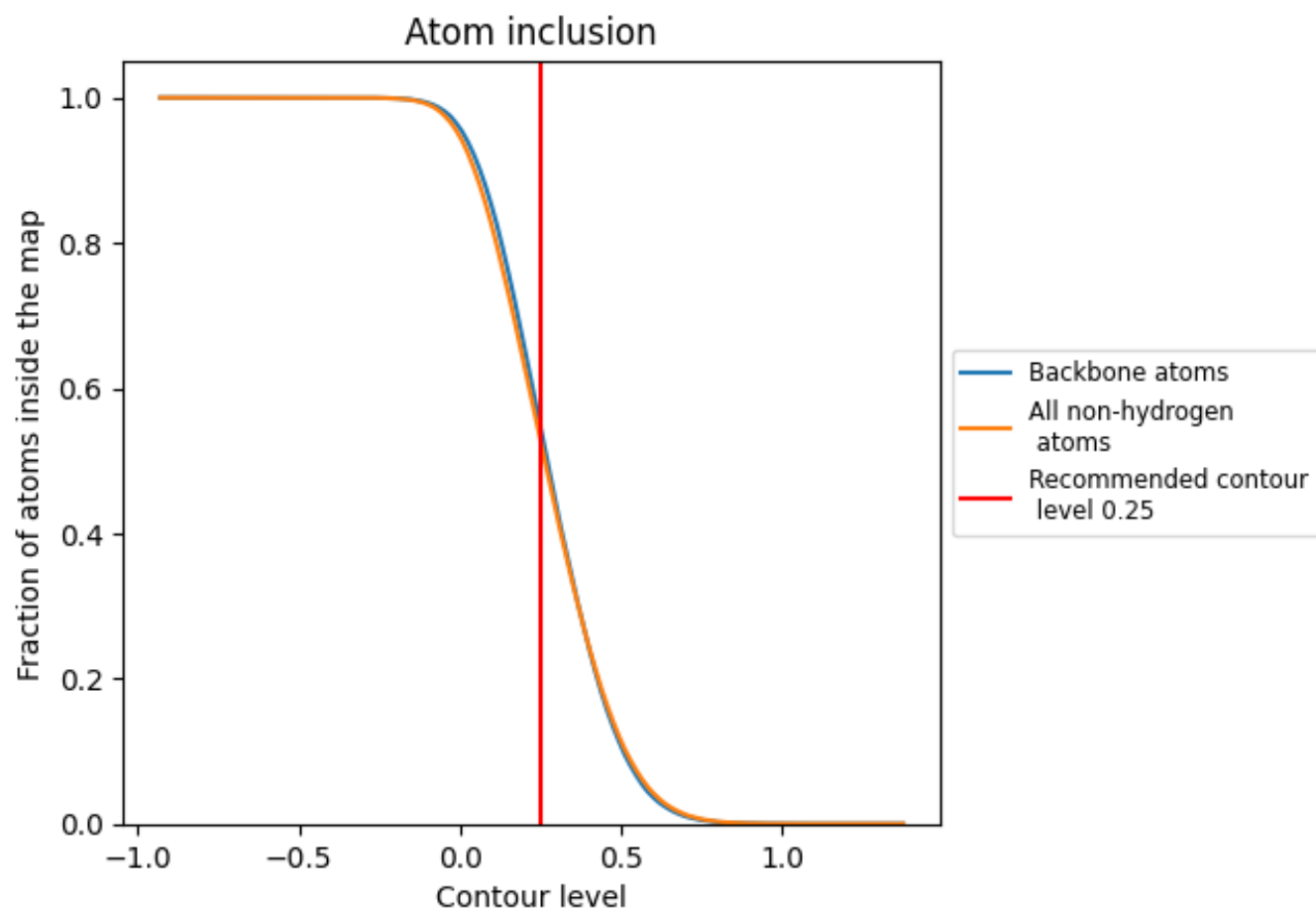
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.5273	 0.2420
A0	 0.2183	 0.1500
A1	 0.3322	 0.2030
A2	 0.1111	 0.0850
A3	 0.3065	 0.1190
A4	 0.3682	 0.2220
A5	 0.0551	 0.0540
A6	 0.1455	 0.1050
A7	 0.0259	 0.0790
AA	 0.3778	 0.1600
AB	 0.1708	 0.1110
AC	 0.4440	 0.2240
AD	 0.1735	 0.1070
AE	 0.4030	 0.1750
AF	 0.1668	 0.1060
AG	 0.2610	 0.0990
AH	 0.3967	 0.2020
AI	 0.3591	 0.1500
AJ	 0.4456	 0.2230
AK	 0.1689	 0.0790
AL	 0.4509	 0.2490
AM	 0.0364	 -0.0000
AN	 0.4669	 0.2480
AO	 0.1450	 0.1020
AP	 0.1745	 0.0870
AQ	 0.2326	 0.1700
AR	 0.2900	 0.1420
AS	 0.1974	 0.1080
AT	 0.2831	 0.1880
AU	 0.1641	 0.1250
AV	 0.3931	 0.1690
AW	 0.5321	 0.2900
AX	 0.5027	 0.3100
AY	 0.3641	 0.1540
AZ	 0.1152	 0.0760

























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Chain	Atom inclusion	Q-score
B2	 0.5407	 0.2310
B5	 0.7096	 0.3000
B7	 0.7169	 0.2600
B8	 0.7569	 0.3200
BA	 0.4044	 0.1650
BB	 0.6064	 0.3180
BC	 0.5800	 0.3070
BD	 0.5057	 0.2520
BE	 0.5360	 0.2680
BF	 0.6146	 0.3410
BG	 0.4645	 0.2000
BH	 0.5658	 0.3090
BI	 0.5351	 0.2970
BJ	 0.4745	 0.2450
BK	 0.1012	 0.0740
BL	 0.4899	 0.2450
BM	 0.5736	 0.2720
BN	 0.5278	 0.2690
BO	 0.6196	 0.3580
BP	 0.6113	 0.3320
BQ	 0.5434	 0.2750
BR	 0.3970	 0.1560
BS	 0.6049	 0.3220
BT	 0.5548	 0.3410
BU	 0.3678	 0.1280
BV	 0.5434	 0.3280
BW	 0.2658	 0.1480
BX	 0.4707	 0.2250
BY	 0.5569	 0.2910
BZ	 0.3324	 0.0810
Ba	 0.5482	 0.2710
Bb	 0.5199	 0.2800
Bc	 0.3113	 0.0810
Bd	 0.4901	 0.2340
Be	 0.5936	 0.3510
Bf	 0.6090	 0.3240
Bg	 0.3960	 0.1360
Bh	 0.5218	 0.2380
Bi	 0.4946	 0.2450
Bj	 0.5899	 0.2960
Bk	 0.3261	 0.1190
Bl	 0.4988	 0.2270

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Chain	Atom inclusion	Q-score
Bm	 0.5891	 0.3320
Bn	 0.1279	 0.0630
Bo	 0.5181	 0.3150
Bq	 0.1867	 0.1280
Br	 0.0381	 0.0850
Bs	 0.0043	 0.0850
By	 0.0422	 0.1160
CL	 0.0172	 0.0430
CN	 0.1003	 0.0590
CP	 0.3952	 0.2720
CW	 0.2227	 0.2310