wwPDB EM Validation Summary Report

Mar 6, 2026 – 12:36 AM UTC

PDB ID	:	6I7O / pdb_00006i7o
EMDB ID	:	EMD-4427
Title	:	The structure of a di-ribosome (disome) as a unit for RQC and NGD quality control pathways recognition.
Authors	:	Tesina, P.; Cheng, J.; Becker, T.; Beckmann, R.
Deposited on	:	2018-11-16
Resolution	:	5.30 Å(reported)

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

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

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

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

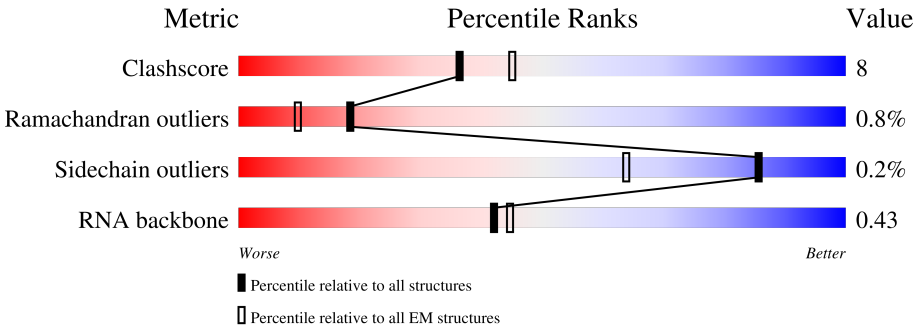
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

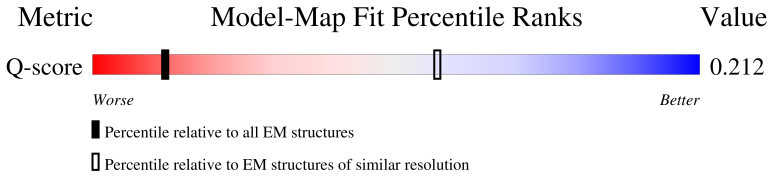
1 Overall quality at a glance

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

The reported resolution of this entry is 5.30 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	625 (4.80 - 5.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	BQ	3396	58% 28% 6% 8%
1	YQ	3396	56% 29% 7% 8%
2	BR	121	64% 30% 6%

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Mol	Chain	Length	Quality of chain
2	YR	121	71% 25%
3	BS	157	61% 33% 6%
3	YS	157	61% 31% 8%
4	AW	252	76% 24%
4	XW	252	72% 28%
5	BA	386	80% 20%
5	YA	386	83% 17%
6	BE	361	82% 16%
6	YE	361	81% 18%
7	BI	294	86% 14%
7	YI	294	88% 12%
8	BM	176	74% 15% 11%
8	YM	176	73% 16% 11%
9	BO	223	83% 17%
9	YO	223	80% 20%
10	AA	231	6% 78% 22%
10	XA	231	74% 26%
11	AD	190	86% 14%
11	XD	190	74% 26%
12	BD	221	81% 14% 5%
12	YD	221	74% 20% 5%
13	AG	169	67% 31%
13	XG	169	70% 28%
14	AJ	194	79% 17%
14	XJ	194	77% 21%

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Mol	Chain	Length	Quality of chain
15	AM	137	74% 26%
15	XM	137	71% 28%
16	AQ	203	71% 28%
16	XQ	203	74% 25%
17	AU	197	75% 25%
17	XU	197	78% 22%
18	2	1800	51% 34% 12%
18	2b	1800	52% 34% 11%
19	P	206	74% 25%
19	Pb	206	63% 36%
20	Q	216	7% 75% 25%
20	Qb	216	70% 29%
21	R	217	69% 30%
21	Rb	217	67% 32%
22	A	223	81% 17%
22	Ab	223	79% 20%
23	S	260	68% 31%
23	Sb	260	8% 63% 37%
24	B	206	78% 21%
24	Bb	206	77% 21%
25	T	218	77% 20%
25	Tb	218	76% 24%
26	U	185	79% 19%
26	Ub	185	76% 22%
27	V	200	69% 25% 6%

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Mol	Chain	Length	Quality of chain
27	Vb	200	68% 26% 6%
28	W	185	74% 26%
28	Wb	185	10% 72% 27%
29	C	92	72% 26%
29	Cb	92	70% 28%
30	X	146	8% 76% 23%
30	Xb	146	8% 71% 29%
31	D	124	11% 68% 29%
31	Db	124	12% 69% 26%
32	Y	150	85% 14%
32	Yb	150	81% 19%
33	Z	128	5% 82% 18%
33	Zb	128	77% 23%
34	E	119	66% 31%
34	Eb	119	67% 29%
35	F	141	60% 40%
35	Fb	141	68% 28%
36	G	125	6% 60% 40%
36	Gb	125	61% 38%
37	H	145	60% 38%
37	Hb	145	61% 36%
38	I	143	73% 27%
38	Ib	143	76% 23%
39	J	101	61% 36%
39	Jb	101	64% 33%

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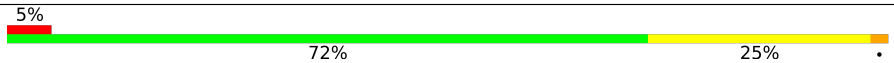
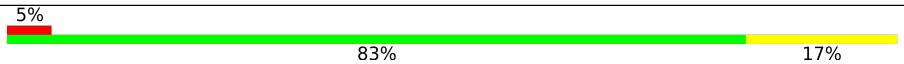
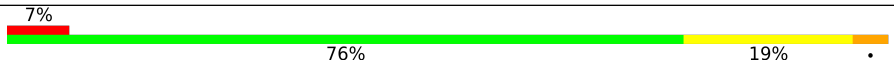
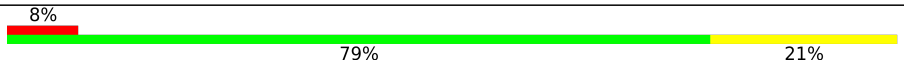
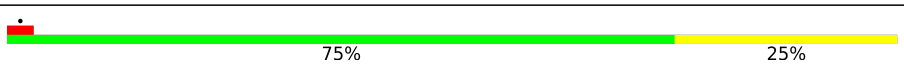
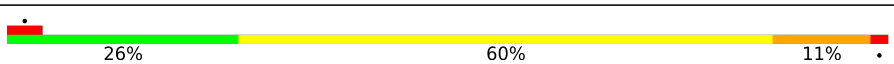
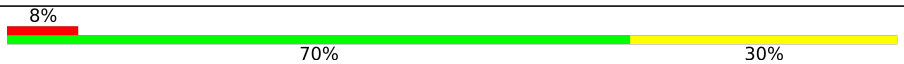
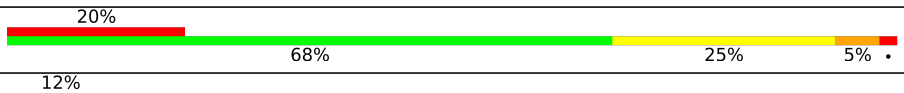
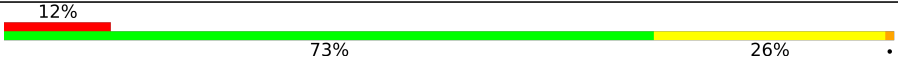
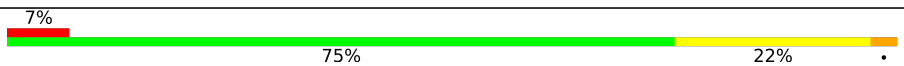
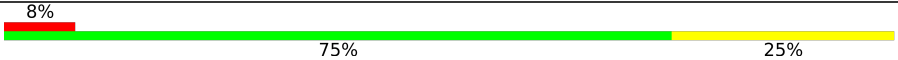
Mol	Chain	Length	Quality of chain
40	a	87	
40	ab	87	
41	b	129	
41	bb	129	
42	c	144	
42	cb	144	
43	d	134	
43	db	134	
44	K	69	
44	Kb	69	
45	e	97	
45	eb	97	
46	f	81	
46	fb	81	
47	L	63	
47	Lb	63	
48	M	53	
48	Mb	53	
49	g	60	
49	gb	60	
50	N	73	
50	Nb	73	
51	O	313	
51	Ob	313	
52	AX	184	

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Mol	Chain	Length	Quality of chain
52	XX	184	75% 20% 5%
53	BB	185	80% 19%
53	YB	185	86% 14%
54	BF	188	81% 15%
54	YF	188	84% 16%
55	BH	172	85% 15%
55	YH	172	83% 17%
56	BJ	159	80% 20%
56	YJ	159	79% 19%
57	BL	98	86% 13%
57	YL	98	85% 15%
58	AB	134	77% 23%
58	XB	134	76% 24%
59	AE	135	43% 83% 13%
59	XE	135	26% 84% 16%
60	AH	120	83% 17%
60	XH	120	82% 17%
61	AK	124	82% 18%
61	XK	124	77% 23%
62	AN	135	70% 28%
62	XN	135	77% 22%
63	AR	148	73% 26%
63	XR	148	81% 18%
64	AV	58	10% 71% 26%
64	XV	58	9% 76% 22%

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Mol	Chain	Length	Quality of chain
65	AY	100	6% 91% 9%
65	XY	100	7% 87% 12%
66	BC	109	89% 11%
66	YC	109	81% 18%
67	BG	127	5% 87% 13%
67	YG	127	88% 12%
68	BK	106	85% 15%
68	YK	106	86% 14%
69	BN	112	9% 81% 19%
69	YN	112	90% 10%
70	BP	119	90% 10%
70	YP	119	85% 14%
71	AC	99	5% 83% 16%
71	XC	99	80% 19%
72	AF	82	74% 26%
72	XF	82	72% 28%
73	AI	77	87% 12%
73	XI	77	82% 17%
74	AL	50	80% 20%
74	XL	50	82% 18%
75	AO	52	79% 21%
75	XO	52	19% 79% 21%
76	AS	25	84% 16%
76	XS	25	16% 80% 20%
77	AP	105	79% 21%

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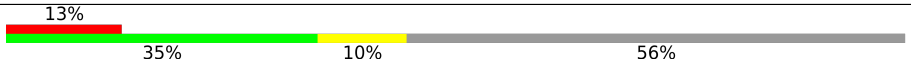
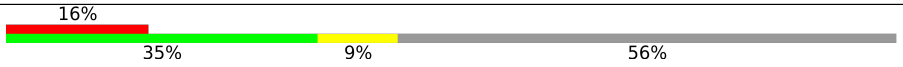
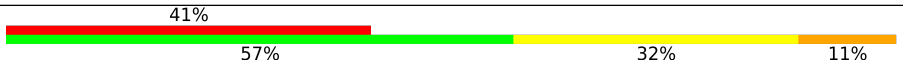
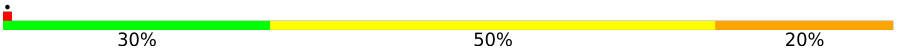
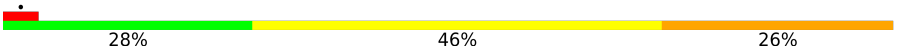
Mol	Chain	Length	Quality of chain
77	XP	105	
78	AT	91	
78	XT	91	
79	BU	312	
79	YU	312	
80	n	76	
81	m	75	
82	nb	76	
83	mb	77	
84	l	57	

2 Entry composition (i)

There are 85 unique types of molecules in this entry. The entry contains 405889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BQ	3127	Total 66891	C 29878	N 12066	O 21820	P 3127	0	0
1	YQ	3127	Total 66891	C 29878	N 12066	O 21820	P 3127	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BR	121	Total 2579	C 1152	N 461	O 845	P 121	0	0
2	YR	121	Total 2579	C 1152	N 461	O 845	P 121	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BS	157	Total 3333	C 1491	N 584	O 1101	P 157	0	0
3	YS	157	Total 3333	C 1491	N 584	O 1101	P 157	0	0

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AW	252	Total 1912	C 1190	N 388	O 333	S 1	0	0
4	XW	252	Total 1912	C 1190	N 388	O 333	S 1	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		
5	YA	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BE	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		
6	YE	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BI	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		
7	YI	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BM	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		
8	YM	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BO	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		
9	YO	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

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

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

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AD	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		
11	XD	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BD	209	Total	C	N	O	S	0	0
			1696	1077	321	293	5		
12	YD	209	Total	C	N	O	S	0	0
			1696	1077	321	293	5		

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AG	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		
13	XG	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AJ	194	Total	C	N	O	0	0
			1548	965	316	267		
14	XJ	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		
15	XM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		
16	XQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AU	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		
17	XU	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 18 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	1758	Total	C	N	O	P	0	0
			37455	16745	6624	12328	1758		
18	2b	1758	Total	C	N	O	P	0	0
			37455	16745	6624	12328	1758		

- Molecule 19 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		
19	Pb	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 20 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	216	Total	C	N	O	S	0	0
			1722	1091	312	315	4		
20	Qb	216	Total	C	N	O	S	0	0
			1722	1091	312	315	4		

- Molecule 21 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		
21	Rb	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 22 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		
22	Ab	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 23 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 24 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		
24	Bb	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 25 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		
25	Tb	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 26 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	185	Total	C	N	O	0	0
			1486	954	266	266		

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Mol	Chain	Residues	Atoms				AltConf	Trace
26	Ub	185	Total 1486	C 954	N 266	O 266	0	0

- Molecule 27 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	188	Total 1489	C 925	N 298	O 264	S 2	0	0
27	Vb	188	Total 1489	C 925	N 298	O 264	S 2	0	0

- Molecule 28 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	185	Total 1494	C 943	N 289	O 261	S 1	0	0
28	Wb	185	Total 1494	C 943	N 289	O 261	S 1	0	0

- Molecule 29 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	C	92	Total 741	C 478	N 121	O 140	S 2	0	0
29	Cb	92	Total 741	C 478	N 121	O 140	S 2	0	0

- Molecule 30 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	146	Total 1168	C 747	N 221	O 197	S 3	0	0
30	Xb	146	Total 1168	C 747	N 221	O 197	S 3	0	0

- Molecule 31 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D	124	Total 890	C 560	N 156	O 172	S 2	0	0
31	Db	124	Total 890	C 560	N 156	O 172	S 2	0	0

- Molecule 32 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		
32	Yb	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 33 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	128	Total	C	N	O	S	0	0
			949	582	188	176	3		
33	Zb	128	Total	C	N	O	S	0	0
			949	582	188	176	3		

- Molecule 34 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	E	119	Total	C	N	O	S	0	0
			939	595	176	161	7		
34	Eb	119	Total	C	N	O	S	0	0
			939	595	176	161	7		

- Molecule 35 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	F	141	Total	C	N	O	0	0
			1105	708	203	194		
35	Fb	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 36 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	G	125	Total	C	N	O	S	0	0
			1001	625	188	186	2		
36	Gb	125	Total	C	N	O	S	0	0
			1001	625	188	186	2		

- Molecule 37 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	H	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		
37	Hb	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 38 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	I	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		
38	Ib	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 39 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	J	101	Total	C	N	O	S	0	0
			805	512	145	147	1		
39	Jb	101	Total	C	N	O	S	0	0
			805	512	145	147	1		

- Molecule 40 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	a	87	Total	C	N	O	S	0	0
			684	420	125	137	2		
40	ab	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 41 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		
41	bb	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 42 is a protein called 40S ribosomal protein S23-A.

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

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

- Molecule 43 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	d	134	Total 1073	C 676	N 208	O 189	0	0
43	db	134	Total 1073	C 676	N 208	O 189	0	0

- Molecule 44 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	K	69	Total 558	C 357	N 103	O 98	0	0
44	Kb	69	Total 558	C 357	N 103	O 98	0	0

- Molecule 45 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	e	97	Total 769	C 475	N 160	O 129	S 5	0	0
45	eb	97	Total 769	C 475	N 160	O 129	S 5	0	0

- Molecule 46 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	f	81	Total 610	C 382	N 110	O 113	S 5	0	0
46	fb	81	Total 610	C 382	N 110	O 113	S 5	0	0

- Molecule 47 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L	63	Total 497	C 306	N 99	O 91	S 1	0	0
47	Lb	63	Total 497	C 306	N 99	O 91	S 1	0	0

- Molecule 48 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 49 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	g	60	Total	C	N	O	S	0	0
			475	299	98	77	1		
49	gb	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 50 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	N	73	Total	C	N	O	S	0	0
			556	352	105	95	4		
50	Nb	73	Total	C	N	O	S	0	0
			556	352	105	95	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	97	ALA	LYS	conflict	UNP P05759
Nb	97	ALA	LYS	conflict	UNP P05759

- Molecule 51 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	O	313	Total	C	N	O	S	0	0
			2403	1521	411	463	8		
51	Ob	313	Total	C	N	O	S	0	0
			2403	1521	411	463	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	161	ALA	LYS	conflict	UNP P38011
Ob	161	ALA	LYS	conflict	UNP P38011

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	AX	175	Total	C	N	O	0	0
			1378	856	273	249		
52	XX	175	Total	C	N	O	0	0
			1378	856	273	249		

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BB	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		
53	YB	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	BF	183	Total	C	N	O	0	0
			1482	911	320	251		
54	YF	188	Total	C	N	O	0	0
			1522	935	326	261		

- Molecule 55 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BH	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		
55	YH	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BJ	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		
56	YJ	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	BL	98	Total 778	C 505	N 127	O 146	0	0
57	YL	98	Total 778	C 505	N 127	O 146	0	0

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AB	134	Total 993	C 623	N 187	O 176	S 7	0	0
58	XB	134	Total 993	C 623	N 187	O 176	S 7	0	0

- Molecule 59 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AE	135	Total 1089	C 682	N 219	O 187	S 1	0	0
59	XE	135	Total 1089	C 682	N 219	O 187	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AH	120	Total 959	C 617	N 168	O 172	S 2	0	0
60	XH	120	Total 959	C 617	N 168	O 172	S 2	0	0

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	AK	124	Total 976	C 614	N 190	O 172	0	0
61	XK	124	Total 976	C 614	N 190	O 172	0	0

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

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

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

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AR	148	Total 1173	C 749	N 231	O 190	S 3	0	0
63	XR	148	Total 1173	C 749	N 231	O 190	S 3	0	0

- Molecule 64 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	AV	58	Total 462	C 289	N 100	O 73	0	0
64	XV	58	Total 462	C 289	N 100	O 73	0	0

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AY	100	Total 767	C 492	N 128	O 146	S 1	0	0
65	XY	100	Total 767	C 492	N 128	O 146	S 1	0	0

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BC	109	Total 883	C 559	N 167	O 156	S 1	0	0
66	YC	109	Total 883	C 559	N 167	O 156	S 1	0	0

- Molecule 67 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BG	127	Total 1020	C 647	N 205	O 167	S 1	0	0
67	YG	127	Total 1020	C 647	N 205	O 167	S 1	0	0

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BK	106	Total	C	N	O	S	0	0
			850	540	165	144	1		
68	YK	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BN	112	Total	C	N	O	S	0	0
			880	545	179	152	4		
69	YN	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BP	119	Total	C	N	O	S	0	0
			965	612	185	167	1		
70	YP	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AC	99	Total	C	N	O	S	0	0
			770	481	156	131	2		
71	XC	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AF	82	Total	C	N	O	S	0	0
			650	396	142	107	5		
72	XF	82	Total	C	N	O	S	0	0
			650	396	142	107	5		

- Molecule 73 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	AI	77	Total 608	C 388	N 114	O 106	0	0
73	XI	77	Total 608	C 388	N 114	O 106	0	0

- Molecule 74 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AL	50	Total 436	C 272	N 97	O 65	S 2	0	0
74	XL	50	Total 436	C 272	N 97	O 65	S 2	0	0

- Molecule 75 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AO	52	Total 417	C 259	N 86	O 67	S 5	0	0
75	XO	52	Total 417	C 259	N 86	O 67	S 5	0	0

- Molecule 76 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AS	25	Total 233	C 142	N 63	O 27	S 1	0	0
76	XS	25	Total 233	C 142	N 63	O 27	S 1	0	0

- Molecule 77 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AP	105	Total 847	C 534	N 170	O 138	S 5	0	0
77	XP	105	Total 847	C 534	N 170	O 138	S 5	0	0

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AT	91	Total 694	C 429	N 138	O 121	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
78	XT	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 79 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	BU	138	Total	C	N	O	S	0	0
			1052	672	187	190	3		
79	YU	138	Total	C	N	O	S	0	0
			1052	672	187	190	3		

- Molecule 80 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	n	76	Total	C	N	O	P	0	0
			1621	723	291	531	76		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	74	C	-	insertion	GB 1329886529
n	75	C	-	insertion	GB 1329886529
n	76	A	-	insertion	GB 1329886529

- Molecule 81 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	m	75	Total	C	N	O	P	0	0
			1589	710	279	525	75		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	11	C	U	conflict	GB 176418

- Molecule 82 is a RNA chain called A/P hybrid tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	nb	76	Total	C	N	O	P	0	0
			1620	723	290	532	75		

- Molecule 83 is a RNA chain called P/E hybrid tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	mb	77	Total	C	N	O	P	0	0
			1644	732	297	538	77		

- Molecule 84 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	l	57	Total	C	N	O	P	0	0
			1182	530	171	424	57		

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

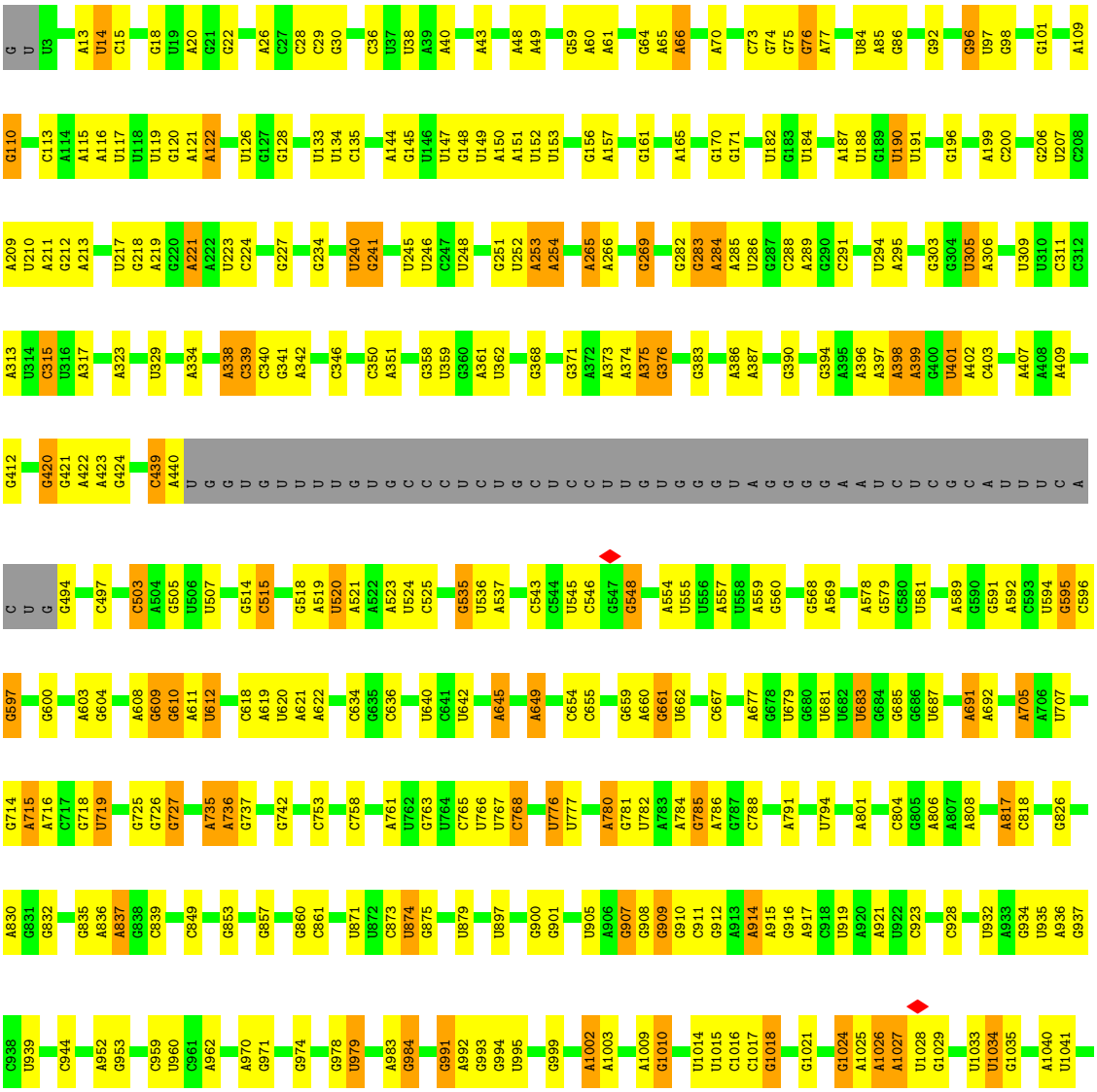
Mol	Chain	Residues	Atoms		AltConf
85	e	1	Total	Zn	0
			1	1	
85	f	1	Total	Zn	0
			1	1	
85	M	1	Total	Zn	0
			1	1	
85	N	1	Total	Zn	0
			1	1	
85	AO	1	Total	Zn	0
			1	1	
85	AP	1	Total	Zn	0
			1	1	
85	AT	1	Total	Zn	0
			1	1	
85	eb	1	Total	Zn	0
			1	1	
85	fb	1	Total	Zn	0
			1	1	
85	Mb	1	Total	Zn	0
			1	1	
85	YN	1	Total	Zn	0
			1	1	
85	XF	1	Total	Zn	0
			1	1	
85	XO	1	Total	Zn	0
			1	1	
85	XP	1	Total	Zn	0
			1	1	
85	XT	1	Total	Zn	0
			1	1	

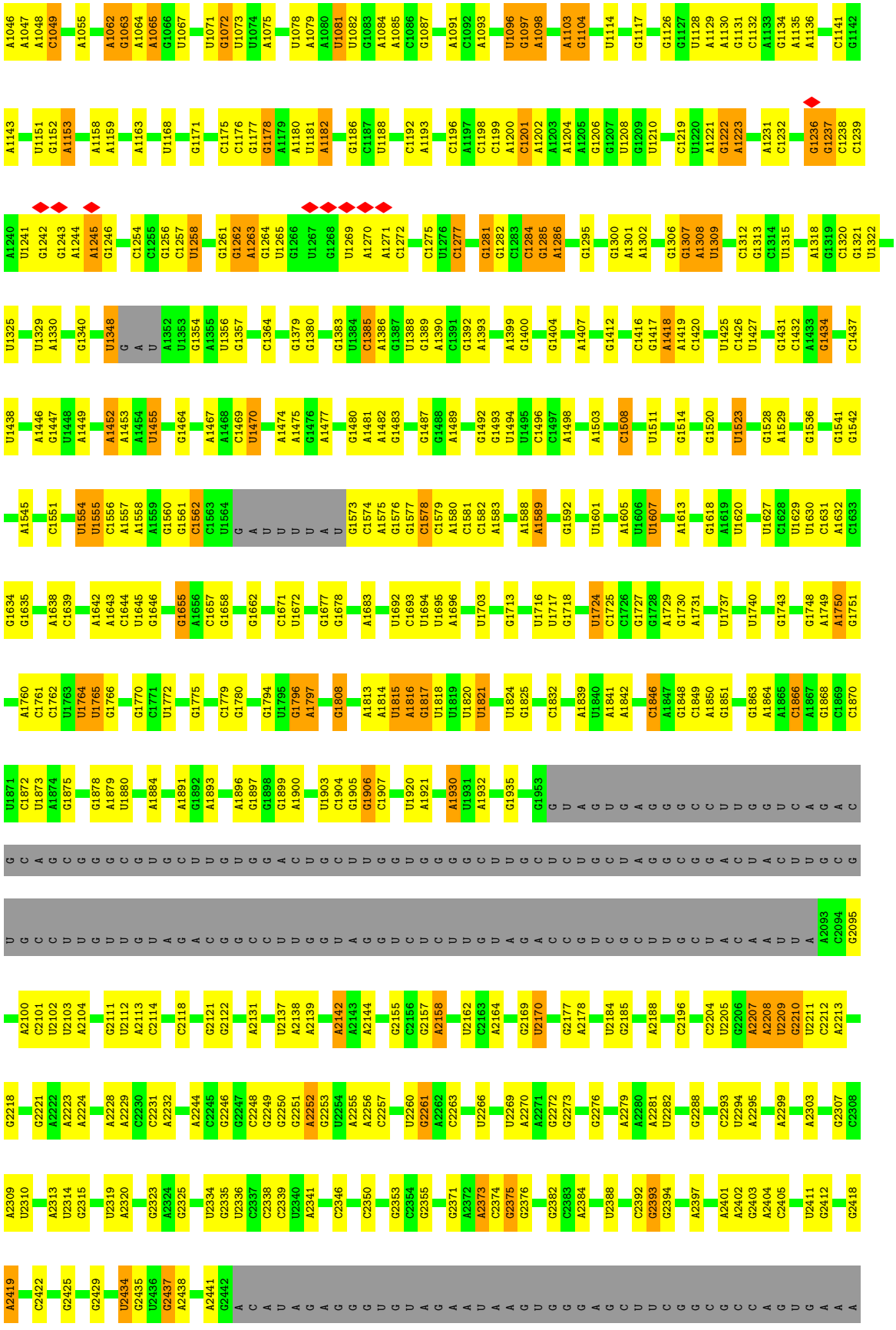
3 Residue-property plots (i)

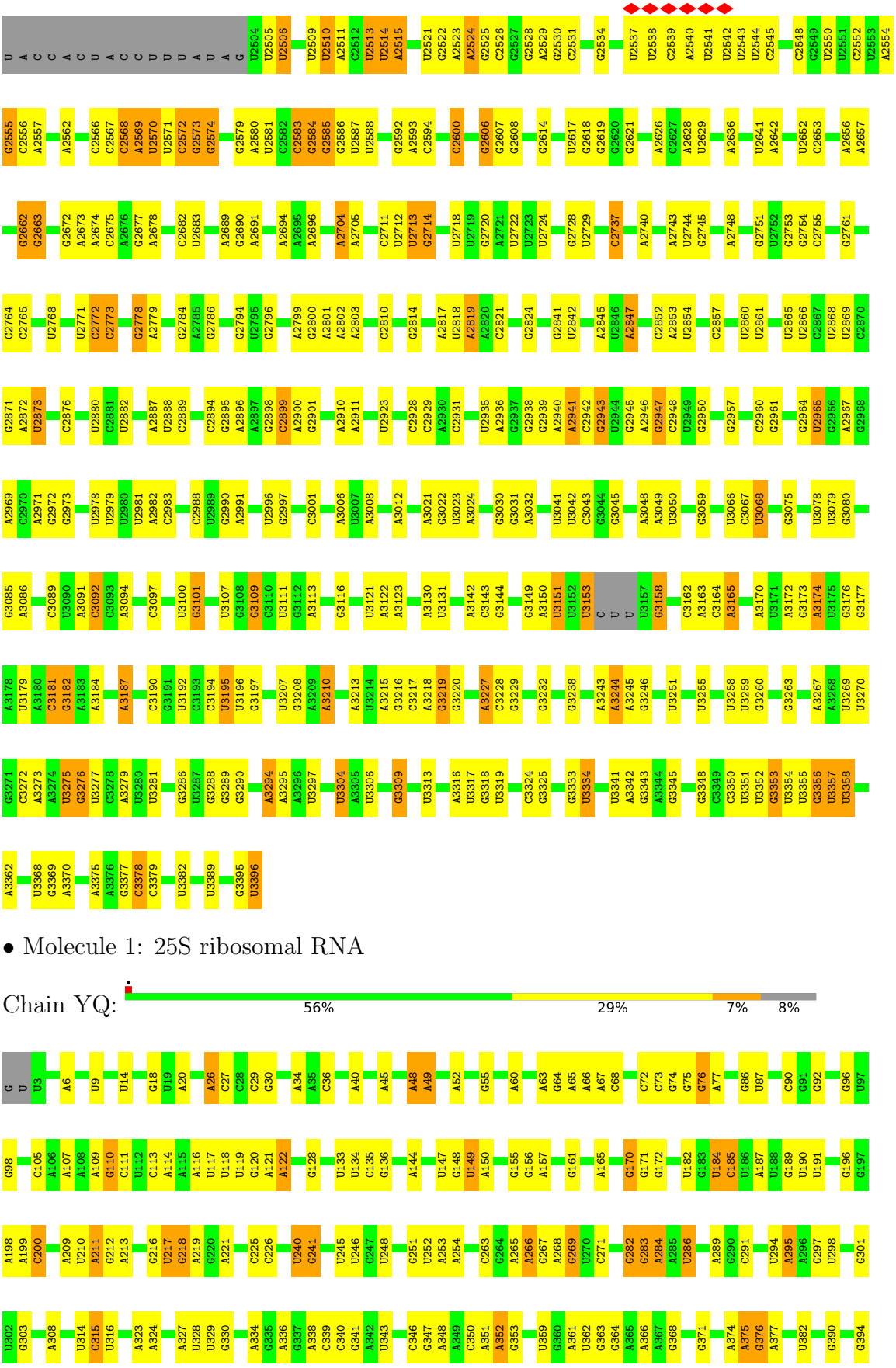
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 25S ribosomal RNA

Chain BQ:

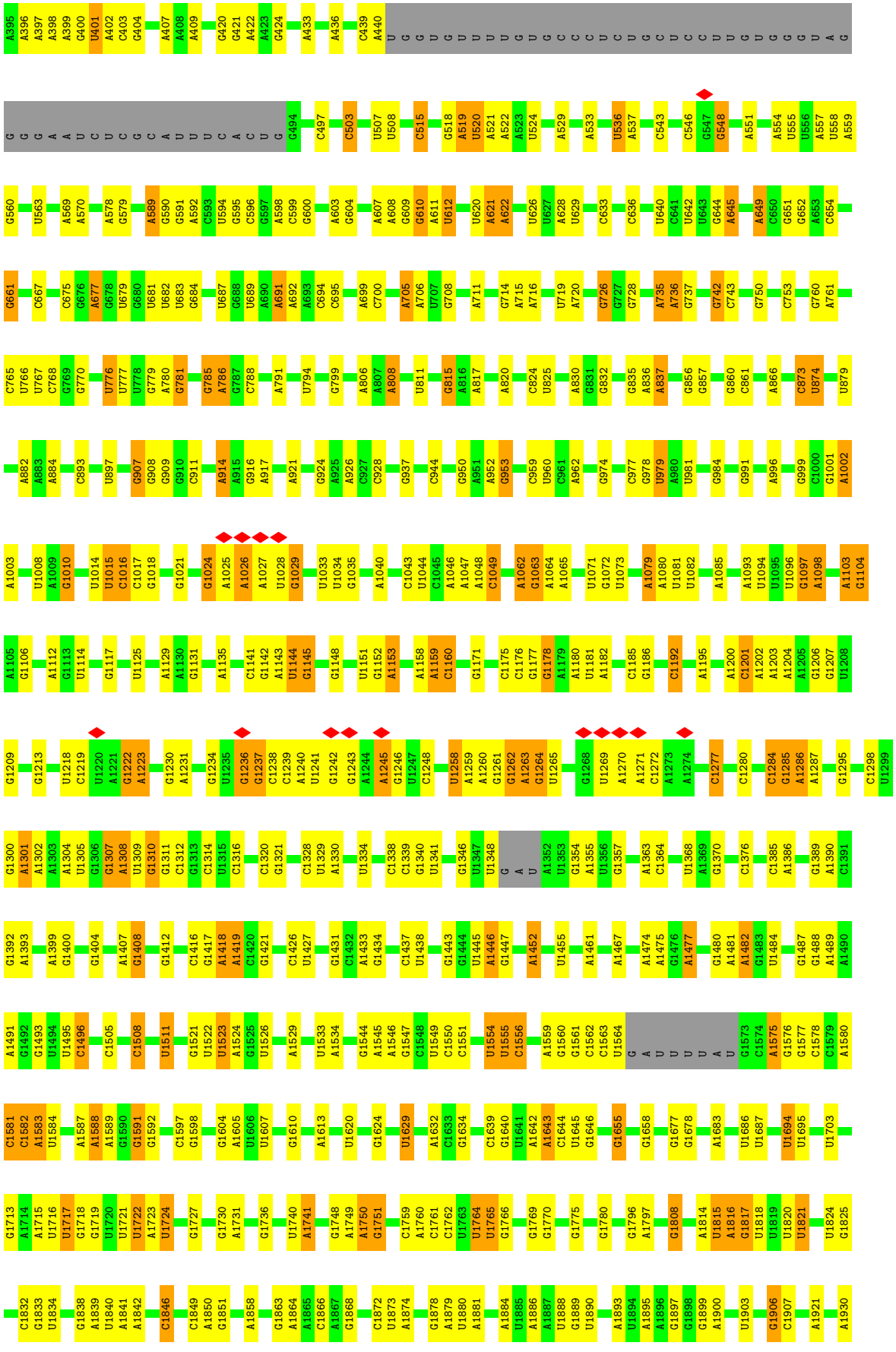


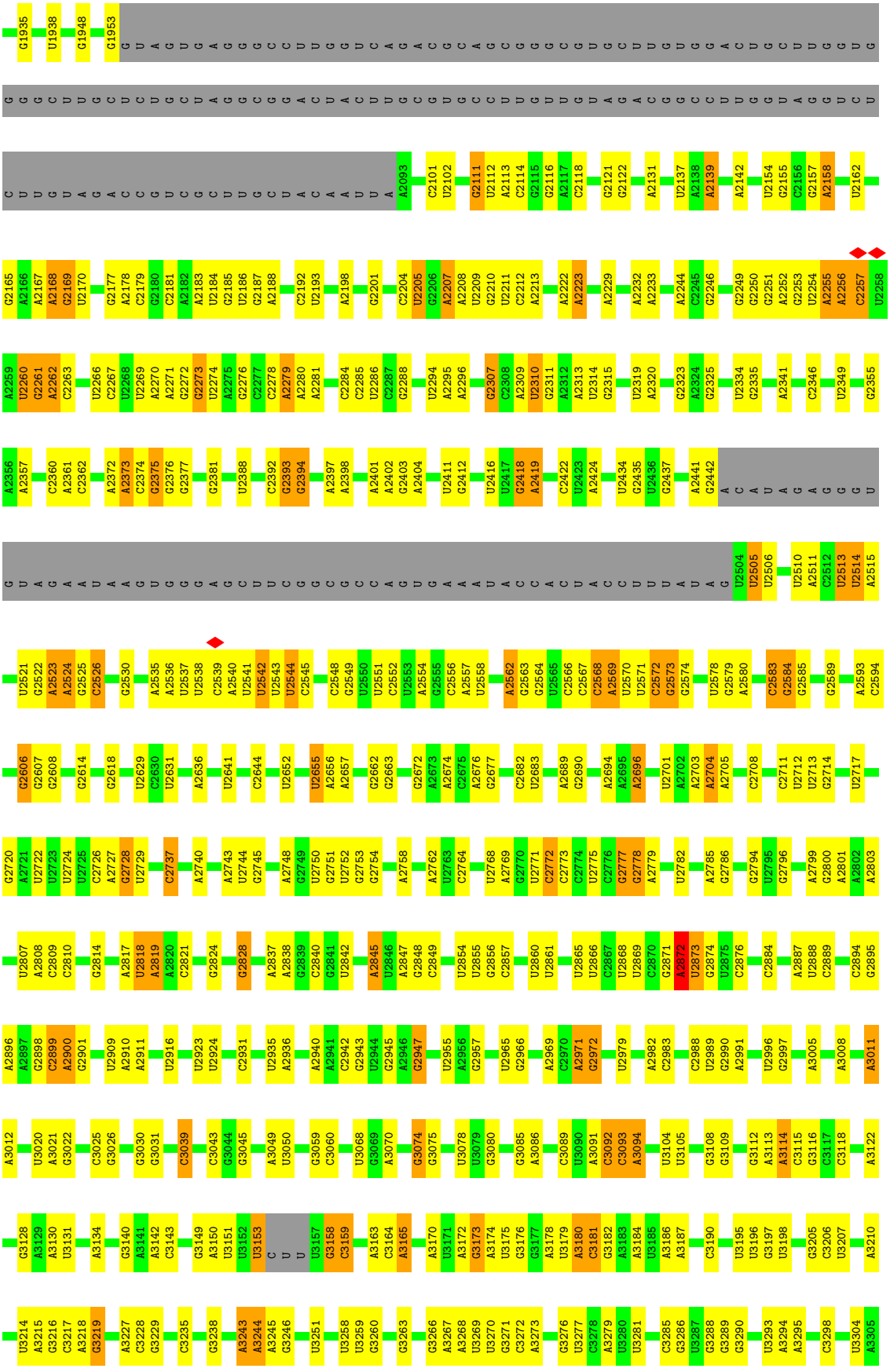


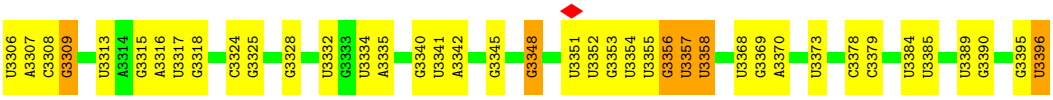


• Molecule 1: 25S ribosomal RNA

Chain YQ:

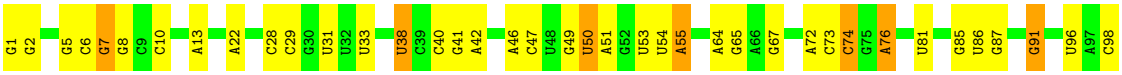


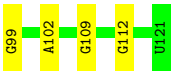




• Molecule 2: 5S ribosomal RNA

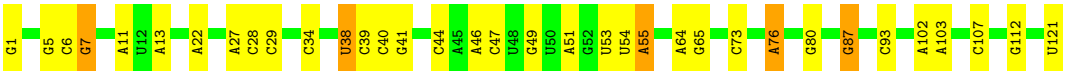
Chain BR:





• Molecule 2: 5S ribosomal RNA

Chain YR:

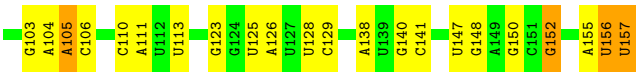


• Molecule 3: 5.8S ribosomal RNA

Chain BS:

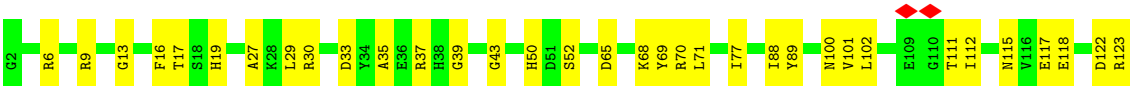
• Molecule 3: 5.8S ribosomal RNA

Chain YS:



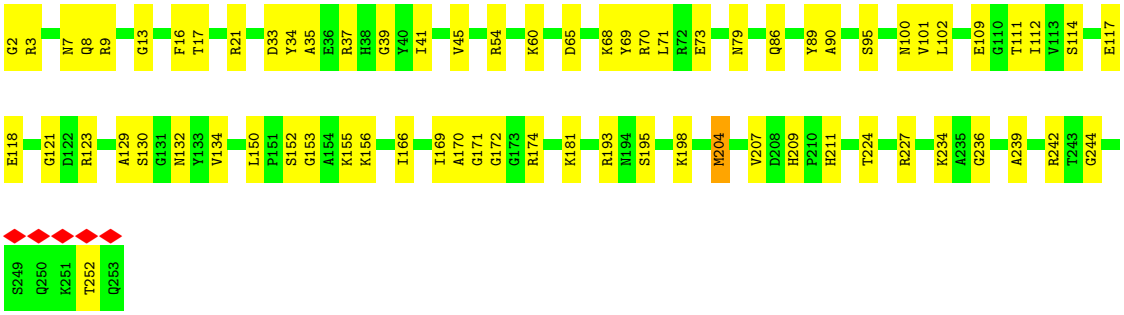
• Molecule 4: 60S ribosomal protein L2-A

Chain AW:



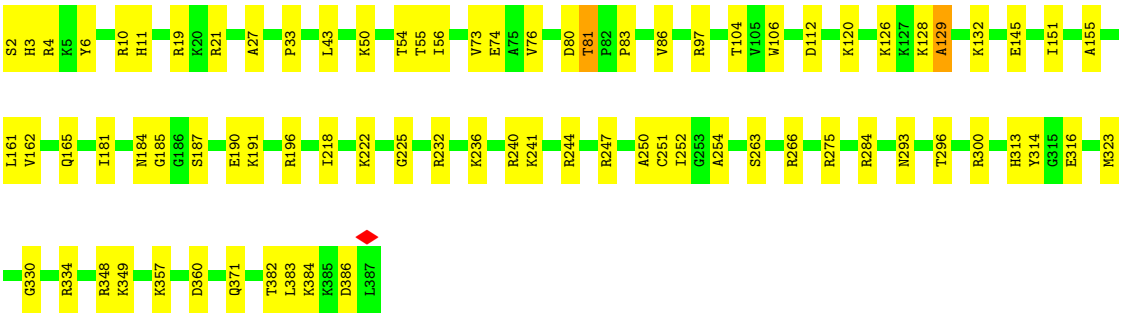
• Molecule 4: 60S ribosomal protein L2-A

Chain XW:



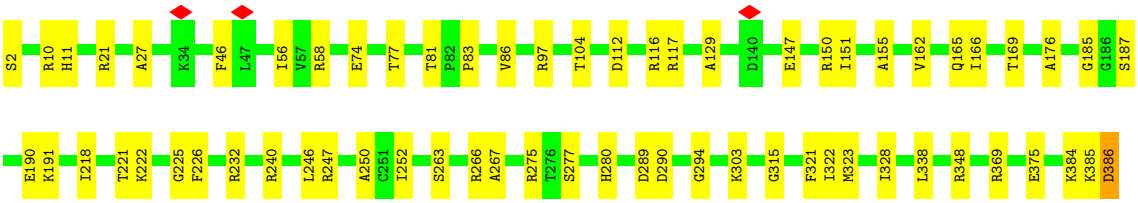
• Molecule 5: 60S ribosomal protein L3

Chain BA:



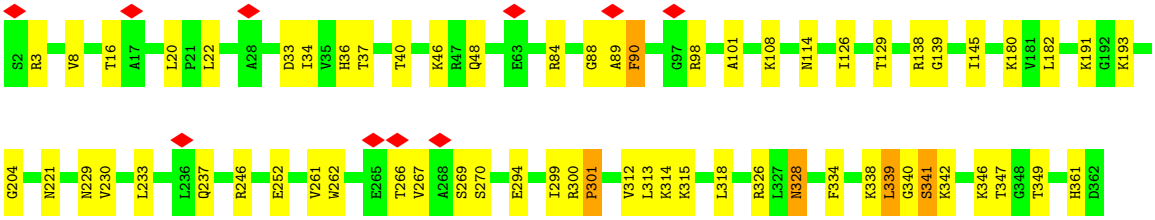
• Molecule 5: 60S ribosomal protein L3

Chain YA:



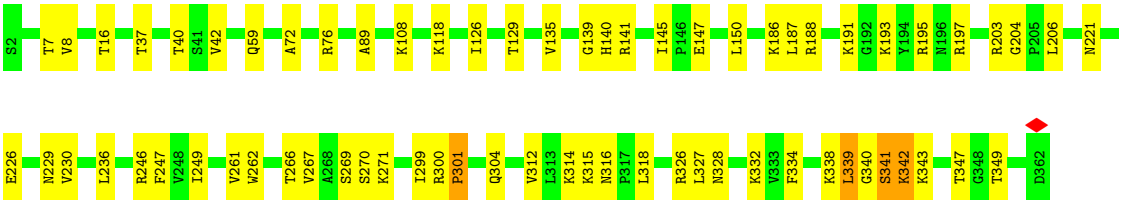
• Molecule 6: 60S ribosomal protein L4-A

Chain BE:



• Molecule 6: 60S ribosomal protein L4-A

Chain YE:

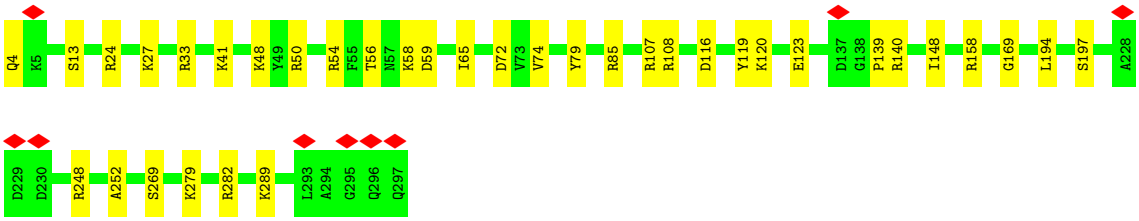


• Molecule 7: 60S ribosomal protein L5

Chain BI:

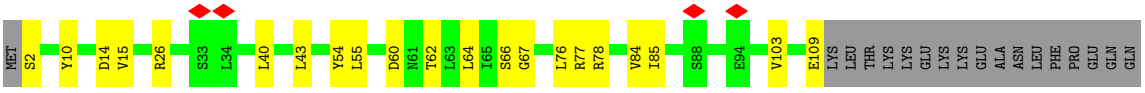
• Molecule 7: 60S ribosomal protein L5

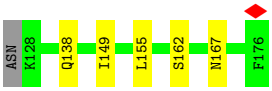
Chain YI:



• Molecule 8: 60S ribosomal protein L6-A

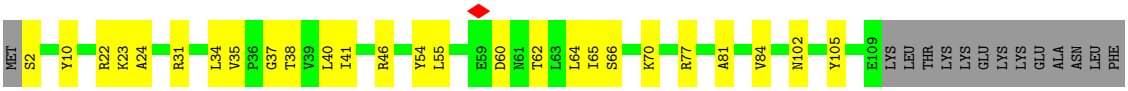
Chain BM:

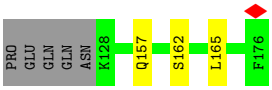




• Molecule 8: 60S ribosomal protein L6-A

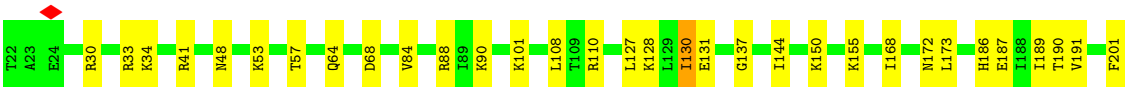
Chain YM:





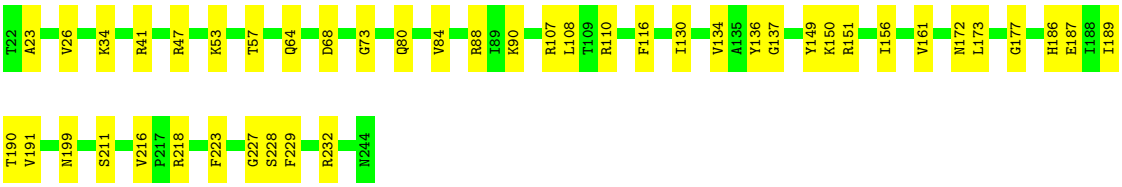
• Molecule 9: 60S ribosomal protein L7-A

Chain BO:



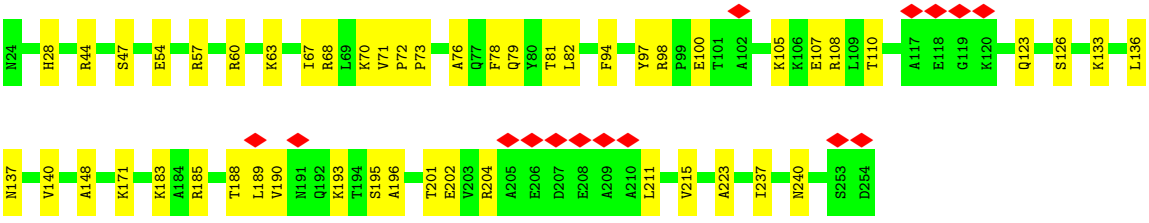
• Molecule 9: 60S ribosomal protein L7-A

Chain YO:



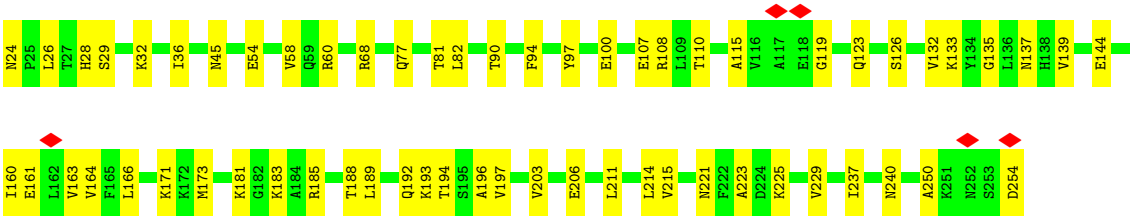
• Molecule 10: 60S ribosomal protein L8-A

Chain AA:



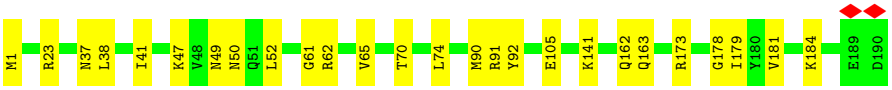
• Molecule 10: 60S ribosomal protein L8-A

Chain XA:



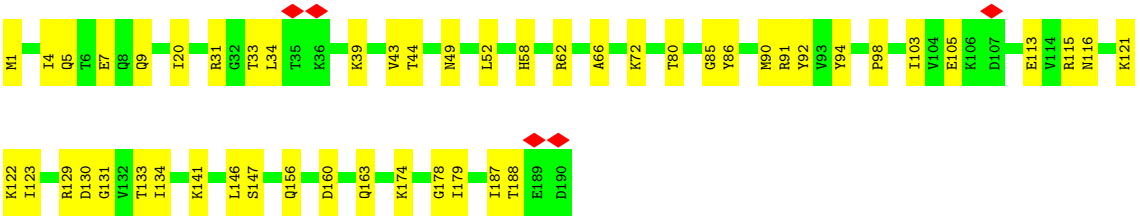
• Molecule 11: 60S ribosomal protein L9-A

Chain AD:



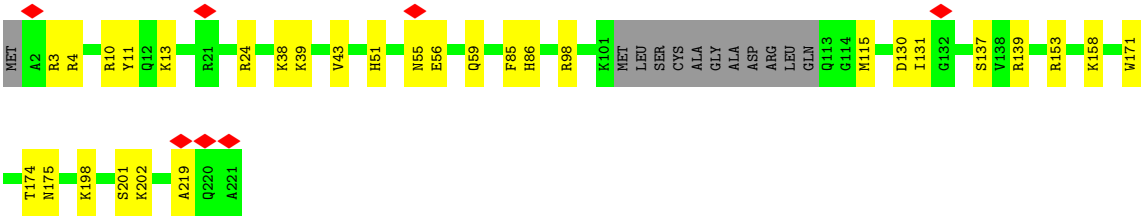
• Molecule 11: 60S ribosomal protein L9-A

Chain XD:



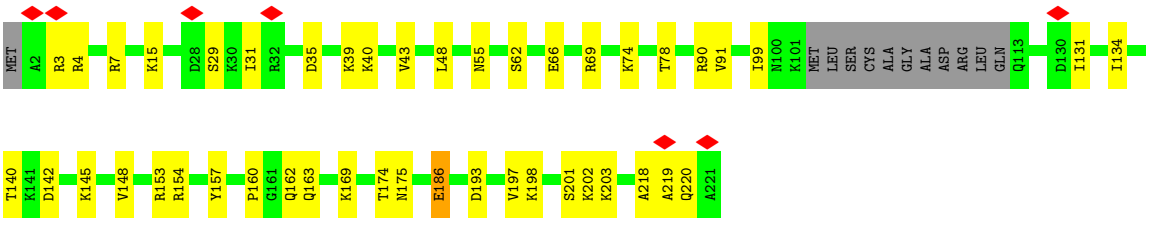
• Molecule 12: 60S ribosomal protein L10

Chain BD:



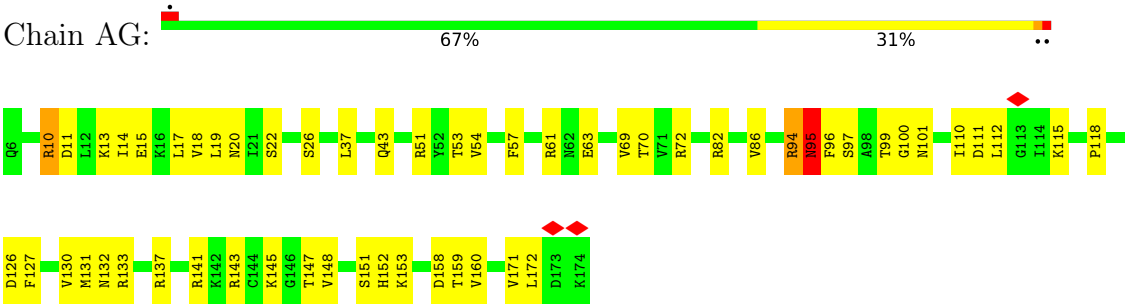
• Molecule 12: 60S ribosomal protein L10

Chain YD:



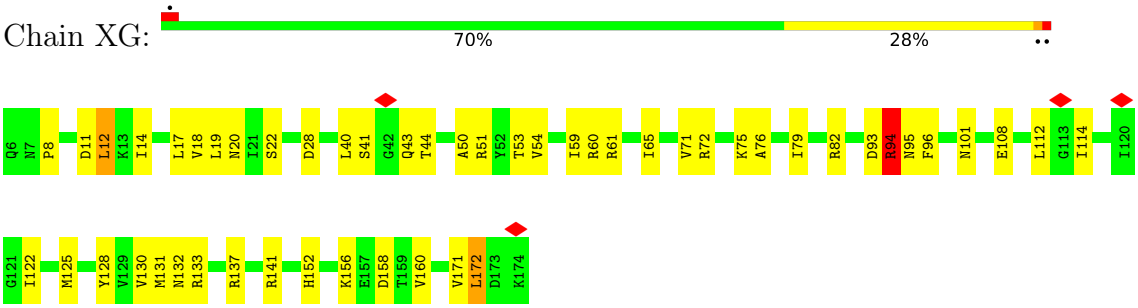
• Molecule 13: 60S ribosomal protein L11-B

Chain AG:



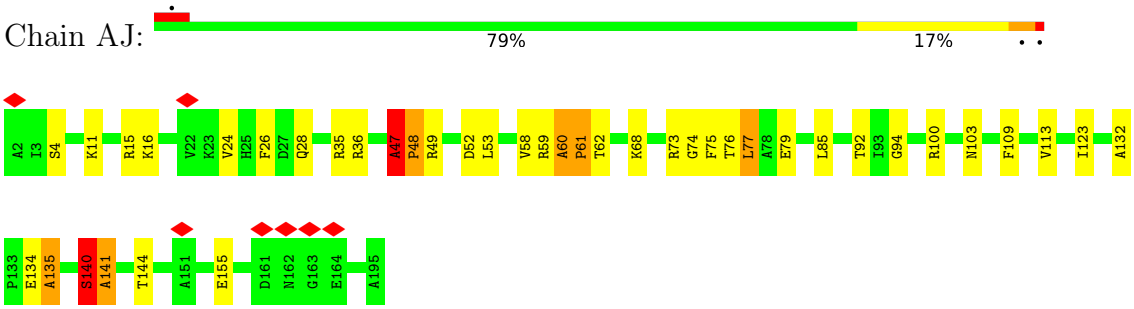
• Molecule 13: 60S ribosomal protein L11-B

Chain XG:



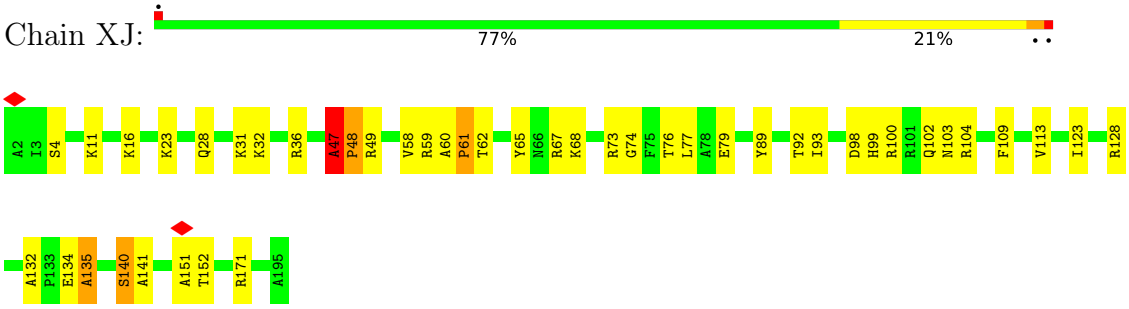
• Molecule 14: 60S ribosomal protein L13-A

Chain AJ:



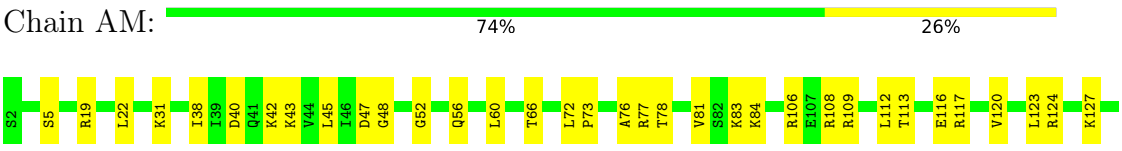
• Molecule 14: 60S ribosomal protein L13-A

Chain XJ:



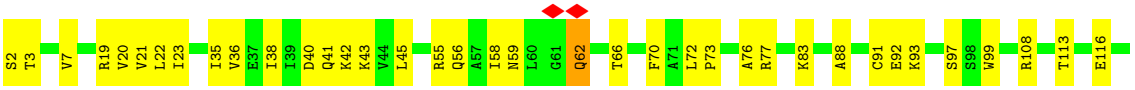
• Molecule 15: 60S ribosomal protein L14-A

Chain AM:



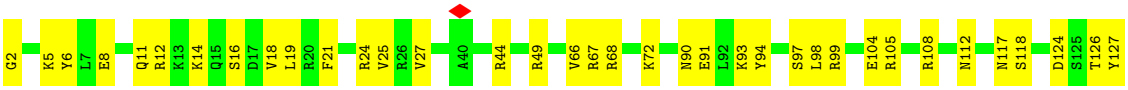
• Molecule 15: 60S ribosomal protein L14-A

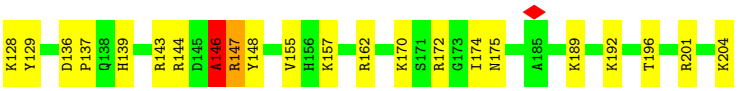
Chain XM:



• Molecule 16: 60S ribosomal protein L15-A

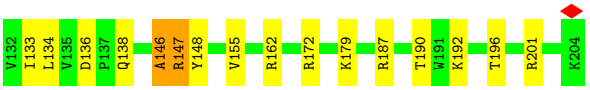
Chain AQ:





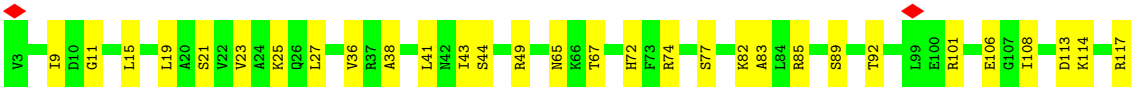
• Molecule 16: 60S ribosomal protein L15-A

Chain XQ:



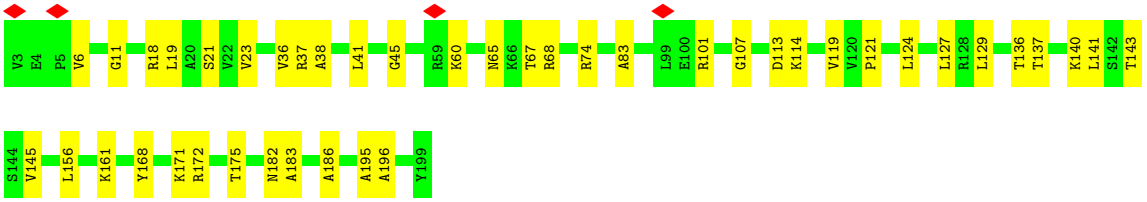
• Molecule 17: 60S ribosomal protein L16-A

Chain AU:



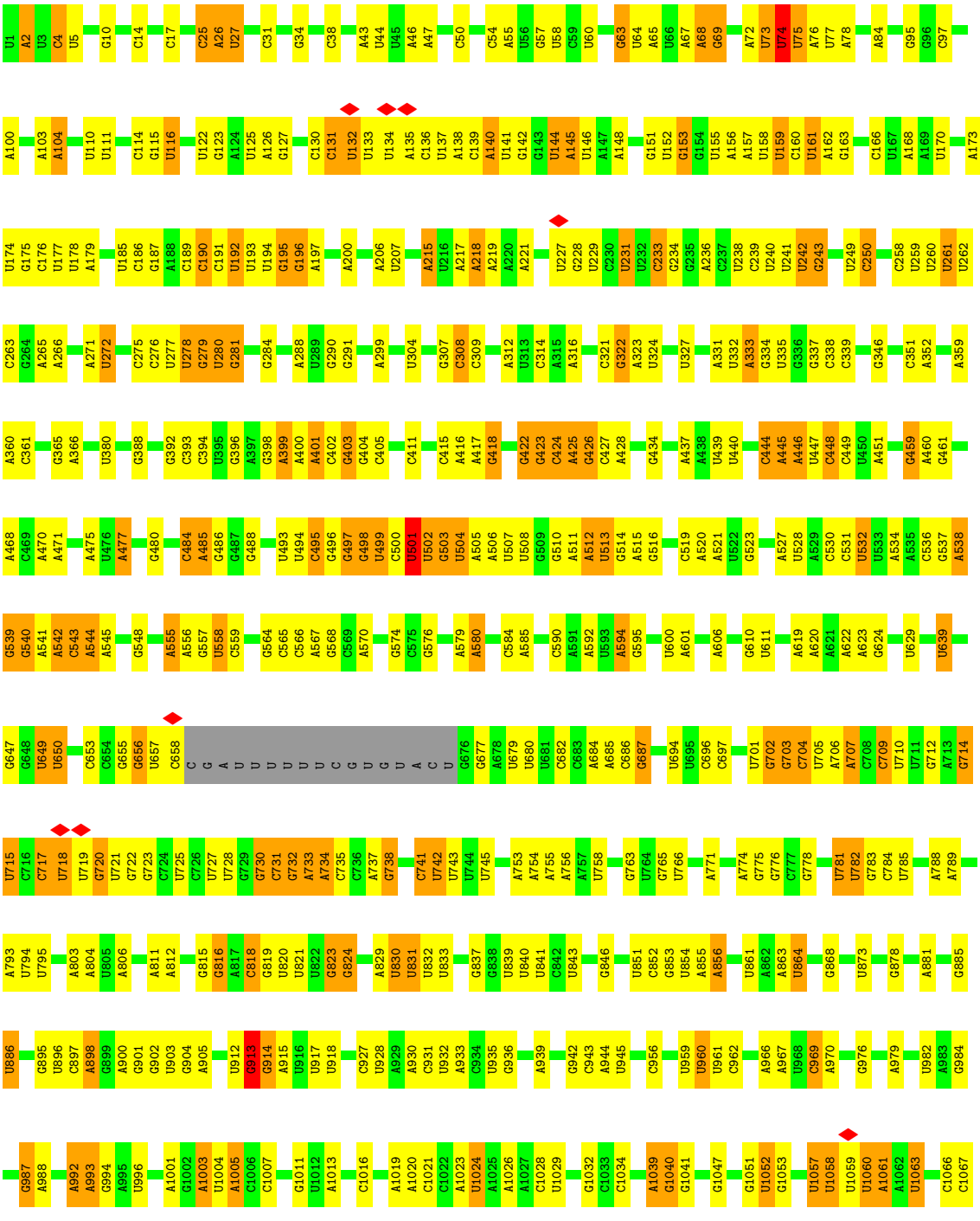
• Molecule 17: 60S ribosomal protein L16-A

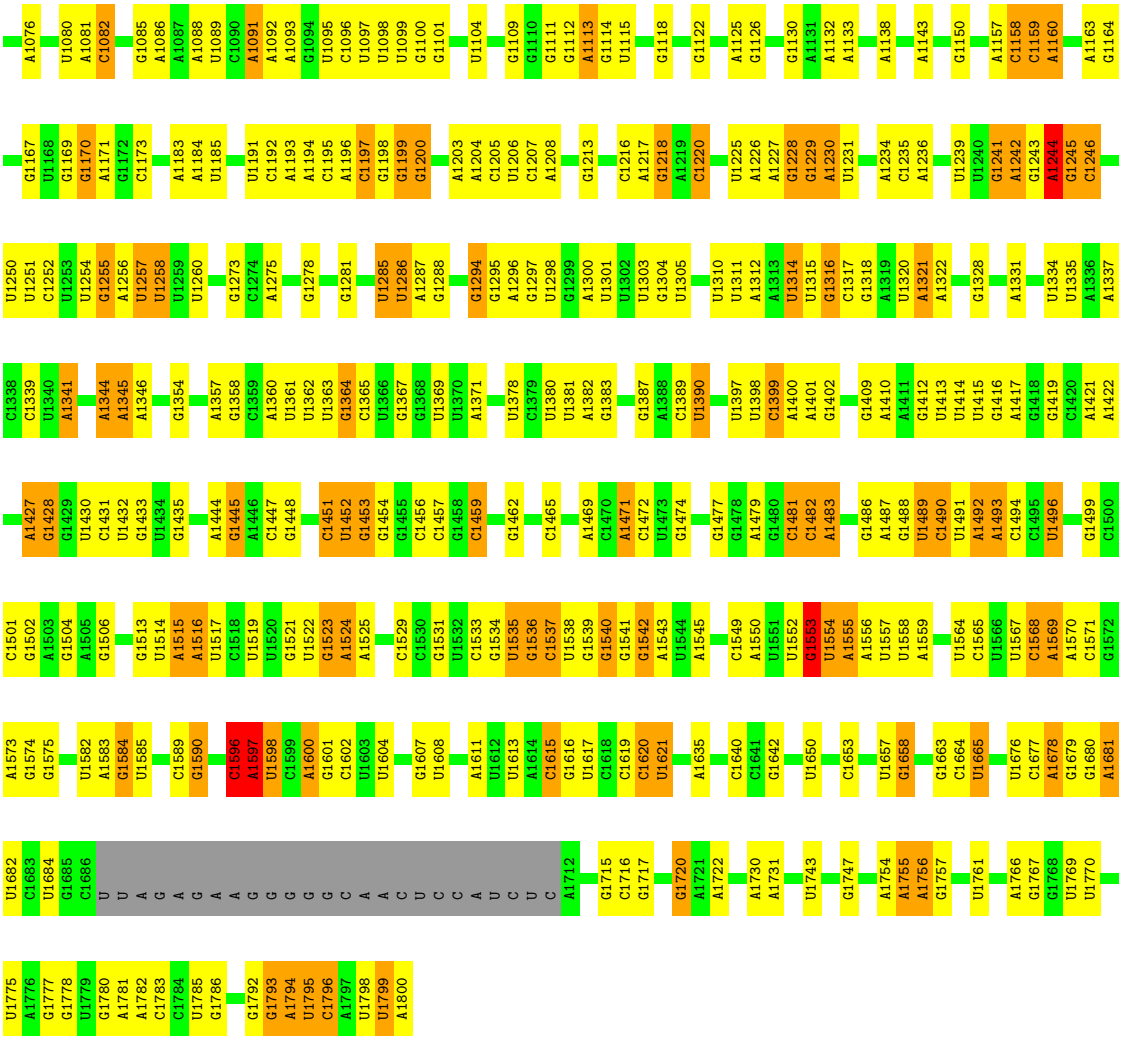
Chain XU:



• Molecule 18: 18S ribosomal RNA

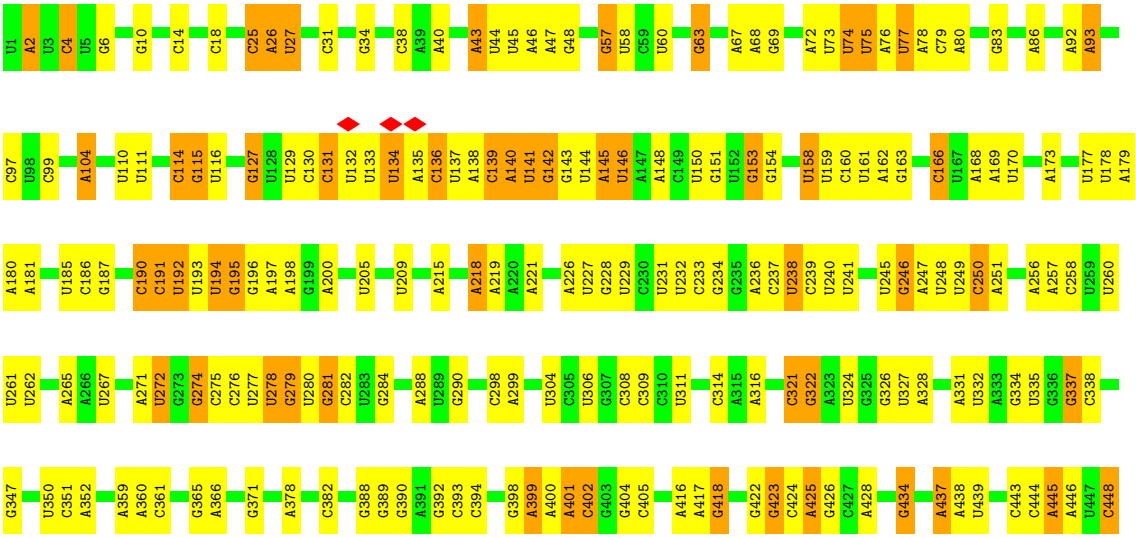
Chain 2:

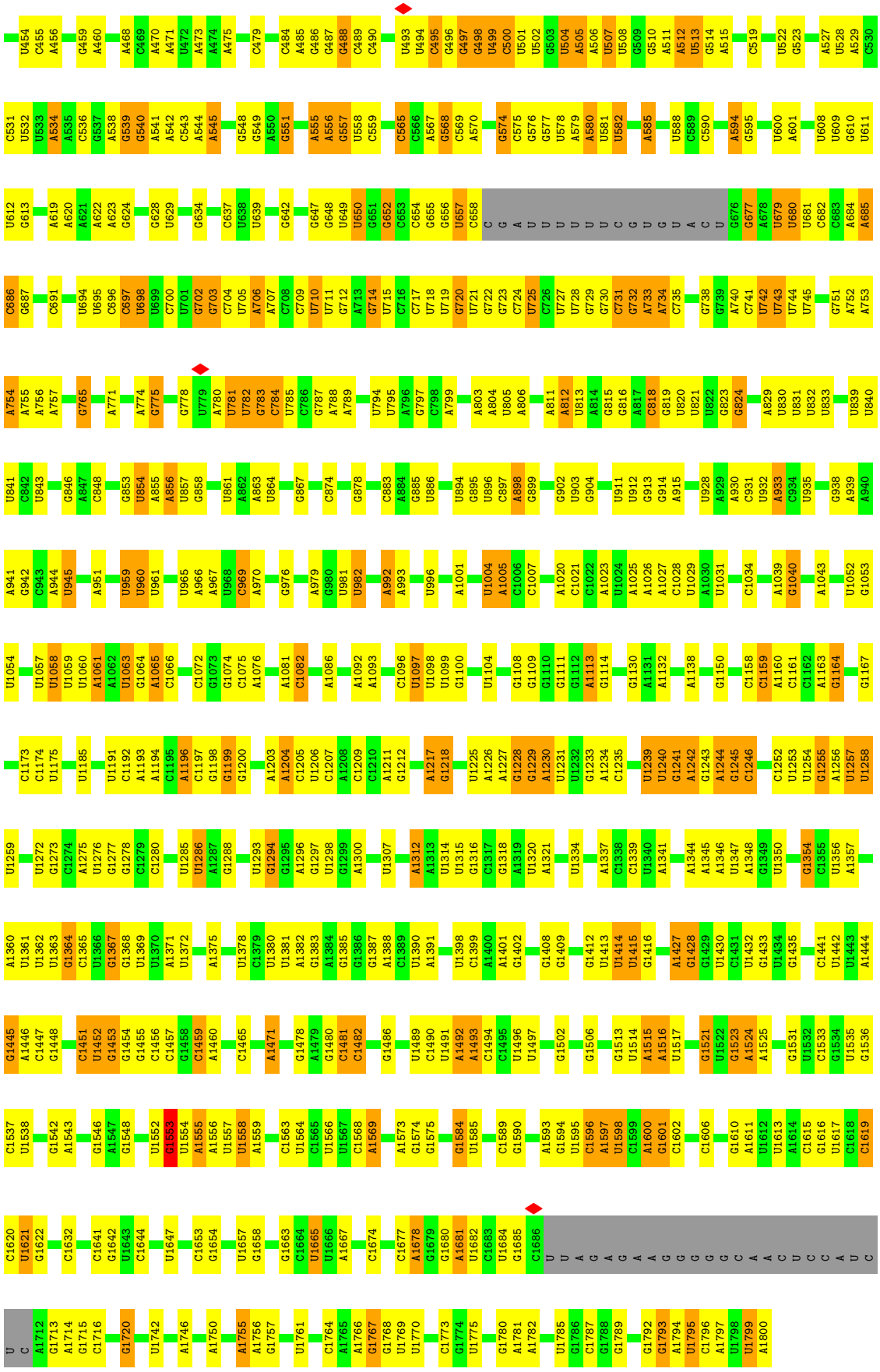




• Molecule 18: 18S ribosomal RNA

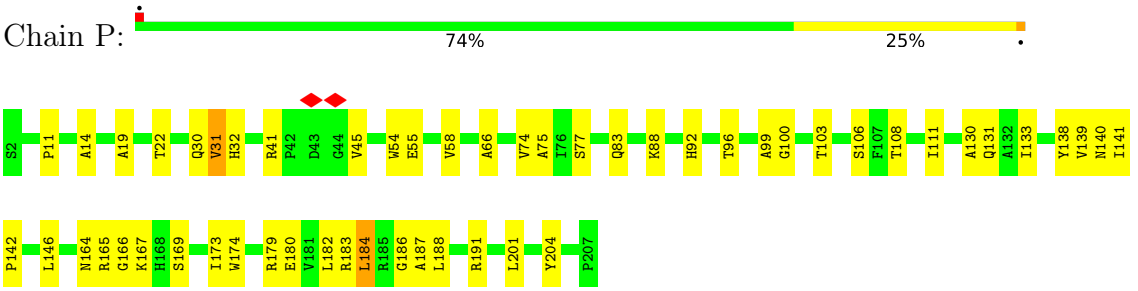
Chain 2b:





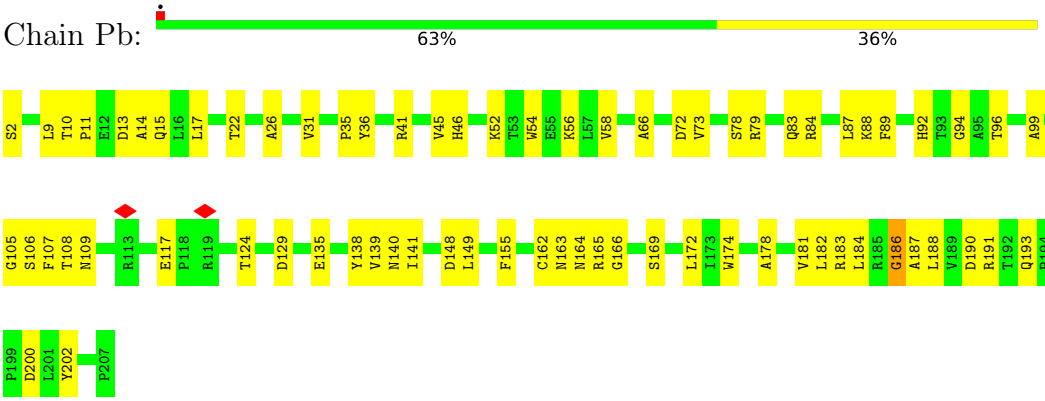
• Molecule 19: 40S ribosomal protein S0-A

Chain P:



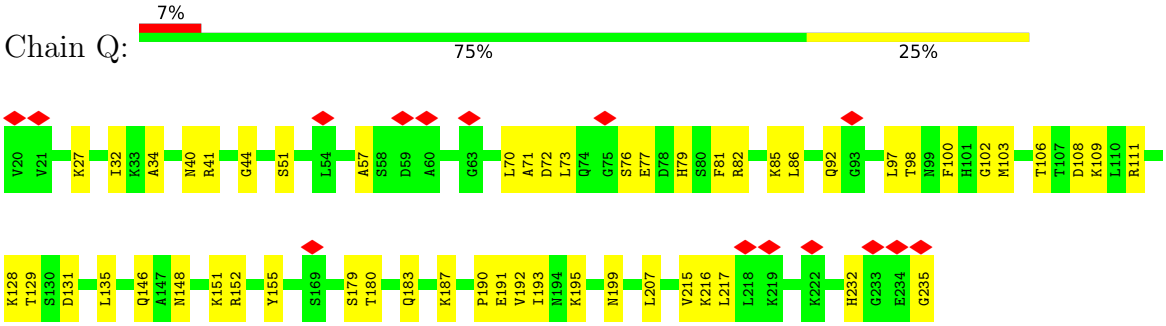
• Molecule 19: 40S ribosomal protein S0-A

Chain Pb:



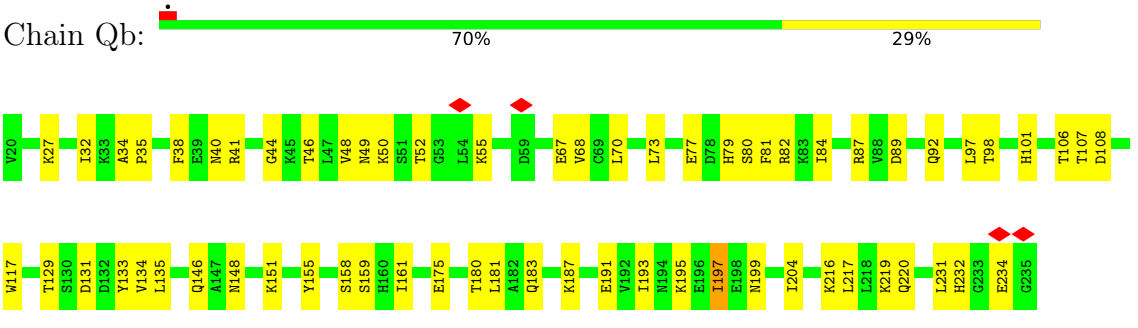
• Molecule 20: 40S ribosomal protein S1-A

Chain Q:



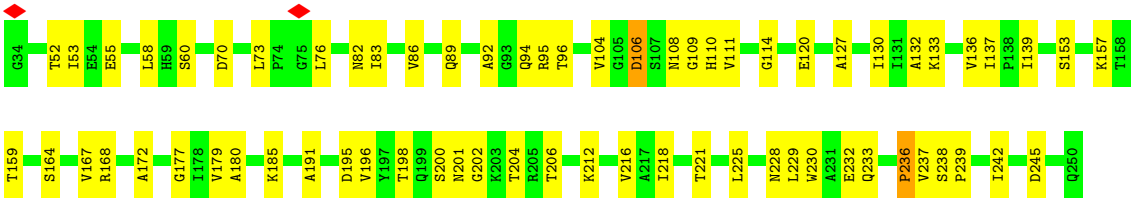
• Molecule 20: 40S ribosomal protein S1-A

Chain Qb:



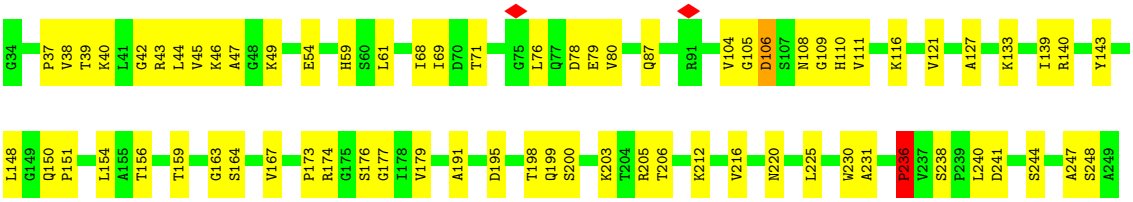
• Molecule 21: 40S ribosomal protein S2

Chain R:



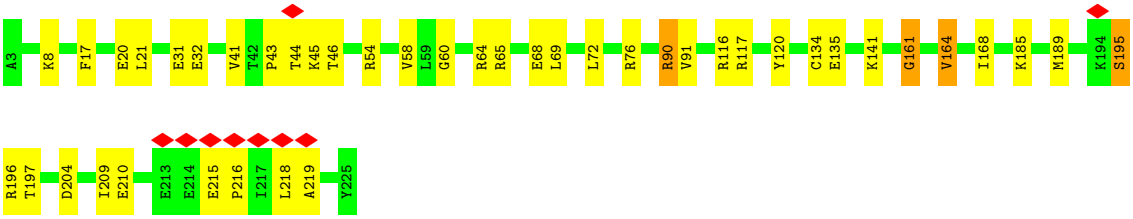
• Molecule 21: 40S ribosomal protein S2

Chain Rb:



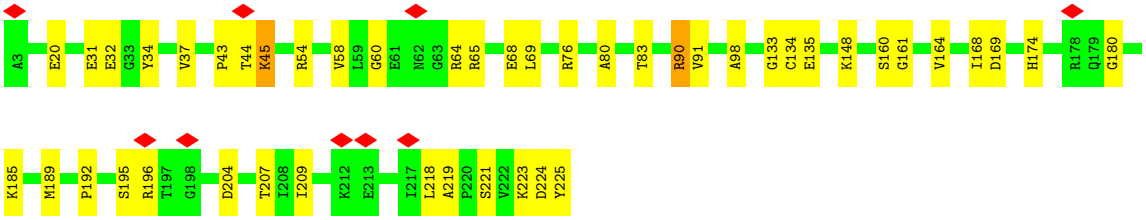
• Molecule 22: 40S ribosomal protein S3

Chain A:



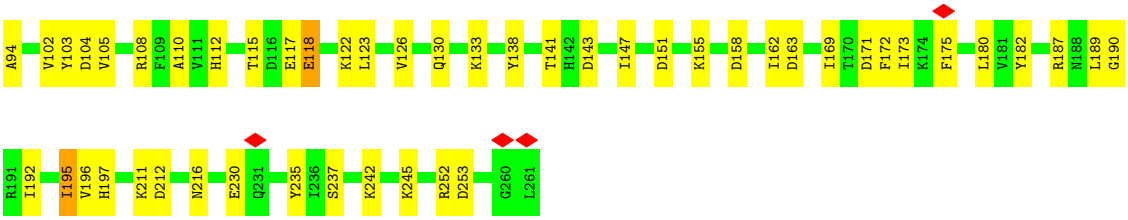
• Molecule 22: 40S ribosomal protein S3

Chain Ab:

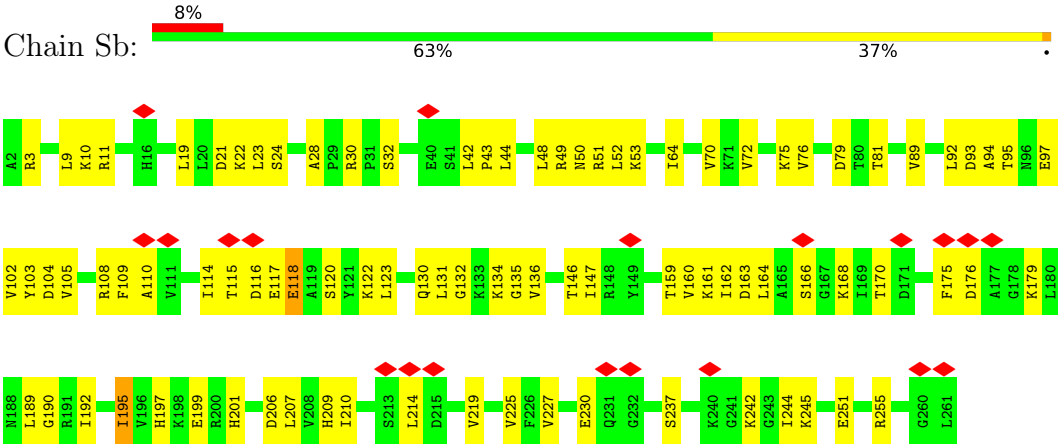


• Molecule 23: 40S ribosomal protein S4-A

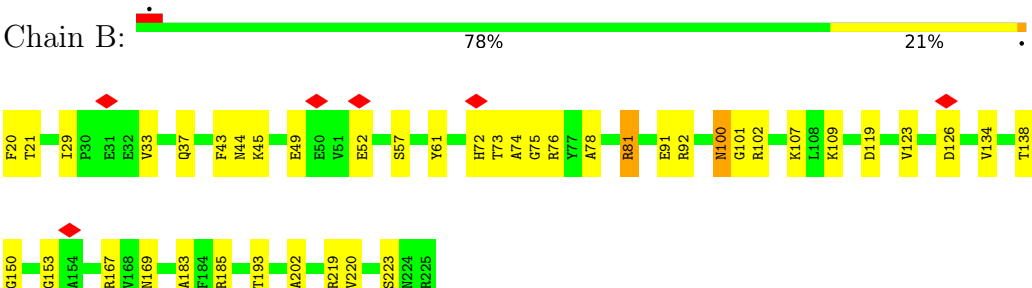
Chain S:



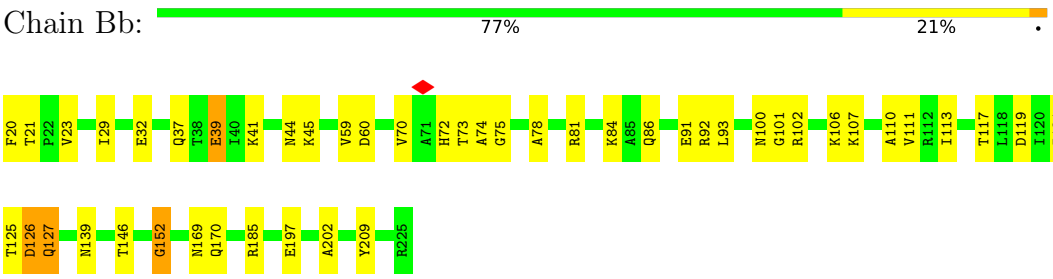
• Molecule 23: 40S ribosomal protein S4-A



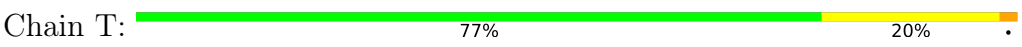
• Molecule 24: 40S ribosomal protein S5

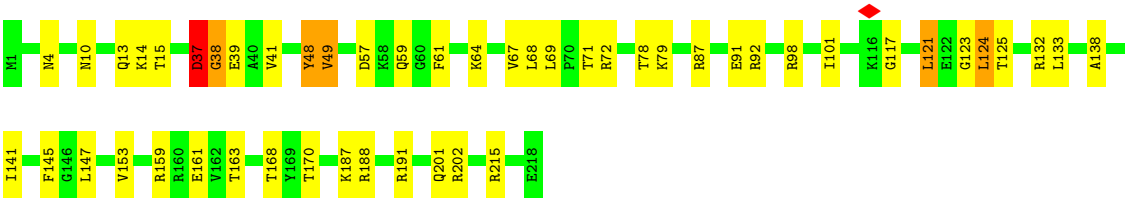


• Molecule 24: 40S ribosomal protein S5



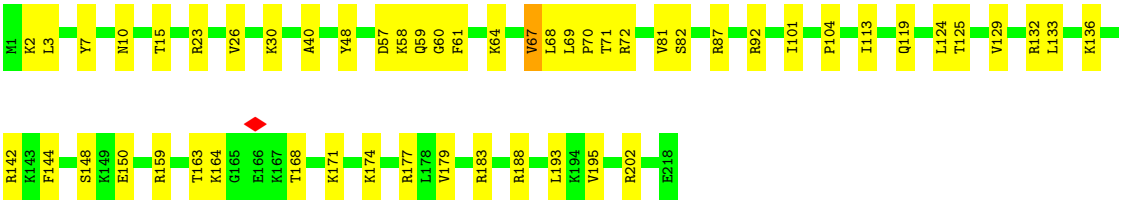
• Molecule 25: 40S ribosomal protein S6-A





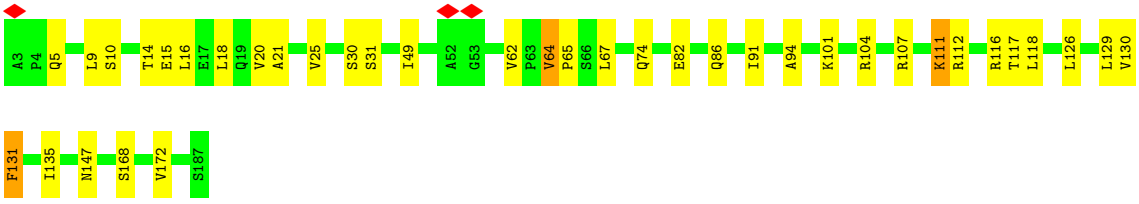
• Molecule 25: 40S ribosomal protein S6-A

Chain Tb:



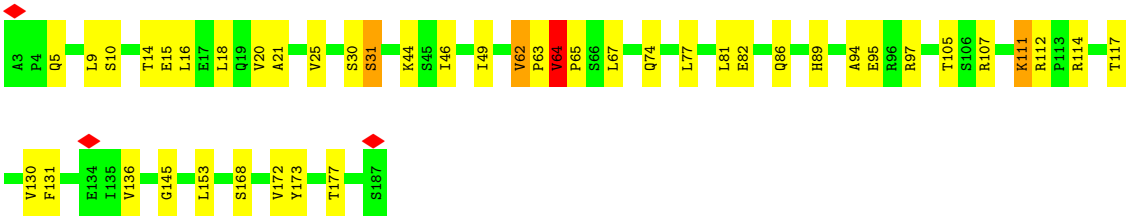
• Molecule 26: 40S ribosomal protein S7-A

Chain U:



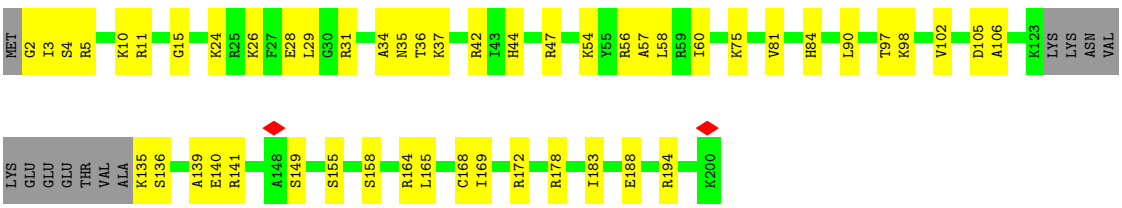
• Molecule 26: 40S ribosomal protein S7-A

Chain Ub:



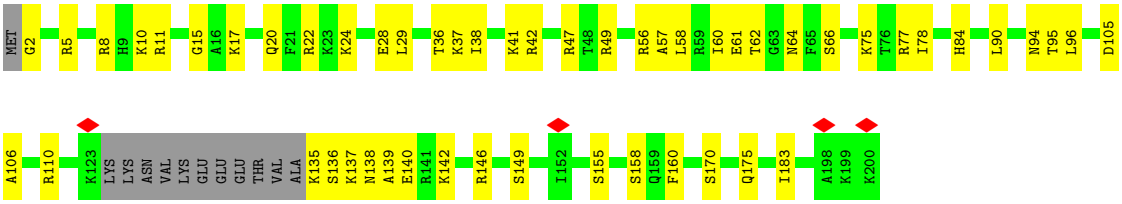
• Molecule 27: 40S ribosomal protein S8-A

Chain V:



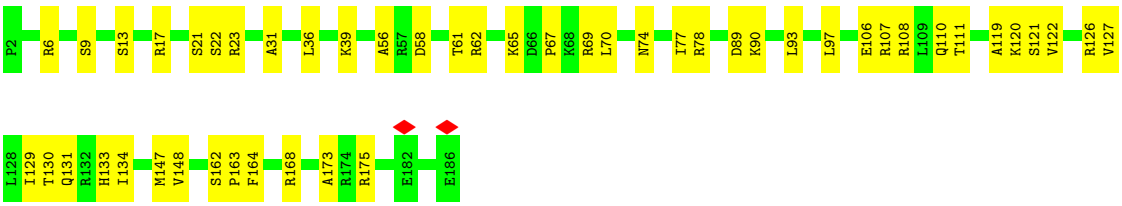
• Molecule 27: 40S ribosomal protein S8-A

Chain Vb:



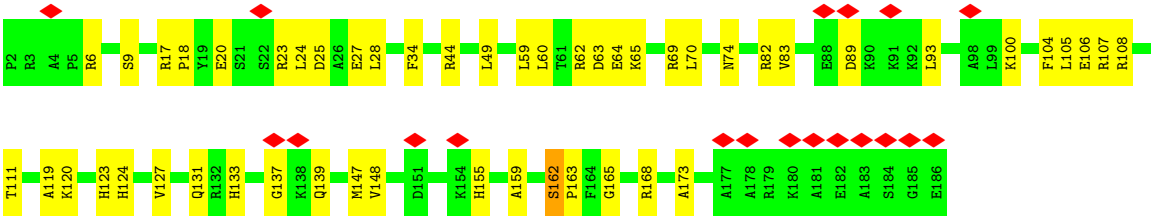
• Molecule 28: 40S ribosomal protein S9-A

Chain W:



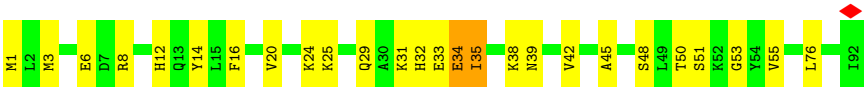
• Molecule 28: 40S ribosomal protein S9-A

Chain Wb:



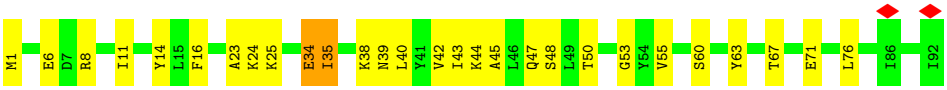
• Molecule 29: 40S ribosomal protein S10-A

Chain C:



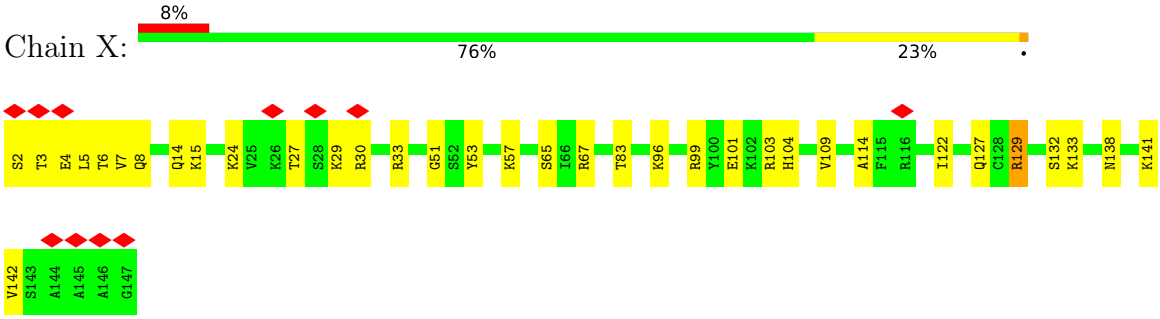
• Molecule 29: 40S ribosomal protein S10-A

Chain Cb:



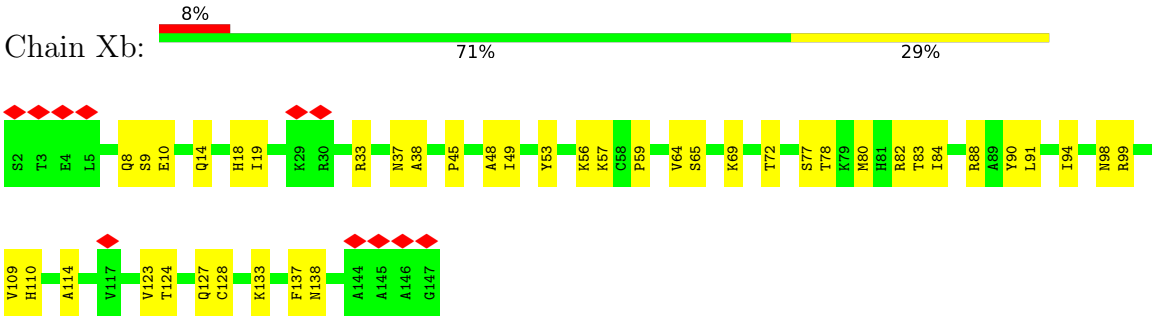
• Molecule 30: 40S ribosomal protein S11-A

Chain X:



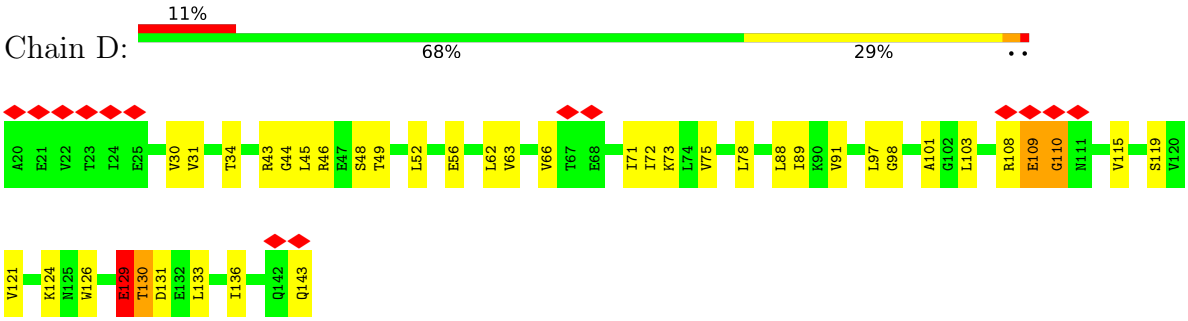
• Molecule 30: 40S ribosomal protein S11-A

Chain Xb:



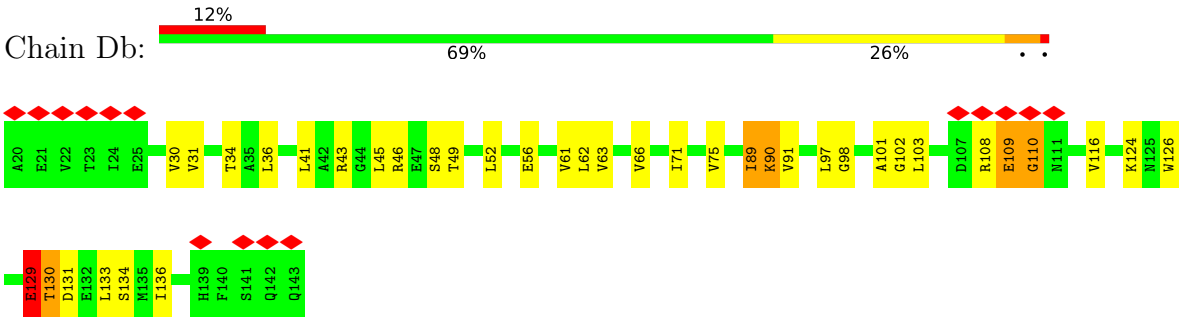
• Molecule 31: 40S ribosomal protein S12

Chain D:



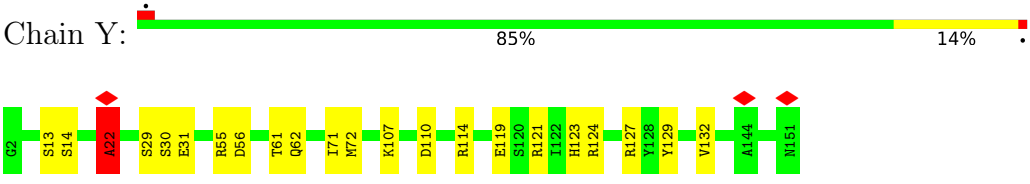
• Molecule 31: 40S ribosomal protein S12

Chain Db:



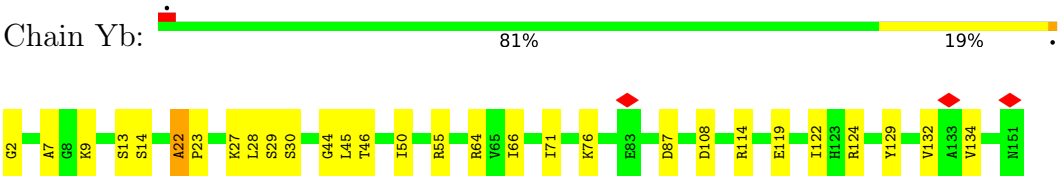
• Molecule 32: 40S ribosomal protein S13

Chain Y:



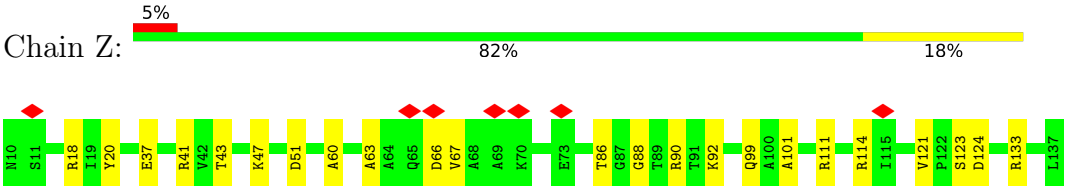
• Molecule 32: 40S ribosomal protein S13

Chain Yb:



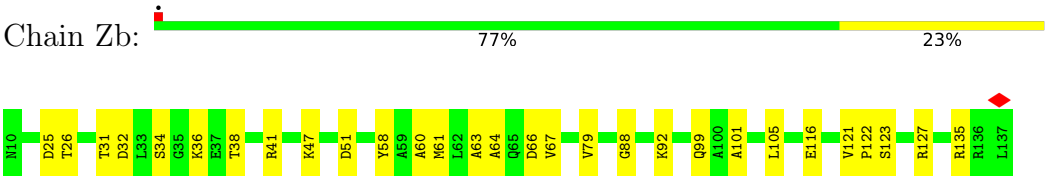
• Molecule 33: 40S ribosomal protein S14-B

Chain Z:



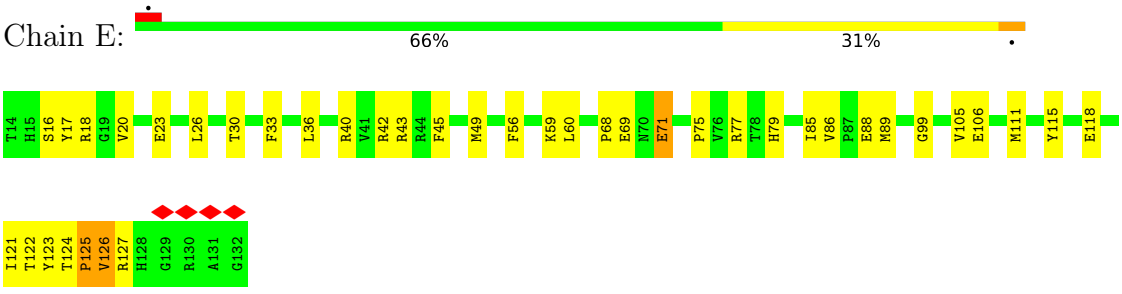
• Molecule 33: 40S ribosomal protein S14-B

Chain Zb:



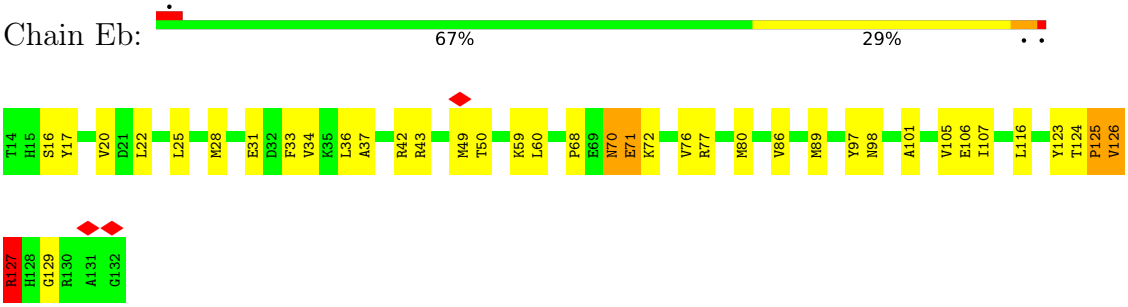
• Molecule 34: 40S ribosomal protein S15

Chain E:



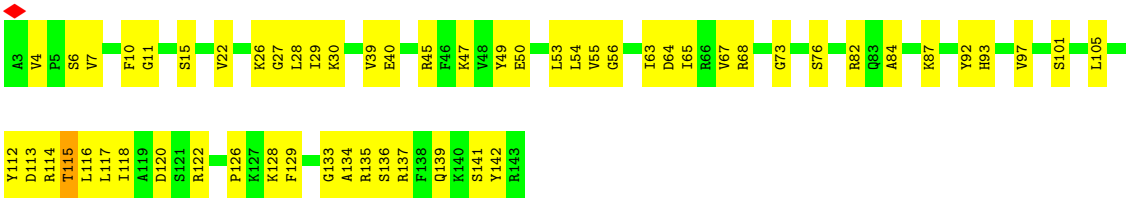
• Molecule 34: 40S ribosomal protein S15

Chain Eb:



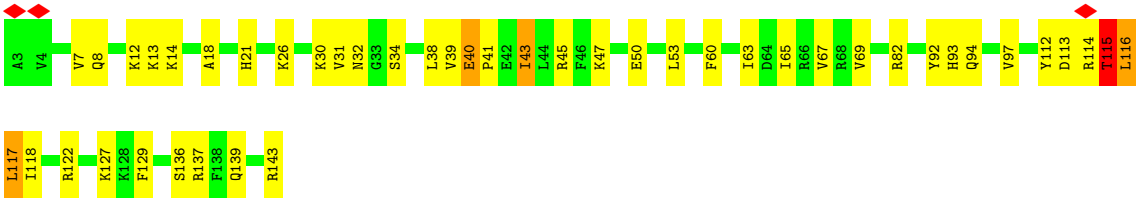
• Molecule 35: 40S ribosomal protein S16-A

Chain F:



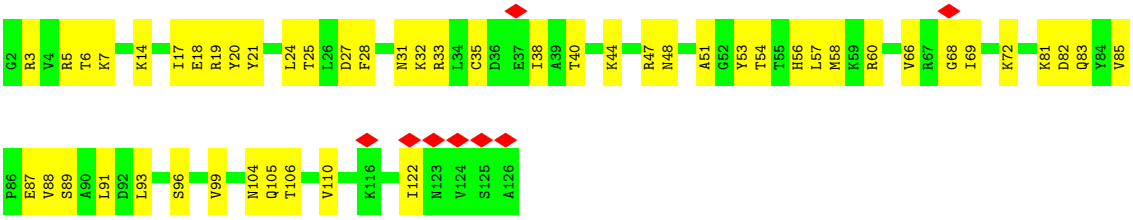
• Molecule 35: 40S ribosomal protein S16-A

Chain Fb:



• Molecule 36: 40S ribosomal protein S17-A

Chain G:

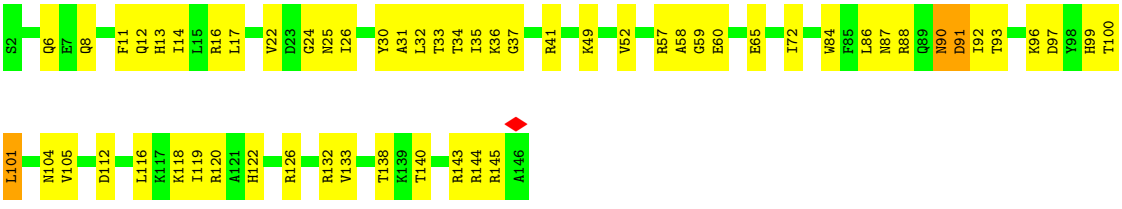


• Molecule 36: 40S ribosomal protein S17-A

Chain Gb:

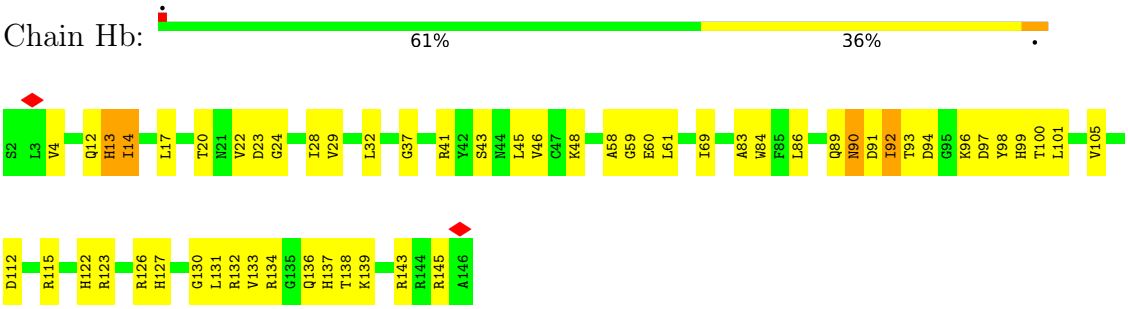
• Molecule 37: 40S ribosomal protein S18-A

Chain H:



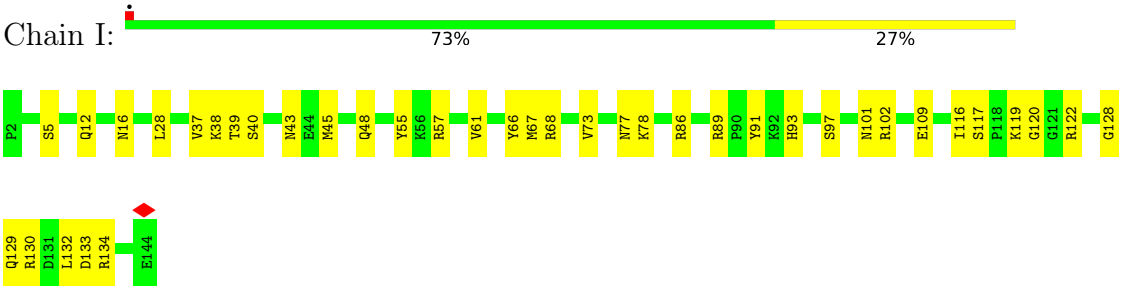
• Molecule 37: 40S ribosomal protein S18-A

Chain Hb:



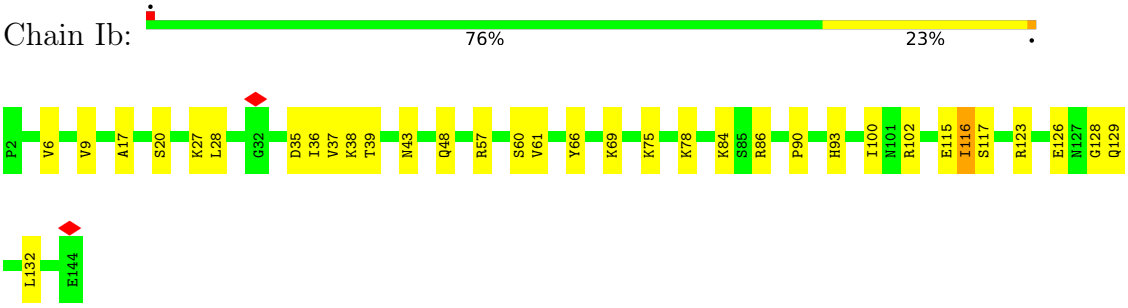
• Molecule 38: 40S ribosomal protein S19-A

Chain I:



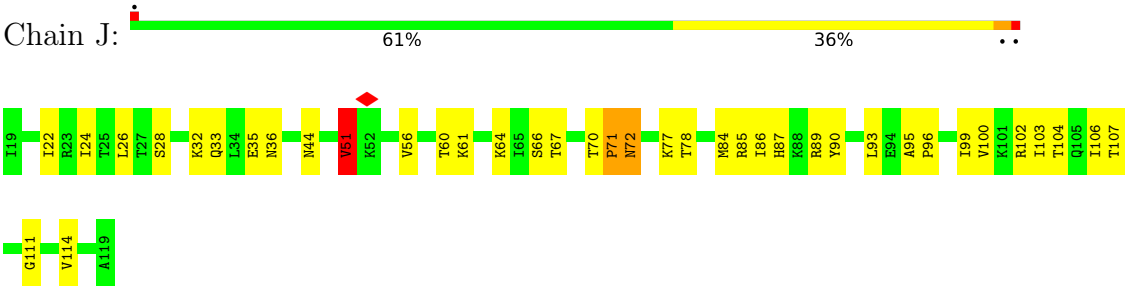
• Molecule 38: 40S ribosomal protein S19-A

Chain Ib:



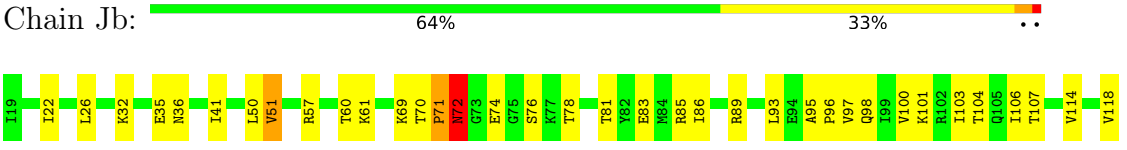
• Molecule 39: 40S ribosomal protein S20

Chain J:



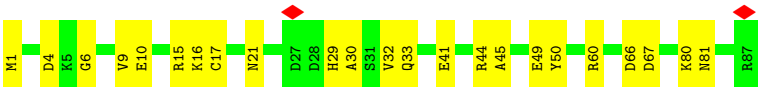
• Molecule 39: 40S ribosomal protein S20

Chain Jb:



• Molecule 40: 40S ribosomal protein S21-A

Chain a:



• Molecule 40: 40S ribosomal protein S21-A

Chain ab:

• Molecule 41: 40S ribosomal protein S22-A

Chain b:

• Molecule 41: 40S ribosomal protein S22-A

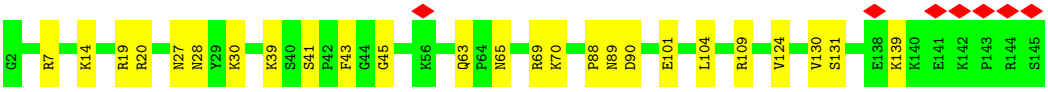
Chain bb:

• Molecule 42: 40S ribosomal protein S23-A

Chain c:

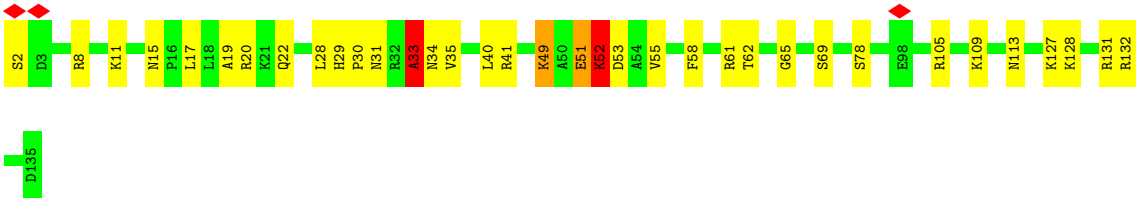
• Molecule 42: 40S ribosomal protein S23-A

Chain cb:

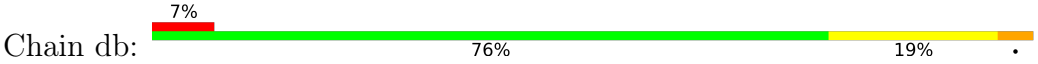


• Molecule 43: 40S ribosomal protein S24-A

Chain d:



• Molecule 43: 40S ribosomal protein S24-A

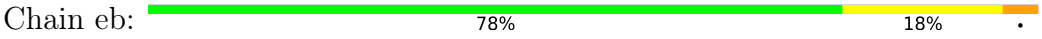


• Molecule 44: 40S ribosomal protein S25-A

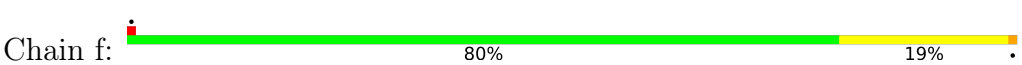
• Molecule 44: 40S ribosomal protein S25-A

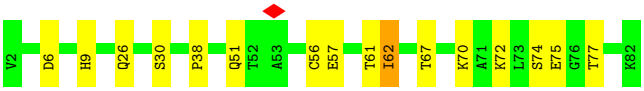
• Molecule 45: 40S ribosomal protein S26-B

• Molecule 45: 40S ribosomal protein S26-B



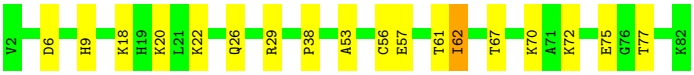
• Molecule 46: 40S ribosomal protein S27-A





• Molecule 46: 40S ribosomal protein S27-A

Chain fb:

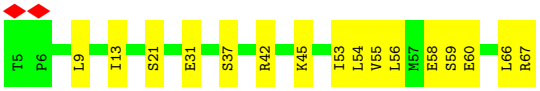


• Molecule 47: 40S ribosomal protein S28-A

Chain L:

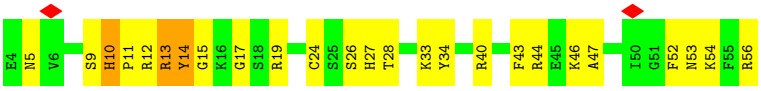
• Molecule 47: 40S ribosomal protein S28-A

Chain Lb:



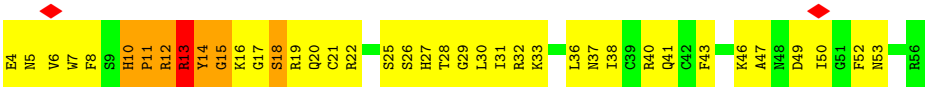
• Molecule 48: 40S ribosomal protein S29-A

Chain M:



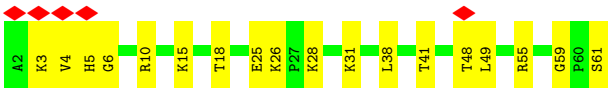
• Molecule 48: 40S ribosomal protein S29-A

Chain Mb:



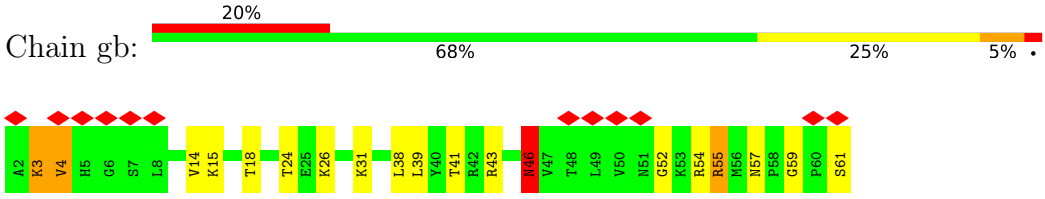
• Molecule 49: 40S ribosomal protein S30-A

Chain g:



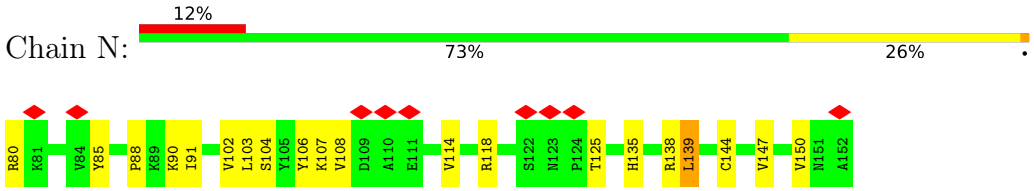
• Molecule 49: 40S ribosomal protein S30-A

Chain gb:



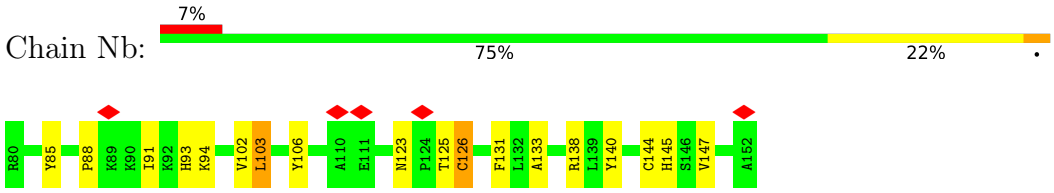
• Molecule 50: Ubiquitin-40S ribosomal protein S31

Chain N:



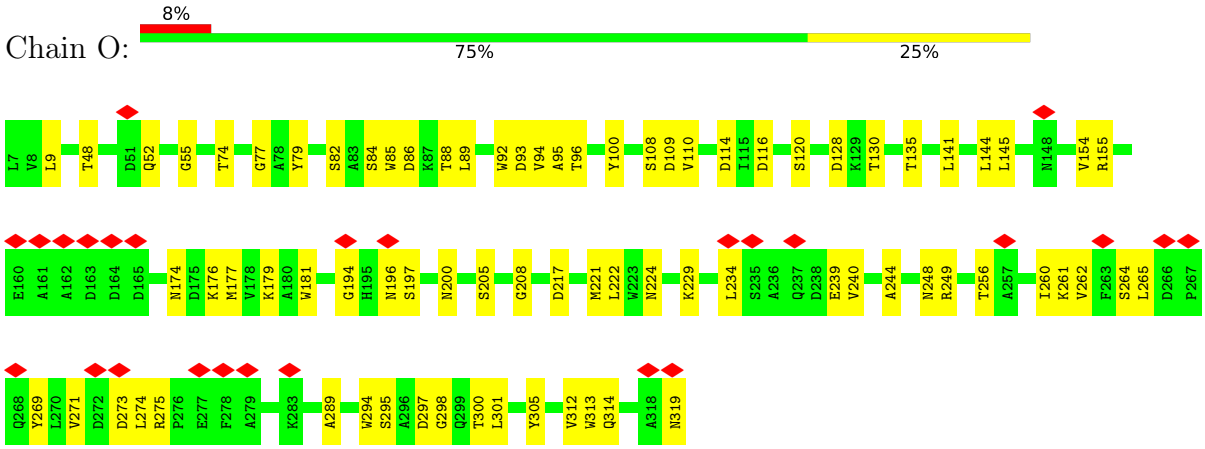
• Molecule 50: Ubiquitin-40S ribosomal protein S31

Chain Nb:



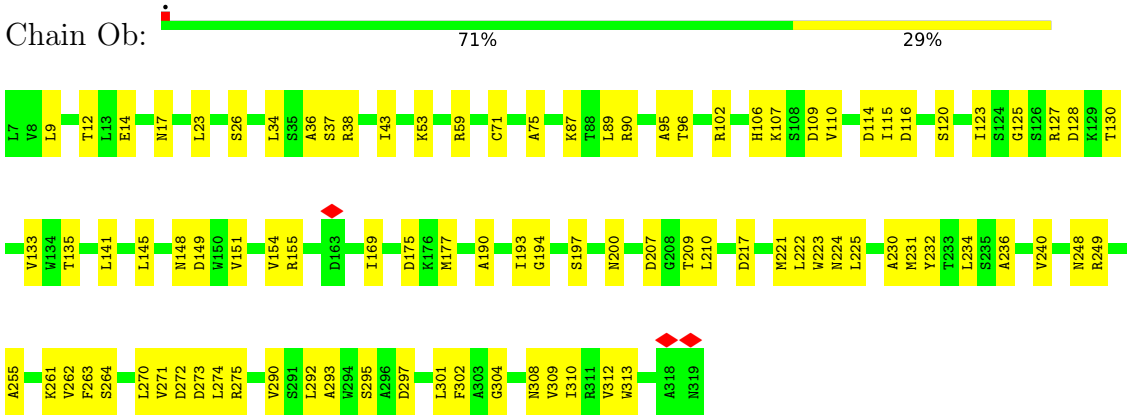
• Molecule 51: Guanine nucleotide-binding protein subunit beta-like protein

Chain O:



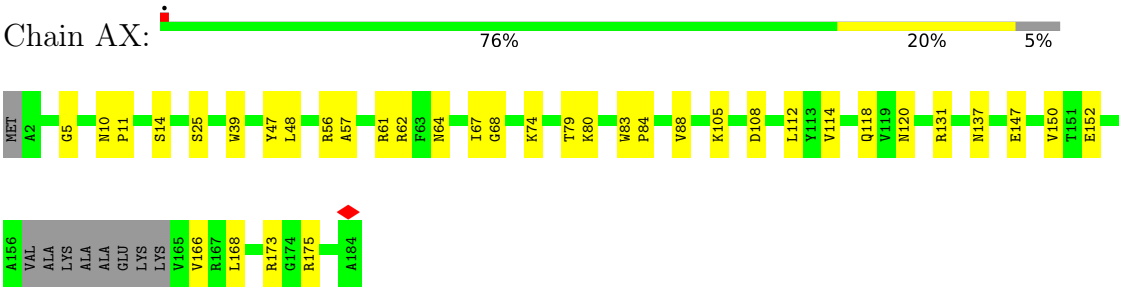
• Molecule 51: Guanine nucleotide-binding protein subunit beta-like protein

Chain Ob:



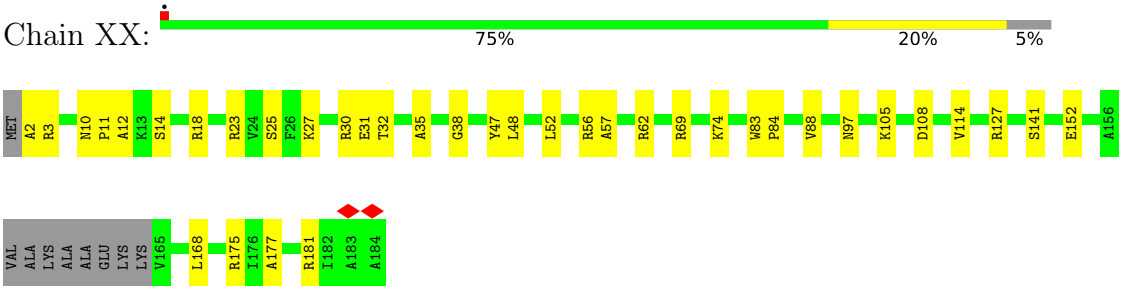
• Molecule 52: 60S ribosomal protein L17-A

Chain AX:



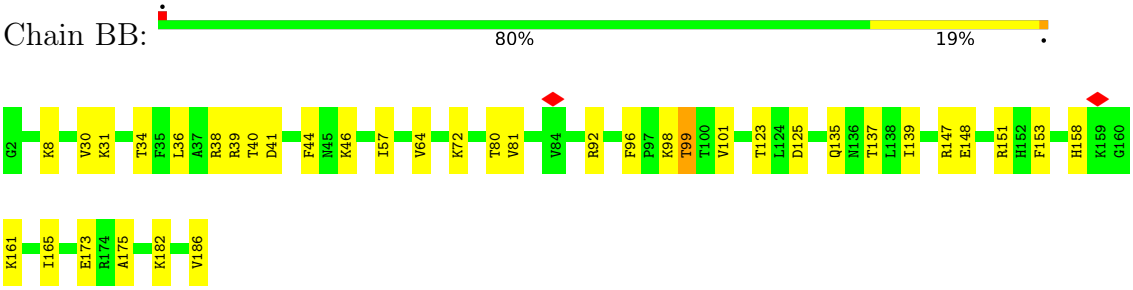
• Molecule 52: 60S ribosomal protein L17-A

Chain XX:



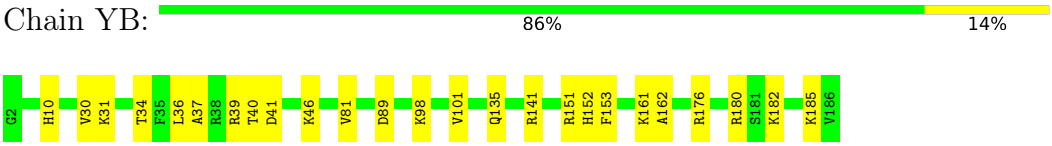
• Molecule 53: 60S ribosomal protein L18-A

Chain BB:



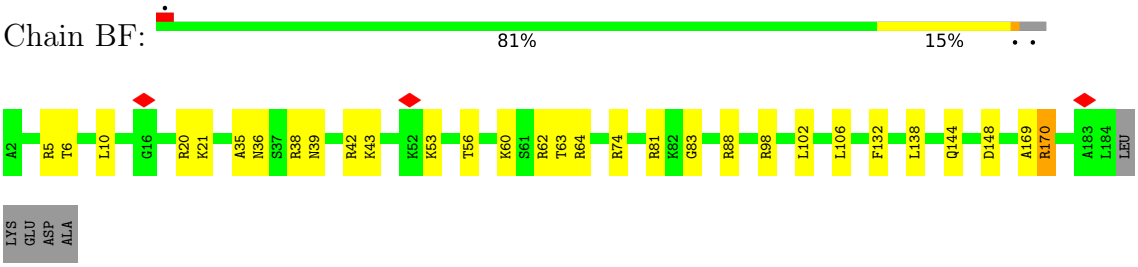
• Molecule 53: 60S ribosomal protein L18-A

Chain YB:



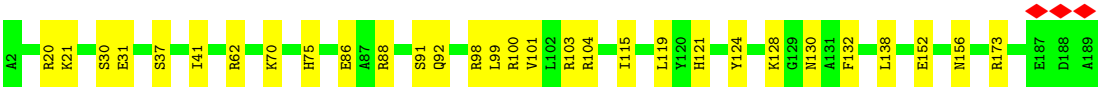
• Molecule 54: 60S ribosomal protein L19-A

Chain BF:



• Molecule 54: 60S ribosomal protein L19-A

Chain YF:

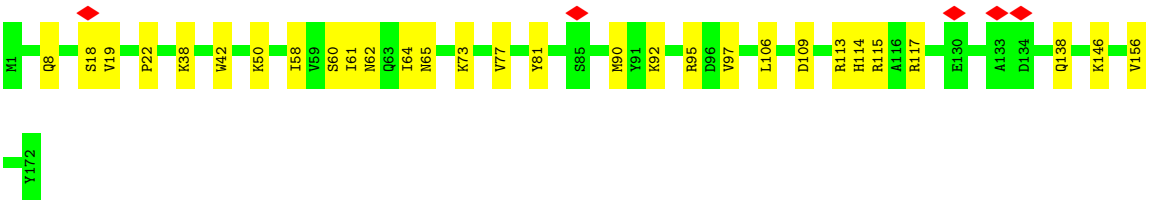


• Molecule 55: 60S ribosomal protein L20-A

Chain BH:

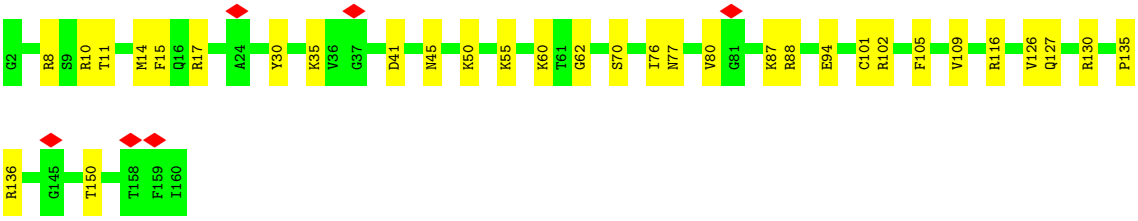
• Molecule 55: 60S ribosomal protein L20-A

Chain YH:



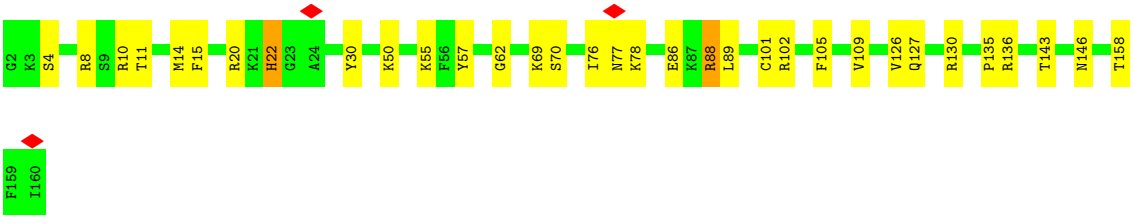
• Molecule 56: 60S ribosomal protein L21-A

Chain BJ:



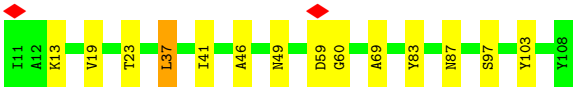
• Molecule 56: 60S ribosomal protein L21-A

Chain YJ:



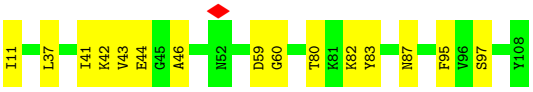
• Molecule 57: 60S ribosomal protein L22-A

Chain BL:



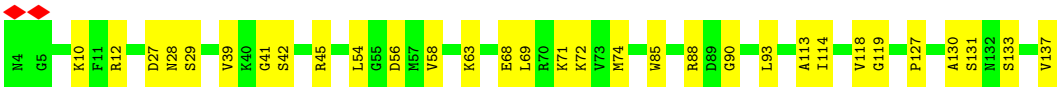
• Molecule 57: 60S ribosomal protein L22-A

Chain YL:



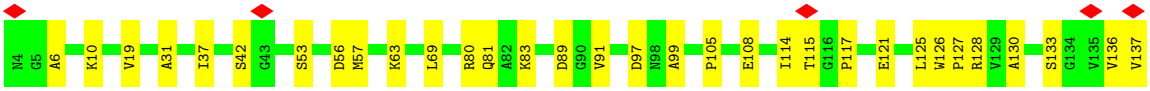
• Molecule 58: 60S ribosomal protein L23-A

Chain AB:



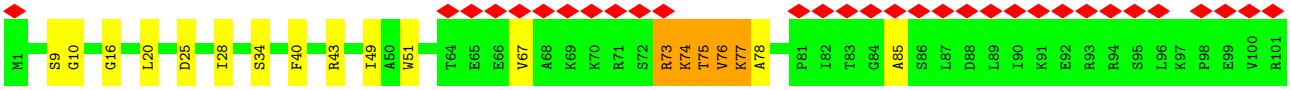
• Molecule 58: 60S ribosomal protein L23-A

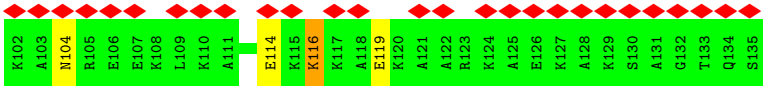
Chain XB:



• Molecule 59: 60S ribosomal protein L24-A

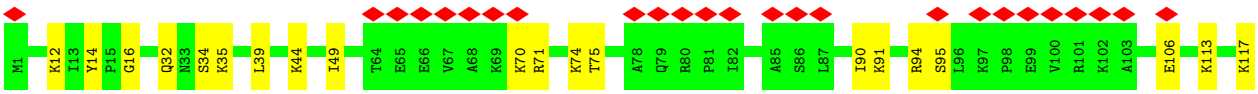
Chain AE:

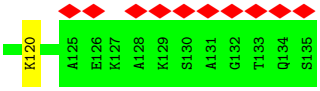




• Molecule 59: 60S ribosomal protein L24-A

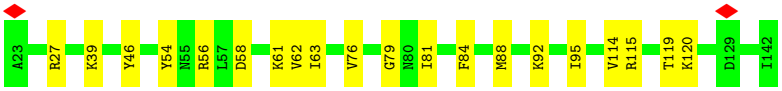
Chain XE:





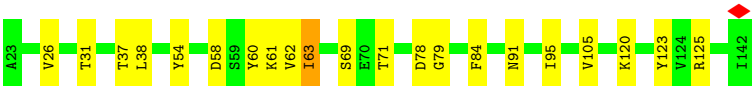
• Molecule 60: 60S ribosomal protein L25

Chain AH:



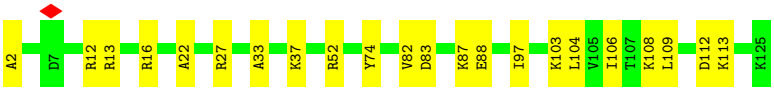
• Molecule 60: 60S ribosomal protein L25

Chain XH:



• Molecule 61: 60S ribosomal protein L26-A

Chain AK:

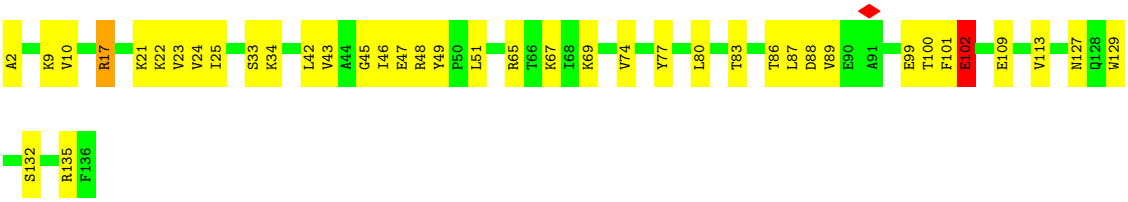


• Molecule 61: 60S ribosomal protein L26-A

Chain XK:

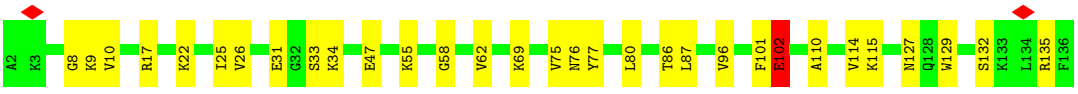
• Molecule 62: 60S ribosomal protein L27-A

Chain AN:



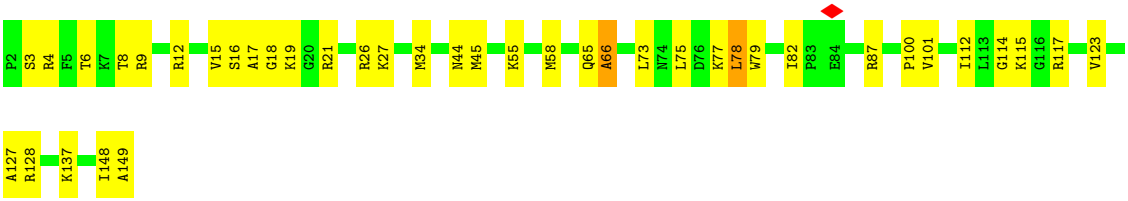
• Molecule 62: 60S ribosomal protein L27-A

Chain XN:

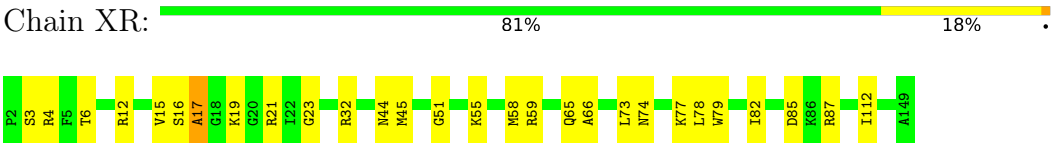


• Molecule 63: 60S ribosomal protein L28

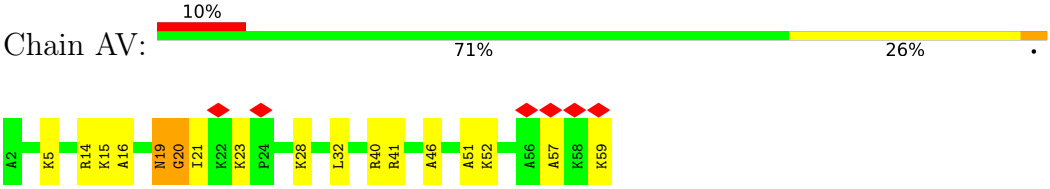
Chain AR:



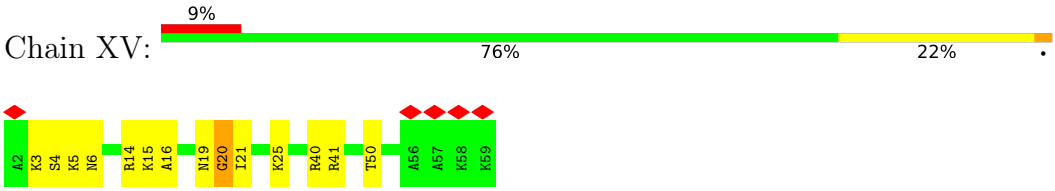
• Molecule 63: 60S ribosomal protein L28



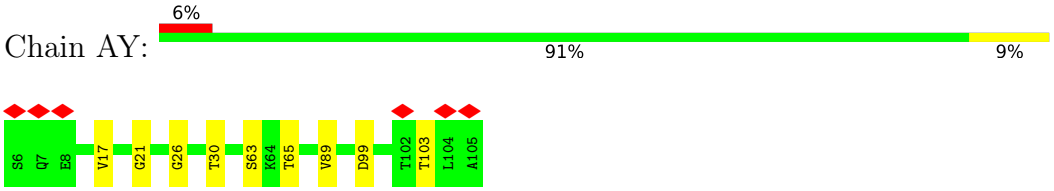
• Molecule 64: 60S ribosomal protein L29



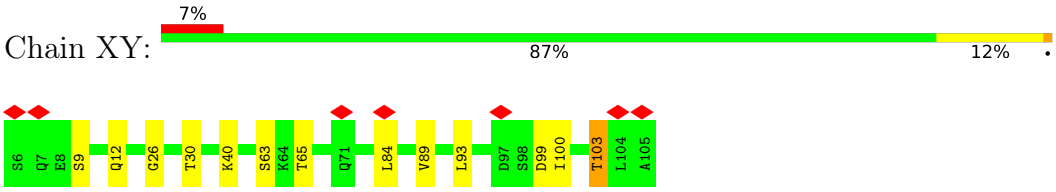
• Molecule 64: 60S ribosomal protein L29



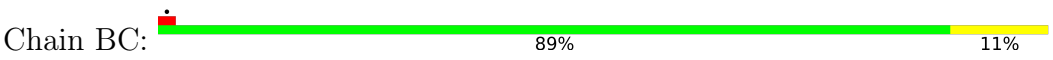
• Molecule 65: 60S ribosomal protein L30

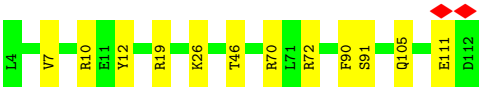


• Molecule 65: 60S ribosomal protein L30

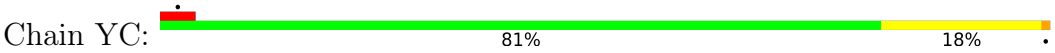


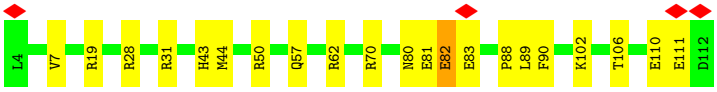
• Molecule 66: 60S ribosomal protein L31-A



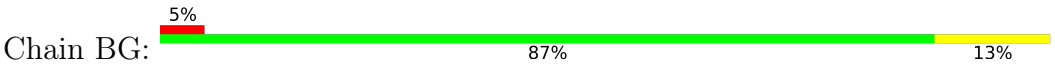


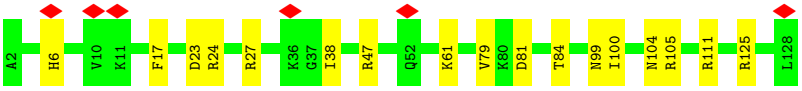
• Molecule 66: 60S ribosomal protein L31-A



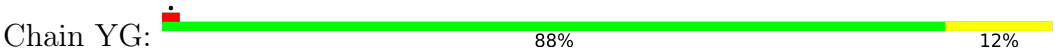


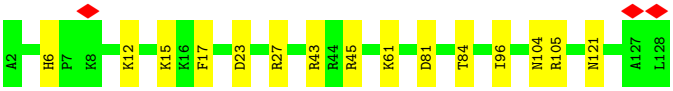
• Molecule 67: 60S ribosomal protein L32



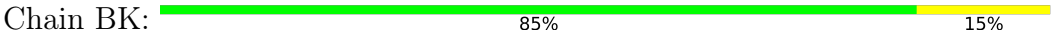


• Molecule 67: 60S ribosomal protein L32

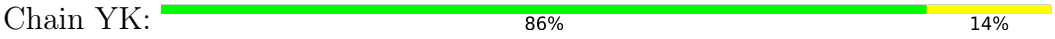




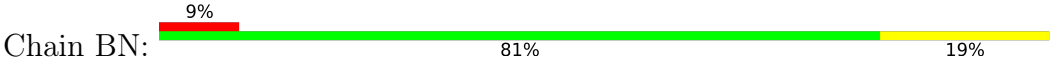
• Molecule 68: 60S ribosomal protein L33-A

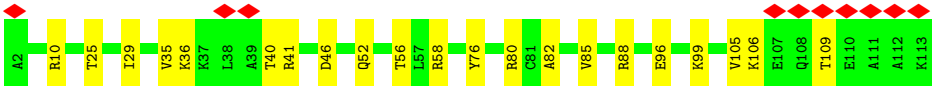


• Molecule 68: 60S ribosomal protein L33-A



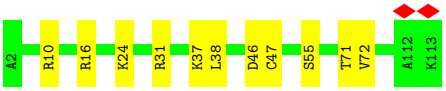
• Molecule 69: 60S ribosomal protein L34-A





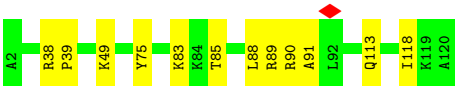
• Molecule 69: 60S ribosomal protein L34-A

Chain YN:



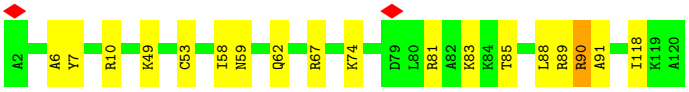
• Molecule 70: 60S ribosomal protein L35-A

Chain BP:



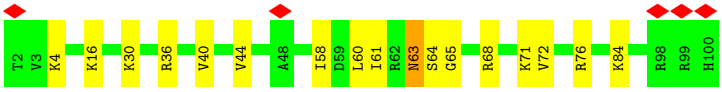
• Molecule 70: 60S ribosomal protein L35-A

Chain YP:



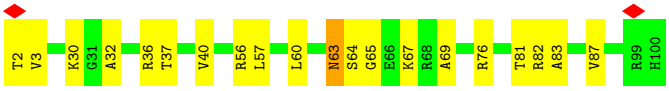
• Molecule 71: 60S ribosomal protein L36-A

Chain AC:



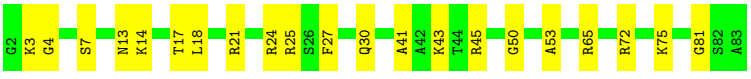
• Molecule 71: 60S ribosomal protein L36-A

Chain XC:



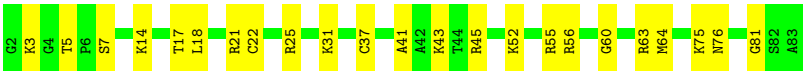
• Molecule 72: 60S ribosomal protein L37-A

Chain AF:



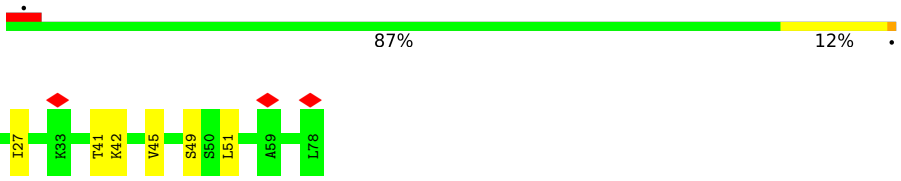
• Molecule 72: 60S ribosomal protein L37-A

Chain XF:



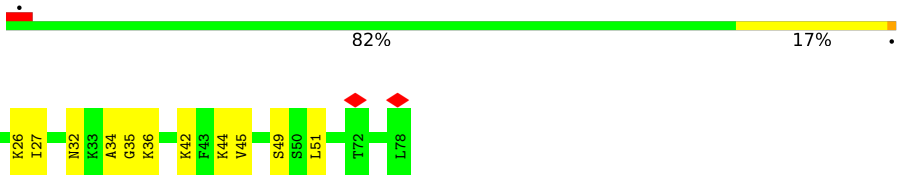
• Molecule 73: 60S ribosomal protein L38

Chain AI:



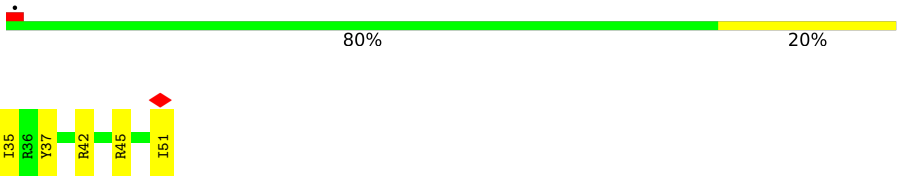
• Molecule 73: 60S ribosomal protein L38

Chain XI:



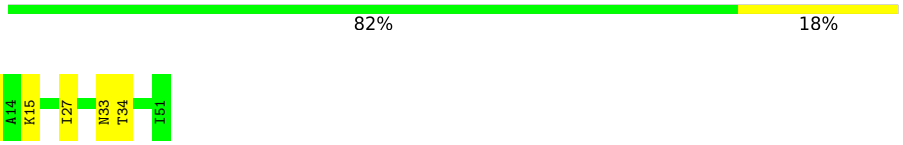
• Molecule 74: 60S ribosomal protein L39

Chain AL:



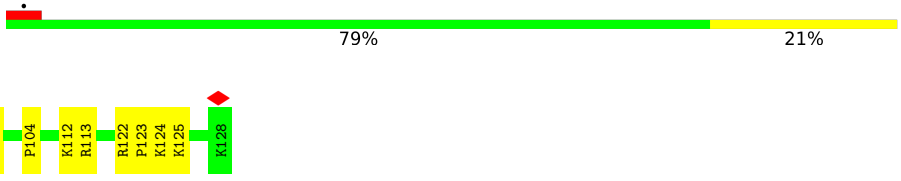
• Molecule 74: 60S ribosomal protein L39

Chain XL:



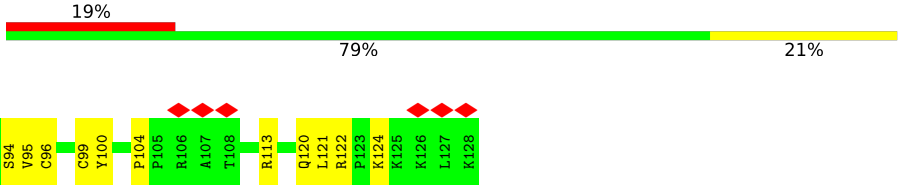
• Molecule 75: Ubiquitin-60S ribosomal protein L40

Chain AO:



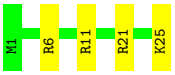
• Molecule 75: Ubiquitin-60S ribosomal protein L40

Chain XO:



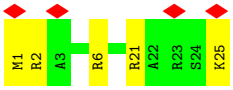
• Molecule 76: 60S ribosomal protein L41-B

Chain AS:



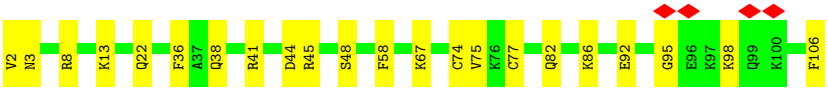
• Molecule 76: 60S ribosomal protein L41-B

Chain XS:



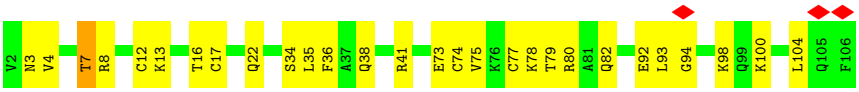
• Molecule 77: 60S ribosomal protein L42-A

Chain AP:



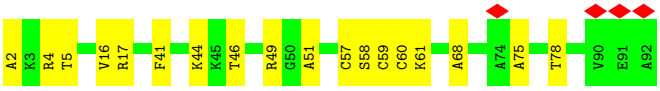
• Molecule 77: 60S ribosomal protein L42-A

Chain XP:



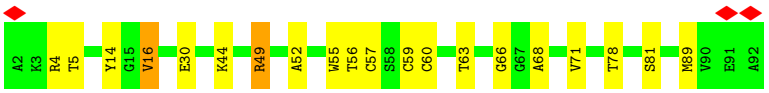
• Molecule 78: 60S ribosomal protein L43-A

Chain AT:



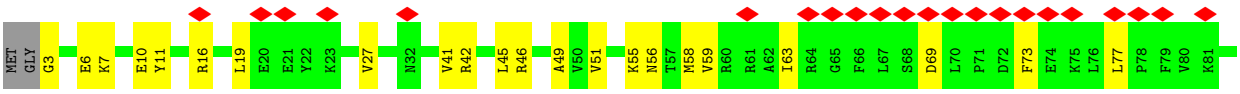
• Molecule 78: 60S ribosomal protein L43-A

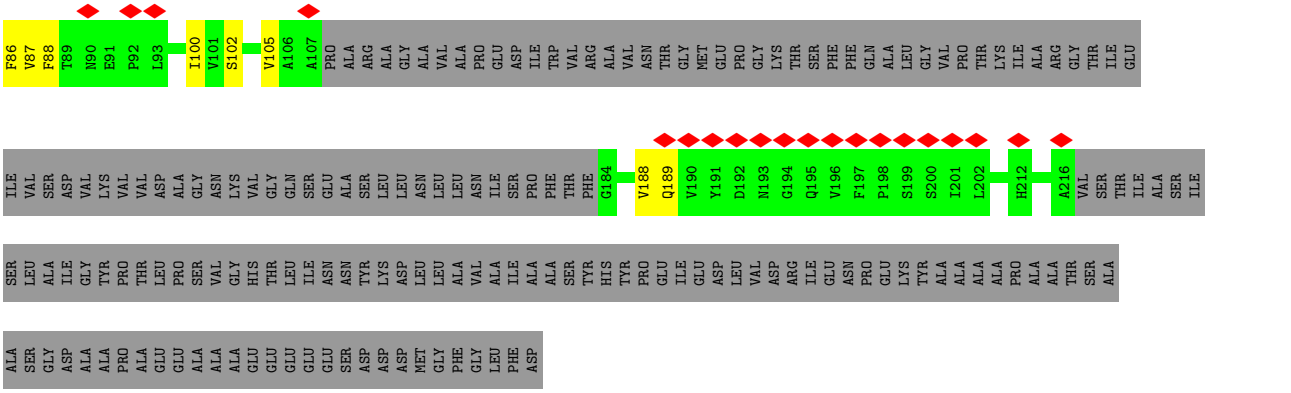
Chain XT:



• Molecule 79: 60S acidic ribosomal protein P0

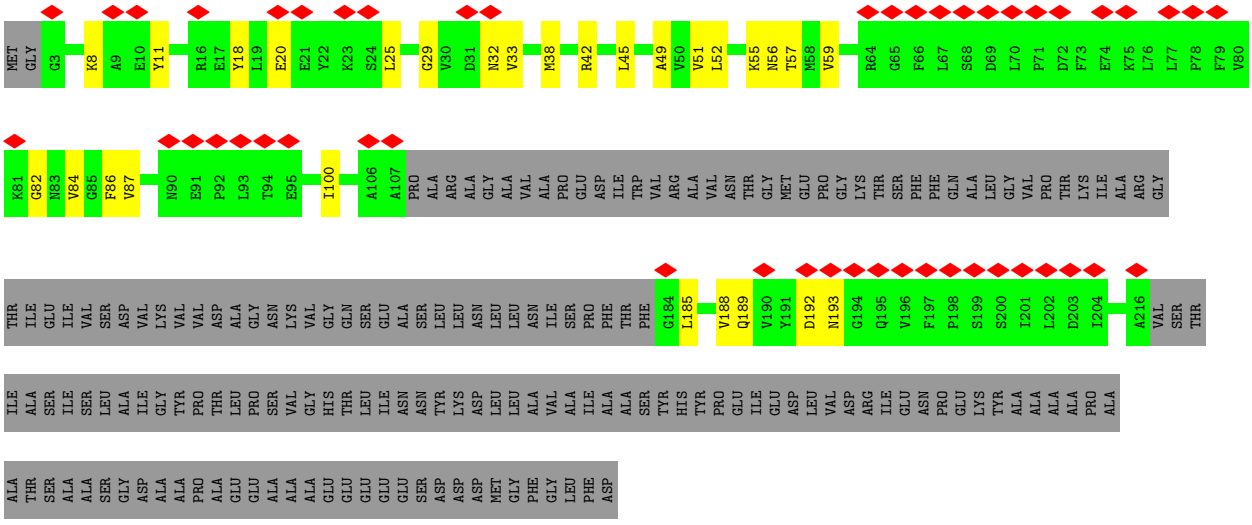
Chain BU:





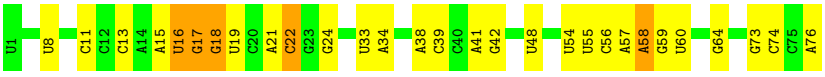
• Molecule 79: 60S acidic ribosomal protein P0

Chain YU:



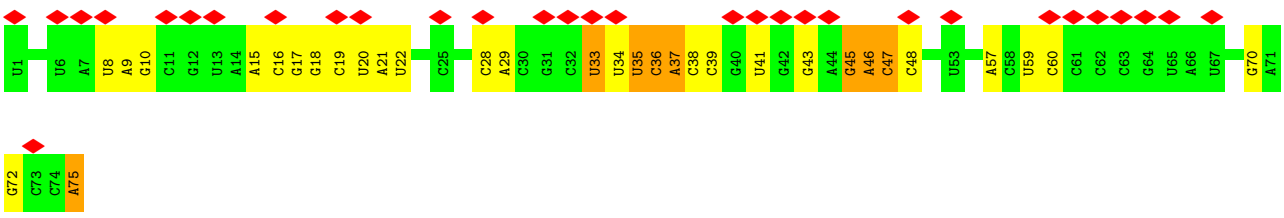
• Molecule 80: P-site tRNA

Chain n:



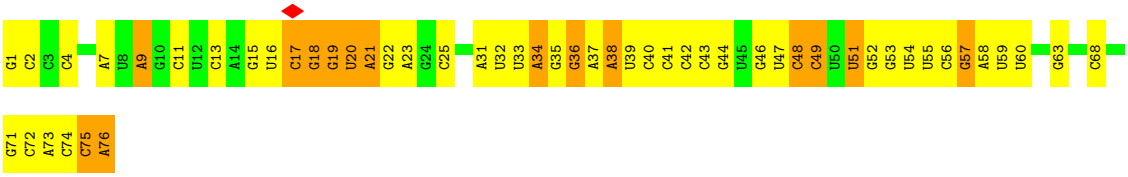
• Molecule 81: E-site tRNA

Chain m:



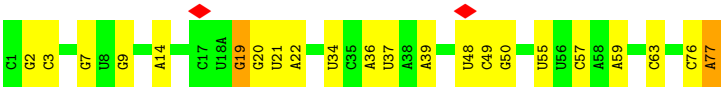
• Molecule 82: A/P hybrid tRNA

Chain nb:



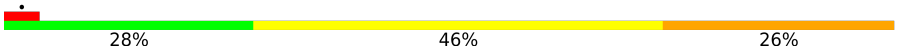
• Molecule 83: P/E hybrid tRNA

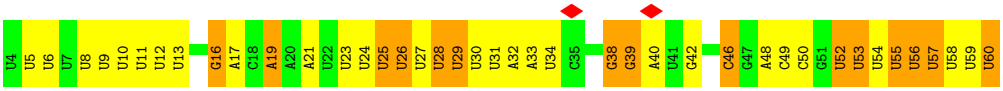
Chain mb:



• Molecule 84: mRNA

Chain l:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.160	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	758.7976, 758.7976, 758.7976	wwPDB
Map dimensions	506, 506, 506	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4996, 1.4996, 1.4996	Depositor

5 Model quality

5.1 Standard geometry

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

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	BQ	0.50	0/74873	0.46	0/116727
1	YQ	0.59	0/74873	0.51	3/116727 (0.0%)
2	BR	0.43	0/2883	0.40	0/4491
2	YR	0.50	0/2883	0.43	0/4491
3	BS	0.49	0/3724	0.46	0/5798
3	YS	0.59	0/3724	0.52	1/5798 (0.0%)
4	AW	0.65	0/1946	0.67	0/2614
4	XW	0.81	1/1946 (0.1%)	0.75	0/2614
5	BA	0.60	0/3146	0.76	2/4228 (0.0%)
5	YA	0.70	0/3146	0.84	2/4228 (0.0%)
6	BE	0.63	1/2800 (0.0%)	0.85	5/3790 (0.1%)
6	YE	0.73	0/2800	0.89	2/3790 (0.1%)
7	BI	0.48	0/2408	0.74	2/3248 (0.1%)
7	YI	0.54	0/2408	0.77	0/3248
8	BM	0.48	0/1269	0.85	3/1705 (0.2%)
8	YM	0.52	0/1269	0.85	0/1705
9	BO	0.63	0/1828	0.84	1/2461 (0.0%)
9	YO	0.72	0/1828	0.83	0/2461
10	AA	0.47	0/1795	0.61	0/2429
10	XA	0.53	0/1795	0.68	0/2429
11	AD	0.45	0/1531	0.60	0/2062
11	XD	0.52	0/1531	0.61	0/2062
12	BD	0.51	0/1732	0.73	0/2323
12	YD	0.62	0/1732	0.81	0/2323
13	AG	0.40	0/1374	0.71	0/1842
13	XG	0.46	0/1374	0.73	0/1842
14	AJ	0.56	0/1573	0.74	1/2113 (0.0%)
14	XJ	0.64	0/1573	0.77	1/2113 (0.0%)
15	AM	0.48	0/1074	0.63	0/1446
15	XM	0.50	0/1074	0.62	1/1446 (0.1%)
16	AQ	0.63	0/1757	0.65	0/2354
16	XQ	0.77	0/1757	0.70	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AU	0.61	0/1585	0.57	0/2128
17	XU	0.70	0/1585	0.61	0/2128
18	2	0.68	12/41891 (0.0%)	0.49	9/65273 (0.0%)
18	2b	0.70	6/41891 (0.0%)	0.53	6/65273 (0.0%)
19	P	0.47	0/1623	0.69	1/2222 (0.0%)
19	Pb	0.58	0/1623	0.75	0/2222
20	Q	0.48	0/1748	0.64	1/2352 (0.0%)
20	Qb	0.55	0/1748	0.63	0/2352
21	R	0.54	0/1665	0.62	0/2263
21	Rb	0.68	0/1665	0.68	0/2263
22	A	0.48	0/1759	0.87	2/2368 (0.1%)
22	Ab	0.63	0/1759	0.91	1/2368 (0.0%)
23	S	0.46	0/2109	0.61	0/2839
23	Sb	0.50	0/2109	0.65	0/2839
24	B	0.48	0/1629	0.95	5/2202 (0.2%)
24	Bb	0.55	0/1629	0.99	3/2202 (0.1%)
25	T	0.39	0/1779	0.68	4/2379 (0.2%)
25	Tb	0.39	0/1779	0.62	0/2379
26	U	0.43	0/1511	0.94	4/2036 (0.2%)
26	Ub	0.52	0/1511	0.95	3/2036 (0.1%)
27	V	0.49	0/1514	0.60	0/2021
27	Vb	0.47	0/1514	0.60	0/2021
28	W	0.48	1/1519 (0.1%)	0.62	0/2035
28	Wb	0.55	0/1519	0.69	0/2035
29	C	0.37	0/757	0.63	0/1022
29	Cb	0.44	0/757	0.70	0/1022
30	X	0.57	0/1194	0.64	0/1610
30	Xb	0.57	0/1194	0.64	0/1610
31	D	0.30	0/898	0.75	2/1220 (0.2%)
31	Db	0.34	0/898	0.79	2/1220 (0.2%)
32	Y	0.57	0/1215	0.67	2/1638 (0.1%)
32	Yb	0.61	0/1215	0.69	1/1638 (0.1%)
33	Z	0.46	0/960	0.61	0/1290
33	Zb	0.55	0/960	0.66	0/1290
34	E	0.36	0/959	0.71	0/1288
34	Eb	0.44	0/959	0.73	2/1288 (0.2%)
35	F	0.44	0/1125	0.69	0/1510
35	Fb	0.53	0/1125	0.76	3/1510 (0.2%)
36	G	0.46	0/1011	0.73	0/1355
36	Gb	0.52	0/1011	0.74	1/1355 (0.1%)
37	H	0.35	0/1211	0.66	0/1628
37	Hb	0.46	0/1211	0.71	0/1628
38	I	0.40	0/1130	0.56	0/1517

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	Ib	0.57	1/1130 (0.1%)	0.58	0/1517
39	J	0.43	0/815	0.63	0/1102
39	Jb	0.56	1/815 (0.1%)	0.68	0/1102
40	a	0.50	0/693	0.89	1/935 (0.1%)
40	ab	0.68	0/693	1.01	3/935 (0.3%)
41	b	0.62	0/1038	0.74	0/1395
41	bb	0.71	0/1038	0.77	0/1395
42	c	0.57	0/1139	0.86	3/1518 (0.2%)
42	cb	0.70	0/1139	0.91	1/1518 (0.1%)
43	d	0.48	0/1087	0.85	0/1449
43	db	0.49	0/1087	0.93	1/1449 (0.1%)
44	K	0.38	0/566	0.65	0/761
44	Kb	0.41	0/566	0.70	0/761
45	e	0.63	0/782	1.04	2/1047 (0.2%)
45	eb	0.70	0/782	0.97	1/1047 (0.1%)
46	f	0.49	0/620	0.79	0/838
46	fb	0.55	0/620	0.83	0/838
47	L	0.40	0/499	0.67	0/670
47	Lb	0.48	0/499	0.66	0/670
48	M	2.06	2/452 (0.4%)	1.97	6/600 (1.0%)
48	Mb	2.20	2/452 (0.4%)	2.08	6/600 (1.0%)
49	g	0.45	0/483	1.12	1/643 (0.2%)
49	gb	0.49	0/483	1.09	2/643 (0.3%)
50	N	0.38	0/567	0.86	0/764
50	Nb	0.48	1/567 (0.2%)	0.88	0/764
51	O	0.30	0/2456	0.53	0/3343
51	Ob	0.43	0/2456	0.59	0/3343
52	AX	0.59	0/1400	0.58	0/1882
52	XX	0.70	0/1400	0.63	0/1882
53	BB	0.57	0/1465	0.75	1/1965 (0.1%)
53	YB	0.71	0/1465	0.82	0/1965
54	BF	0.59	0/1499	0.91	3/1998 (0.2%)
54	YF	0.70	0/1539	0.84	0/2050
55	BH	0.55	0/1481	0.71	0/1990
55	YH	0.65	0/1481	0.76	0/1990
56	BJ	0.57	0/1300	0.76	0/1743
56	YJ	0.68	0/1300	0.85	2/1743 (0.1%)
57	BL	0.44	0/794	0.72	2/1076 (0.2%)
57	YL	0.47	0/794	0.73	2/1076 (0.2%)
58	AB	0.59	0/1008	0.57	0/1356
58	XB	0.70	0/1008	0.61	0/1356
59	AE	2.80	1/1103 (0.1%)	0.79	3/1458 (0.2%)
59	XE	0.53	0/1103	0.69	0/1458

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
60	AH	0.56	0/974	0.61	0/1314
60	XH	0.65	0/974	0.66	0/1314
61	AK	0.52	0/987	0.57	0/1318
61	XK	0.61	0/987	0.64	0/1318
62	AN	0.46	0/1118	0.59	0/1497
62	XN	0.53	0/1118	0.64	0/1497
63	AR	0.57	0/1204	0.65	0/1612
63	XR	0.72	0/1204	0.72	0/1612
64	AV	0.46	0/473	0.64	0/629
64	XV	0.61	0/473	0.77	0/629
65	AY	0.58	0/775	0.69	0/1040
65	XY	0.62	0/775	0.75	0/1040
66	BC	0.56	0/897	0.82	1/1205 (0.1%)
66	YC	0.65	0/897	0.83	1/1205 (0.1%)
67	BG	0.59	0/1041	0.75	0/1394
67	YG	0.72	0/1041	0.79	0/1394
68	BK	0.63	0/868	0.74	0/1168
68	YK	0.77	0/868	0.81	0/1168
69	BN	0.64	0/890	0.75	0/1189
69	YN	0.76	0/890	0.85	0/1189
70	BP	0.52	0/974	0.79	0/1297
70	YP	0.63	0/974	0.78	1/1297 (0.1%)
71	AC	0.46	0/777	0.61	0/1033
71	XC	0.54	0/777	0.70	0/1033
72	AF	0.65	0/665	0.58	0/882
72	XF	0.77	0/665	0.68	0/882
73	AI	0.43	0/614	0.57	0/822
73	XI	0.49	0/614	0.57	0/822
74	AL	0.64	0/443	0.59	0/588
74	XL	0.75	0/443	0.69	0/588
75	AO	0.45	0/423	0.52	0/562
75	XO	0.52	0/423	0.55	0/562
76	AS	0.54	0/234	0.69	0/300
76	XS	0.63	0/234	0.74	0/300
77	AP	0.54	0/860	0.57	0/1136
77	XP	0.65	0/860	0.59	0/1136
78	AT	0.63	0/701	0.70	0/934
78	XT	0.73	0/701	0.72	1/934 (0.1%)
79	BU	0.25	0/1067	0.52	0/1439
79	YU	0.28	0/1067	0.59	0/1439
80	n	0.36	0/1811	0.43	0/2821
81	m	0.18	0/1773	0.39	0/2759
82	nb	0.34	0/1810	0.55	0/2821

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
83	mb	0.42	0/1836	0.41	0/2859
84	l	0.35	0/1312	0.58	0/2033
All	All	0.60	29/436056 (0.0%)	0.60	120/640783 (0.0%)

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
4	AW	0	1
4	XW	0	1
5	BA	0	1
5	YA	0	1
6	BE	0	2
6	YE	0	2
7	BI	0	1
9	BO	0	1
9	YO	0	1
10	AA	0	1
12	YD	0	1
13	AG	0	6
13	XG	0	3
14	AJ	0	5
14	XJ	0	4
15	XM	0	1
16	AQ	0	1
16	XQ	0	1
19	P	0	3
19	Pb	0	5
20	Q	0	1
20	Qb	0	2
21	R	0	2
21	Rb	0	2
22	A	0	2
22	Ab	0	1
23	S	0	4
23	Sb	0	3
24	B	0	2
24	Bb	0	2
25	T	0	3
25	Tb	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	U	0	5
26	Ub	0	4
27	V	0	1
27	Vb	0	1
29	C	0	2
29	Cb	0	2
30	X	0	3
31	D	0	4
31	Db	0	4
32	Y	0	1
32	Yb	0	1
33	Zb	0	2
34	E	0	2
34	Eb	0	4
35	F	0	2
35	Fb	0	2
37	H	0	2
37	Hb	0	3
39	J	0	2
39	Jb	0	4
40	a	0	1
41	b	0	1
41	bb	0	1
42	c	0	1
42	cb	0	1
43	d	0	3
43	db	0	5
44	Kb	0	1
45	e	0	5
45	eb	0	5
48	M	0	1
48	Mb	0	2
49	g	0	1
49	gb	0	2
50	N	0	3
50	Nb	0	3
53	BB	0	1
53	YB	0	2
58	AB	0	1
59	AE	0	4
59	XE	0	2
62	AN	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
62	XN	0	1
63	AR	0	1
63	XR	0	1
64	AV	0	3
64	XV	0	3
70	BP	0	1
70	YP	0	1
71	AC	0	1
71	XC	0	1
78	XT	0	1
All	All	0	180

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AE	116	LYS	CB-CG	91.49	4.26	1.52
18	2b	1597	A	C6-N1	49.28	2.34	1.35
18	2	1597	A	C6-N1	47.71	2.31	1.35
18	2b	1597	A	N1-C2	47.67	2.29	1.34
18	2	1597	A	N1-C2	46.50	2.27	1.34

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Mb	13	ARG	CA-C-N	28.58	164.38	122.93
48	Mb	13	ARG	C-N-CA	28.58	164.38	122.93
48	M	13	ARG	CA-C-N	27.88	164.76	122.94
48	M	13	ARG	C-N-CA	27.88	164.76	122.94
6	YE	341	SER	N-CA-C	-11.45	95.82	111.96

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AW	214	GLY	Peptide
5	BA	112	ASP	Mainchain
6	BE	318	LEU	Peptide
6	BE	89	ALA	Peptide
7	BI	269	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BQ	66891	0	33619	593	0
1	YQ	66891	0	33619	632	0
2	BR	2579	0	1304	33	0
2	YR	2579	0	1304	27	0
3	BS	3333	0	1685	40	0
3	YS	3333	0	1685	52	0
4	AW	1912	0	1976	44	0
4	XW	1912	0	1976	57	0
5	BA	3075	0	3142	62	0
5	YA	3075	0	3142	48	0
6	BE	2748	0	2859	49	0
6	YE	2748	0	2859	50	0
7	BI	2359	0	2311	30	0
7	YI	2359	0	2311	28	0
8	BM	1248	0	1339	19	0
8	YM	1248	0	1339	19	0
9	BO	1791	0	1869	26	0
9	YO	1791	0	1869	31	0
10	AA	1763	0	1819	36	0
10	XA	1763	0	1819	47	0
11	AD	1510	0	1576	21	0
11	XD	1510	0	1576	35	0
12	BD	1696	0	1731	21	0
12	YD	1696	0	1731	35	0
13	AG	1353	0	1383	34	0
13	XG	1353	0	1383	37	0
14	AJ	1548	0	1613	30	0
14	XJ	1548	0	1613	33	0
15	AM	1059	0	1154	27	0
15	XM	1059	0	1154	33	0
16	AQ	1720	0	1779	45	0
16	XQ	1720	0	1779	47	0
17	AU	1555	0	1659	37	0
17	XU	1555	0	1659	36	0
18	2	37455	0	18845	557	0
18	2b	37455	0	18845	529	0
19	P	1583	0	1578	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Pb	1583	0	1578	54	0
20	Q	1722	0	1793	40	0
20	Qb	1722	0	1793	45	0
21	R	1635	0	1723	51	0
21	Rb	1635	0	1723	55	0
22	A	1734	0	1817	29	0
22	Ab	1734	0	1817	30	0
23	S	2068	0	2154	59	0
23	Sb	2068	0	2154	80	0
24	B	1609	0	1675	27	0
24	Bb	1609	0	1675	36	0
25	T	1755	0	1846	40	0
25	Tb	1755	0	1846	47	0
26	U	1486	0	1576	21	0
26	Ub	1486	0	1576	30	0
27	V	1489	0	1525	42	0
27	Vb	1489	0	1525	39	0
28	W	1494	0	1573	35	0
28	Wb	1494	0	1573	37	0
29	C	741	0	691	18	0
29	Cb	741	0	691	20	0
30	X	1168	0	1233	25	0
30	Xb	1168	0	1233	31	0
31	D	890	0	887	35	0
31	Db	890	0	887	28	0
32	Y	1192	0	1255	18	0
32	Yb	1192	0	1255	20	0
33	Z	949	0	985	21	0
33	Zb	949	0	985	21	0
34	E	939	0	968	29	0
34	Eb	939	0	968	25	0
35	F	1105	0	1166	42	0
35	Fb	1105	0	1166	40	0
36	G	1001	0	1063	42	0
36	Gb	1001	0	1063	42	0
37	H	1192	0	1222	50	0
37	Hb	1192	0	1222	41	0
38	I	1112	0	1124	34	0
38	Ib	1112	0	1124	28	0
39	J	805	0	874	32	0
39	Jb	805	0	874	29	0
40	a	684	0	672	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	ab	684	0	672	21	0
41	b	1021	0	1060	14	0
41	bb	1021	0	1060	11	0
42	c	1121	0	1196	17	0
42	cb	1121	0	1196	18	0
43	d	1073	0	1132	35	0
43	db	1073	0	1132	24	0
44	K	558	0	598	17	0
44	Kb	558	0	598	23	0
45	e	769	0	815	23	0
45	eb	769	0	815	17	0
46	f	610	0	633	11	0
46	fb	610	0	633	13	0
47	L	497	0	535	8	0
47	Lb	497	0	535	12	0
48	M	442	0	427	55	0
48	Mb	442	0	428	67	0
49	g	475	0	525	12	0
49	gb	475	0	525	13	0
50	N	556	0	548	20	0
50	Nb	556	0	552	15	0
51	O	2403	0	2353	49	0
51	Ob	2403	0	2353	65	0
52	AX	1378	0	1404	23	0
52	XX	1378	0	1404	30	0
53	BB	1441	0	1543	24	0
53	YB	1441	0	1543	17	0
54	BF	1482	0	1578	26	0
54	YF	1522	0	1617	26	0
55	BH	1445	0	1487	26	0
55	YH	1445	0	1487	22	0
56	BJ	1276	0	1323	27	0
56	YJ	1276	0	1323	26	0
57	BL	778	0	791	7	0
57	YL	778	0	791	9	0
58	AB	993	0	1040	22	0
58	XB	993	0	1040	25	0
59	AE	1089	0	1183	30	0
59	XE	1089	0	1183	18	0
60	AH	959	0	1023	15	0
60	XH	959	0	1023	17	0
61	AK	976	0	1064	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	XK	976	0	1064	29	0
62	AN	1092	0	1155	26	0
62	XN	1092	0	1155	26	0
63	AR	1173	0	1215	31	0
63	XR	1173	0	1215	26	0
64	AV	462	0	491	13	0
64	XV	462	0	491	11	0
65	AY	767	0	816	7	0
65	XY	767	0	816	9	0
66	BC	883	0	918	7	0
66	YC	883	0	918	13	0
67	BG	1020	0	1090	13	0
67	YG	1020	0	1090	14	0
68	BK	850	0	880	10	0
68	YK	850	0	880	12	0
69	BN	880	0	945	14	0
69	YN	880	0	942	10	0
70	BP	965	0	1067	8	0
70	YP	965	0	1067	15	0
71	AC	770	0	846	14	0
71	XC	770	0	846	18	0
72	AF	650	0	654	19	0
72	XF	650	0	650	20	0
73	AI	608	0	671	9	0
73	XI	608	0	671	12	0
74	AL	436	0	475	10	0
74	XL	436	0	475	9	0
75	AO	417	0	455	9	0
75	XO	417	0	455	8	0
76	AS	233	0	284	6	0
76	XS	233	0	284	5	0
77	AP	847	0	915	17	0
77	XP	847	0	915	23	0
78	AT	694	0	734	15	0
78	XT	694	0	734	14	0
79	BU	1052	0	1028	24	0
79	YU	1052	0	1028	20	0
80	n	1621	0	822	14	0
81	m	1589	0	810	21	0
82	nb	1620	0	822	18	0
83	mb	1644	0	836	10	0
84	l	1182	0	594	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	AO	1	0	0	0	0
85	AP	1	0	0	0	0
85	AT	1	0	0	0	0
85	M	1	0	0	0	0
85	Mb	1	0	0	0	0
85	N	1	0	0	0	0
85	XF	1	0	0	0	0
85	XO	1	0	0	0	0
85	XP	1	0	0	0	0
85	XT	1	0	0	0	0
85	YN	1	0	0	0	0
85	e	1	0	0	0	0
85	eb	1	0	0	0	0
85	f	1	0	0	0	0
85	fb	1	0	0	0	0
All	All	405889	0	299841	4980	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 4980 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:74:U:C2	18:2:74:U:N1	1.70	1.59
18:2:74:U:C4	18:2:74:U:N3	1.70	1.59
18:2:74:U:N1	18:2:74:U:C6	1.68	1.58
18:2:74:U:C2	18:2:74:U:N3	1.69	1.52
18:2b:1597:A:C4	18:2b:1597:A:C5	2.01	1.46

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AW	250/252 (99%)	217 (87%)	33 (13%)	0	100	100
4	XW	250/252 (99%)	218 (87%)	32 (13%)	0	100	100
5	BA	384/386 (100%)	357 (93%)	27 (7%)	0	100	100
5	YA	384/386 (100%)	358 (93%)	25 (6%)	1 (0%)	36	71
6	BE	359/361 (99%)	321 (89%)	33 (9%)	5 (1%)	9	38
6	YE	359/361 (99%)	321 (89%)	33 (9%)	5 (1%)	9	38
7	BI	292/294 (99%)	266 (91%)	25 (9%)	1 (0%)	36	71
7	YI	292/294 (99%)	265 (91%)	27 (9%)	0	100	100
8	BM	153/176 (87%)	146 (95%)	6 (4%)	1 (1%)	18	55
8	YM	153/176 (87%)	146 (95%)	6 (4%)	1 (1%)	18	55
9	BO	221/223 (99%)	206 (93%)	14 (6%)	1 (0%)	24	63
9	YO	221/223 (99%)	207 (94%)	14 (6%)	0	100	100
10	AA	229/231 (99%)	202 (88%)	27 (12%)	0	100	100
10	XA	229/231 (99%)	197 (86%)	32 (14%)	0	100	100
11	AD	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
11	XD	188/190 (99%)	175 (93%)	13 (7%)	0	100	100
12	BD	205/221 (93%)	187 (91%)	17 (8%)	1 (0%)	24	63
12	YD	205/221 (93%)	187 (91%)	17 (8%)	1 (0%)	24	63
13	AG	167/169 (99%)	139 (83%)	26 (16%)	2 (1%)	10	42
13	XG	167/169 (99%)	139 (83%)	24 (14%)	4 (2%)	4	25
14	AJ	192/194 (99%)	159 (83%)	25 (13%)	8 (4%)	2	17
14	XJ	192/194 (99%)	155 (81%)	30 (16%)	7 (4%)	2	19
15	AM	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
15	XM	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
16	AQ	201/203 (99%)	185 (92%)	14 (7%)	2 (1%)	12	47
16	XQ	201/203 (99%)	180 (90%)	20 (10%)	1 (0%)	24	63
17	AU	195/197 (99%)	191 (98%)	4 (2%)	0	100	100
17	XU	195/197 (99%)	186 (95%)	9 (5%)	0	100	100
19	P	204/206 (99%)	171 (84%)	32 (16%)	1 (0%)	24	63
19	Pb	204/206 (99%)	171 (84%)	31 (15%)	2 (1%)	12	47
20	Q	214/216 (99%)	193 (90%)	21 (10%)	0	100	100
20	Qb	214/216 (99%)	189 (88%)	25 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	R	215/217 (99%)	190 (88%)	25 (12%)	0	100	100
21	Rb	215/217 (99%)	187 (87%)	27 (13%)	1 (0%)	24	63
22	A	221/223 (99%)	196 (89%)	21 (10%)	4 (2%)	6	32
22	Ab	221/223 (99%)	199 (90%)	18 (8%)	4 (2%)	6	32
23	S	258/260 (99%)	226 (88%)	31 (12%)	1 (0%)	30	67
23	Sb	258/260 (99%)	219 (85%)	38 (15%)	1 (0%)	30	67
24	B	204/206 (99%)	170 (83%)	31 (15%)	3 (2%)	8	38
24	Bb	204/206 (99%)	173 (85%)	28 (14%)	3 (2%)	8	38
25	T	216/218 (99%)	194 (90%)	20 (9%)	2 (1%)	14	49
25	Tb	216/218 (99%)	202 (94%)	13 (6%)	1 (0%)	24	63
26	U	183/185 (99%)	156 (85%)	23 (13%)	4 (2%)	5	27
26	Ub	183/185 (99%)	157 (86%)	22 (12%)	4 (2%)	5	27
27	V	184/200 (92%)	167 (91%)	17 (9%)	0	100	100
27	Vb	184/200 (92%)	168 (91%)	16 (9%)	0	100	100
28	W	183/185 (99%)	164 (90%)	18 (10%)	1 (0%)	24	63
28	Wb	183/185 (99%)	149 (81%)	32 (18%)	2 (1%)	11	45
29	C	90/92 (98%)	67 (74%)	21 (23%)	2 (2%)	5	27
29	Cb	90/92 (98%)	70 (78%)	18 (20%)	2 (2%)	5	27
30	X	144/146 (99%)	123 (85%)	20 (14%)	1 (1%)	18	55
30	Xb	144/146 (99%)	125 (87%)	19 (13%)	0	100	100
31	D	122/124 (98%)	86 (70%)	31 (25%)	5 (4%)	2	17
31	Db	122/124 (98%)	87 (71%)	30 (25%)	5 (4%)	2	17
32	Y	148/150 (99%)	131 (88%)	15 (10%)	2 (1%)	9	38
32	Yb	148/150 (99%)	132 (89%)	14 (10%)	2 (1%)	9	38
33	Z	126/128 (98%)	110 (87%)	16 (13%)	0	100	100
33	Zb	126/128 (98%)	112 (89%)	14 (11%)	0	100	100
34	E	117/119 (98%)	101 (86%)	12 (10%)	4 (3%)	3	20
34	Eb	117/119 (98%)	102 (87%)	10 (8%)	5 (4%)	2	16
35	F	139/141 (99%)	124 (89%)	14 (10%)	1 (1%)	18	55
35	Fb	139/141 (99%)	123 (88%)	15 (11%)	1 (1%)	18	55
36	G	123/125 (98%)	106 (86%)	16 (13%)	1 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	Gb	123/125 (98%)	103 (84%)	19 (15%)	1 (1%)	16 52
37	H	143/145 (99%)	122 (85%)	19 (13%)	2 (1%)	9 38
37	Hb	143/145 (99%)	128 (90%)	11 (8%)	4 (3%)	4 23
38	I	141/143 (99%)	131 (93%)	10 (7%)	0	100 100
38	Ib	141/143 (99%)	130 (92%)	11 (8%)	0	100 100
39	J	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	6 30
39	Jb	99/101 (98%)	84 (85%)	13 (13%)	2 (2%)	6 30
40	a	85/87 (98%)	72 (85%)	12 (14%)	1 (1%)	10 42
40	ab	85/87 (98%)	74 (87%)	10 (12%)	1 (1%)	10 42
41	b	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
41	bb	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16 52
42	c	142/144 (99%)	129 (91%)	10 (7%)	3 (2%)	5 28
42	cb	142/144 (99%)	128 (90%)	11 (8%)	3 (2%)	5 28
43	d	132/134 (98%)	117 (89%)	10 (8%)	5 (4%)	2 18
43	db	132/134 (98%)	114 (86%)	12 (9%)	6 (4%)	2 16
44	K	67/69 (97%)	61 (91%)	6 (9%)	0	100 100
44	Kb	67/69 (97%)	61 (91%)	6 (9%)	0	100 100
45	e	95/97 (98%)	77 (81%)	17 (18%)	1 (1%)	11 45
45	eb	95/97 (98%)	80 (84%)	14 (15%)	1 (1%)	11 45
46	f	79/81 (98%)	68 (86%)	10 (13%)	1 (1%)	9 40
46	fb	79/81 (98%)	68 (86%)	10 (13%)	1 (1%)	9 40
47	L	61/63 (97%)	51 (84%)	10 (16%)	0	100 100
47	Lb	61/63 (97%)	52 (85%)	9 (15%)	0	100 100
48	M	51/53 (96%)	37 (72%)	14 (28%)	0	100 100
48	Mb	51/53 (96%)	38 (74%)	11 (22%)	2 (4%)	2 18
49	g	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	7 34
49	gb	58/60 (97%)	46 (79%)	11 (19%)	1 (2%)	7 34
50	N	71/73 (97%)	45 (63%)	25 (35%)	1 (1%)	9 38
50	Nb	71/73 (97%)	47 (66%)	24 (34%)	0	100 100
51	O	311/313 (99%)	292 (94%)	19 (6%)	0	100 100
51	Ob	311/313 (99%)	280 (90%)	31 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	AX	171/184 (93%)	163 (95%)	8 (5%)	0	100	100
52	XX	171/184 (93%)	161 (94%)	10 (6%)	0	100	100
53	BB	183/185 (99%)	171 (93%)	11 (6%)	1 (0%)	24	63
53	YB	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
54	BF	181/188 (96%)	173 (96%)	7 (4%)	1 (1%)	21	58
54	YF	186/188 (99%)	178 (96%)	8 (4%)	0	100	100
55	BH	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
55	YH	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
56	BJ	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	9	40
56	YJ	157/159 (99%)	140 (89%)	14 (9%)	3 (2%)	6	30
57	BL	96/98 (98%)	88 (92%)	7 (7%)	1 (1%)	12	47
57	YL	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
58	AB	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
58	XB	132/134 (98%)	122 (92%)	10 (8%)	0	100	100
59	AE	133/135 (98%)	114 (86%)	17 (13%)	2 (2%)	8	38
59	XE	133/135 (98%)	113 (85%)	20 (15%)	0	100	100
60	AH	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
60	XH	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
61	AK	122/124 (98%)	111 (91%)	11 (9%)	0	100	100
61	XK	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
62	AN	133/135 (98%)	119 (90%)	12 (9%)	2 (2%)	8	38
62	XN	133/135 (98%)	118 (89%)	13 (10%)	2 (2%)	8	38
63	AR	146/148 (99%)	122 (84%)	22 (15%)	2 (1%)	9	38
63	XR	146/148 (99%)	119 (82%)	26 (18%)	1 (1%)	18	55
64	AV	56/58 (97%)	45 (80%)	11 (20%)	0	100	100
64	XV	56/58 (97%)	44 (79%)	12 (21%)	0	100	100
65	AY	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
65	XY	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	12	47
66	BC	107/109 (98%)	94 (88%)	12 (11%)	1 (1%)	14	49
66	YC	107/109 (98%)	94 (88%)	11 (10%)	2 (2%)	6	30
67	BG	125/127 (98%)	116 (93%)	7 (6%)	2 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
67	YG	125/127 (98%)	116 (93%)	7 (6%)	2 (2%)	7 36
68	BK	104/106 (98%)	97 (93%)	7 (7%)	0	100 100
68	YK	104/106 (98%)	96 (92%)	8 (8%)	0	100 100
69	BN	110/112 (98%)	105 (96%)	5 (4%)	0	100 100
69	YN	110/112 (98%)	106 (96%)	4 (4%)	0	100 100
70	BP	117/119 (98%)	108 (92%)	8 (7%)	1 (1%)	14 49
70	YP	117/119 (98%)	108 (92%)	8 (7%)	1 (1%)	14 49
71	AC	97/99 (98%)	83 (86%)	14 (14%)	0	100 100
71	XC	97/99 (98%)	91 (94%)	6 (6%)	0	100 100
72	AF	80/82 (98%)	72 (90%)	8 (10%)	0	100 100
72	XF	80/82 (98%)	71 (89%)	9 (11%)	0	100 100
73	AI	75/77 (97%)	70 (93%)	4 (5%)	1 (1%)	9 40
73	XI	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	9 40
74	AL	48/50 (96%)	46 (96%)	2 (4%)	0	100 100
74	XL	48/50 (96%)	43 (90%)	5 (10%)	0	100 100
75	AO	50/52 (96%)	47 (94%)	3 (6%)	0	100 100
75	XO	50/52 (96%)	49 (98%)	1 (2%)	0	100 100
76	AS	23/25 (92%)	23 (100%)	0	0	100 100
76	XS	23/25 (92%)	22 (96%)	1 (4%)	0	100 100
77	AP	103/105 (98%)	94 (91%)	9 (9%)	0	100 100
77	XP	103/105 (98%)	95 (92%)	8 (8%)	0	100 100
78	AT	89/91 (98%)	82 (92%)	7 (8%)	0	100 100
78	XT	89/91 (98%)	82 (92%)	7 (8%)	0	100 100
79	BU	134/312 (43%)	128 (96%)	6 (4%)	0	100 100
79	YU	134/312 (43%)	127 (95%)	7 (5%)	0	100 100
All	All	22169/22946 (97%)	19791 (89%)	2203 (10%)	175 (1%)	18 52

5 of 175 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	BE	90	PHE
6	BE	339	LEU
13	AG	95	ASN

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Mol	Chain	Res	Type
14	AJ	48	PRO
14	AJ	62	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AW	192/194 (99%)	192 (100%)	0	100	100
4	XW	192/194 (99%)	192 (100%)	0	100	100
5	BA	318/322 (99%)	315 (99%)	3 (1%)	70	77
5	YA	318/322 (99%)	316 (99%)	2 (1%)	78	81
6	BE	288/288 (100%)	287 (100%)	1 (0%)	86	84
6	YE	288/288 (100%)	288 (100%)	0	100	100
7	BI	243/243 (100%)	243 (100%)	0	100	100
7	YI	243/243 (100%)	242 (100%)	1 (0%)	84	83
8	BM	135/153 (88%)	135 (100%)	0	100	100
8	YM	135/153 (88%)	134 (99%)	1 (1%)	76	80
9	BO	187/187 (100%)	187 (100%)	0	100	100
9	YO	187/187 (100%)	187 (100%)	0	100	100
10	AA	177/190 (93%)	177 (100%)	0	100	100
10	XA	177/190 (93%)	177 (100%)	0	100	100
11	AD	170/170 (100%)	170 (100%)	0	100	100
11	XD	170/170 (100%)	170 (100%)	0	100	100
12	BD	177/187 (95%)	177 (100%)	0	100	100
12	YD	177/187 (95%)	176 (99%)	1 (1%)	78	81
13	AG	147/147 (100%)	147 (100%)	0	100	100
13	XG	147/147 (100%)	146 (99%)	1 (1%)	76	80
14	AJ	154/154 (100%)	154 (100%)	0	100	100
14	XJ	154/154 (100%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	AM	108/108 (100%)	108 (100%)	0	100 100
15	XM	108/108 (100%)	108 (100%)	0	100 100
16	AQ	175/175 (100%)	175 (100%)	0	100 100
16	XQ	175/175 (100%)	175 (100%)	0	100 100
17	AU	160/160 (100%)	160 (100%)	0	100 100
17	XU	160/160 (100%)	160 (100%)	0	100 100
19	P	165/173 (95%)	165 (100%)	0	100 100
19	Pb	165/173 (95%)	164 (99%)	1 (1%)	78 81
20	Q	192/192 (100%)	192 (100%)	0	100 100
20	Qb	192/192 (100%)	191 (100%)	1 (0%)	81 82
21	R	176/176 (100%)	176 (100%)	0	100 100
21	Rb	176/176 (100%)	176 (100%)	0	100 100
22	A	182/182 (100%)	181 (100%)	1 (0%)	81 82
22	Ab	182/182 (100%)	182 (100%)	0	100 100
23	S	221/221 (100%)	221 (100%)	0	100 100
23	Sb	221/221 (100%)	221 (100%)	0	100 100
24	B	173/173 (100%)	173 (100%)	0	100 100
24	Bb	173/173 (100%)	170 (98%)	3 (2%)	53 67
25	T	187/187 (100%)	187 (100%)	0	100 100
25	Tb	187/187 (100%)	187 (100%)	0	100 100
26	U	165/165 (100%)	165 (100%)	0	100 100
26	Ub	165/165 (100%)	164 (99%)	1 (1%)	78 81
27	V	150/161 (93%)	150 (100%)	0	100 100
27	Vb	150/161 (93%)	150 (100%)	0	100 100
28	W	158/158 (100%)	158 (100%)	0	100 100
28	Wb	158/158 (100%)	158 (100%)	0	100 100
29	C	73/85 (86%)	73 (100%)	0	100 100
29	Cb	73/85 (86%)	73 (100%)	0	100 100
30	X	129/129 (100%)	129 (100%)	0	100 100
30	Xb	129/129 (100%)	129 (100%)	0	100 100
31	D	88/100 (88%)	88 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Db	88/100 (88%)	88 (100%)	0	100	100
32	Y	127/127 (100%)	127 (100%)	0	100	100
32	Yb	127/127 (100%)	127 (100%)	0	100	100
33	Z	97/97 (100%)	97 (100%)	0	100	100
33	Zb	97/97 (100%)	97 (100%)	0	100	100
34	E	98/98 (100%)	98 (100%)	0	100	100
34	Eb	98/98 (100%)	98 (100%)	0	100	100
35	F	117/117 (100%)	117 (100%)	0	100	100
35	Fb	117/117 (100%)	116 (99%)	1 (1%)	70	77
36	G	113/113 (100%)	113 (100%)	0	100	100
36	Gb	113/113 (100%)	113 (100%)	0	100	100
37	H	128/128 (100%)	127 (99%)	1 (1%)	73	78
37	Hb	128/128 (100%)	128 (100%)	0	100	100
38	I	115/115 (100%)	115 (100%)	0	100	100
38	Ib	115/115 (100%)	115 (100%)	0	100	100
39	J	94/94 (100%)	94 (100%)	0	100	100
39	Jb	94/94 (100%)	94 (100%)	0	100	100
40	a	74/74 (100%)	74 (100%)	0	100	100
40	ab	74/74 (100%)	74 (100%)	0	100	100
41	b	110/110 (100%)	109 (99%)	1 (1%)	70	77
41	bb	110/110 (100%)	108 (98%)	2 (2%)	51	66
42	c	119/119 (100%)	119 (100%)	0	100	100
42	cb	119/119 (100%)	119 (100%)	0	100	100
43	d	112/112 (100%)	112 (100%)	0	100	100
43	db	112/112 (100%)	110 (98%)	2 (2%)	51	66
44	K	61/61 (100%)	61 (100%)	0	100	100
44	Kb	61/61 (100%)	61 (100%)	0	100	100
45	e	83/83 (100%)	83 (100%)	0	100	100
45	eb	83/83 (100%)	83 (100%)	0	100	100
46	f	70/70 (100%)	70 (100%)	0	100	100
46	fb	70/70 (100%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	L	56/56 (100%)	56 (100%)	0	100 100
47	Lb	56/56 (100%)	56 (100%)	0	100 100
48	M	47/47 (100%)	46 (98%)	1 (2%)	47 64
48	Mb	47/47 (100%)	44 (94%)	3 (6%)	16 37
49	g	51/51 (100%)	51 (100%)	0	100 100
49	gb	51/51 (100%)	47 (92%)	4 (8%)	11 32
50	N	56/63 (89%)	56 (100%)	0	100 100
50	Nb	56/63 (89%)	56 (100%)	0	100 100
51	O	255/256 (100%)	255 (100%)	0	100 100
51	Ob	255/256 (100%)	255 (100%)	0	100 100
52	AX	139/146 (95%)	139 (100%)	0	100 100
52	XX	139/146 (95%)	139 (100%)	0	100 100
53	BB	150/150 (100%)	150 (100%)	0	100 100
53	YB	150/150 (100%)	150 (100%)	0	100 100
54	BF	149/153 (97%)	148 (99%)	1 (1%)	76 80
54	YF	153/153 (100%)	153 (100%)	0	100 100
55	BH	156/156 (100%)	156 (100%)	0	100 100
55	YH	156/156 (100%)	156 (100%)	0	100 100
56	BJ	136/136 (100%)	135 (99%)	1 (1%)	76 80
56	YJ	136/136 (100%)	136 (100%)	0	100 100
57	BL	85/85 (100%)	84 (99%)	1 (1%)	63 74
57	YL	85/85 (100%)	85 (100%)	0	100 100
58	AB	103/103 (100%)	103 (100%)	0	100 100
58	XB	103/103 (100%)	103 (100%)	0	100 100
59	AE	114/114 (100%)	113 (99%)	1 (1%)	70 77
59	XE	114/114 (100%)	114 (100%)	0	100 100
60	AH	104/104 (100%)	104 (100%)	0	100 100
60	XH	104/104 (100%)	102 (98%)	2 (2%)	50 66
61	AK	107/107 (100%)	107 (100%)	0	100 100
61	XK	107/107 (100%)	107 (100%)	0	100 100
62	AN	115/115 (100%)	114 (99%)	1 (1%)	70 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	XN	115/115 (100%)	115 (100%)	0	100	100
63	AR	118/118 (100%)	118 (100%)	0	100	100
63	XR	118/118 (100%)	118 (100%)	0	100	100
64	AV	46/46 (100%)	46 (100%)	0	100	100
64	XV	46/46 (100%)	46 (100%)	0	100	100
65	AY	84/84 (100%)	84 (100%)	0	100	100
65	XY	84/84 (100%)	84 (100%)	0	100	100
66	BC	94/96 (98%)	94 (100%)	0	100	100
66	YC	94/96 (98%)	93 (99%)	1 (1%)	65	74
67	BG	109/109 (100%)	109 (100%)	0	100	100
67	YG	109/109 (100%)	109 (100%)	0	100	100
68	BK	90/90 (100%)	90 (100%)	0	100	100
68	YK	90/90 (100%)	90 (100%)	0	100	100
69	BN	95/95 (100%)	95 (100%)	0	100	100
69	YN	95/95 (100%)	94 (99%)	1 (1%)	65	74
70	BP	103/104 (99%)	103 (100%)	0	100	100
70	YP	103/104 (99%)	103 (100%)	0	100	100
71	AC	80/81 (99%)	80 (100%)	0	100	100
71	XC	80/81 (99%)	80 (100%)	0	100	100
72	AF	67/67 (100%)	67 (100%)	0	100	100
72	XF	67/67 (100%)	65 (97%)	2 (3%)	36	56
73	AI	67/68 (98%)	67 (100%)	0	100	100
73	XI	67/68 (98%)	67 (100%)	0	100	100
74	AL	45/45 (100%)	45 (100%)	0	100	100
74	XL	45/45 (100%)	45 (100%)	0	100	100
75	AO	47/47 (100%)	47 (100%)	0	100	100
75	XO	47/47 (100%)	47 (100%)	0	100	100
76	AS	23/23 (100%)	23 (100%)	0	100	100
76	XS	23/23 (100%)	23 (100%)	0	100	100
77	AP	90/90 (100%)	90 (100%)	0	100	100
77	XP	90/90 (100%)	89 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	AT	71/71 (100%)	71 (100%)	0	100 100
78	XT	71/71 (100%)	70 (99%)	1 (1%)	59 71
79	BU	105/254 (41%)	105 (100%)	0	100 100
79	YU	105/254 (41%)	104 (99%)	1 (1%)	68 76
All	All	18734/19256 (97%)	18688 (100%)	46 (0%)	85 85

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	gb	39	LEU
12	YD	186	GLU
49	gb	46	ASN
5	YA	221	THR
60	XH	63	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
10	XA	38	GLN
65	XY	12	GLN
12	YD	55	ASN
54	YF	68	GLN
72	XF	76	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	BQ	3121/3396 (91%)	652 (20%)	63 (2%)
1	YQ	3120/3396 (91%)	676 (21%)	58 (1%)
18	2	1755/1800 (97%)	488 (27%)	62 (3%)
18	2b	1755/1800 (97%)	492 (28%)	0
2	BR	120/121 (99%)	15 (12%)	0
2	YR	120/121 (99%)	14 (11%)	0
3	BS	156/157 (99%)	29 (18%)	3 (1%)
3	YS	156/157 (99%)	32 (20%)	2 (1%)
80	n	75/76 (98%)	17 (22%)	0
81	m	74/75 (98%)	21 (28%)	0
82	nb	75/76 (98%)	42 (56%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
83	mb	76/77 (98%)	11 (14%)	0
84	l	56/57 (98%)	37 (66%)	0
All	All	10659/11309 (94%)	2526 (23%)	188 (1%)

5 of 2526 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	BQ	14	U
1	BQ	15	C
1	BQ	26	A
1	BQ	30	G
1	BQ	40	A

5 of 188 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	2	1421	A
1	YQ	1081	U
18	2	1491	U
1	YQ	217	U
1	YQ	1284	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
48	Mb	1
48	M	1
38	Ib	1
4	XW	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Mb	13:ARG	C	14:TYR	N	1.77
1	M	13:ARG	C	14:TYR	N	1.76
1	Ib	116:ILE	C	117:SER	N	1.19
1	XW	204:MET	C	205:ASN	N	1.18

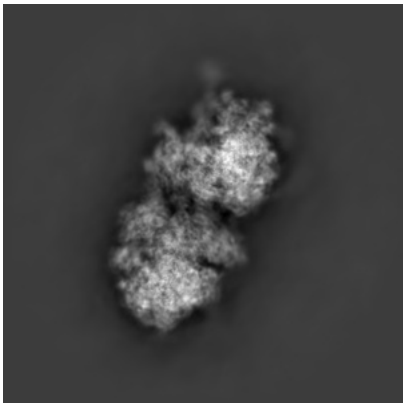
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4427. These allow visual inspection of the internal detail of the map and identification of artifacts.

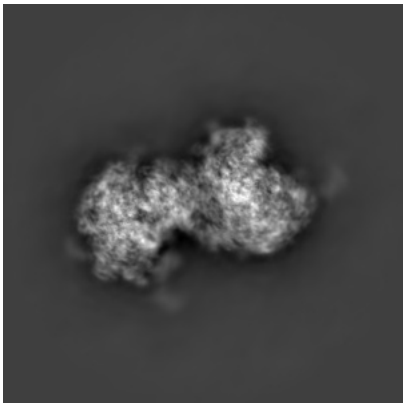
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

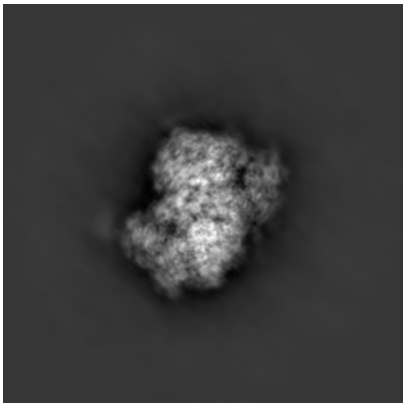
6.1.1 Primary map



X



Y

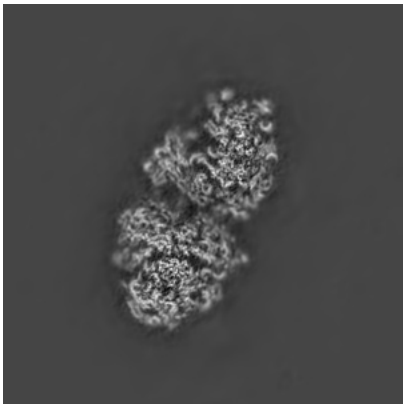


Z

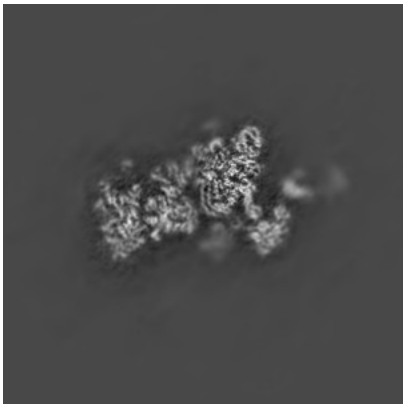
The images above show the map projected in three orthogonal directions.

6.2 Central slices

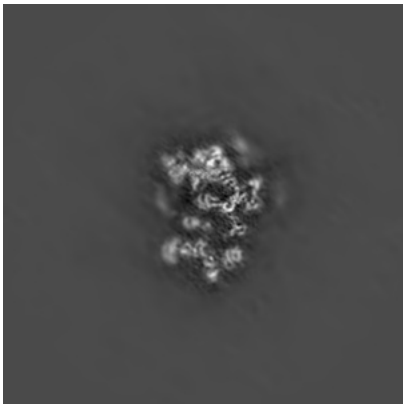
6.2.1 Primary map



X Index: 253



Y Index: 253

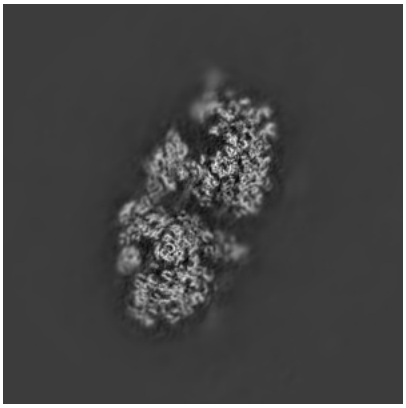


Z Index: 253

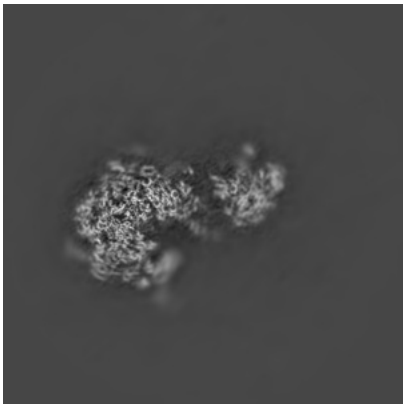
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

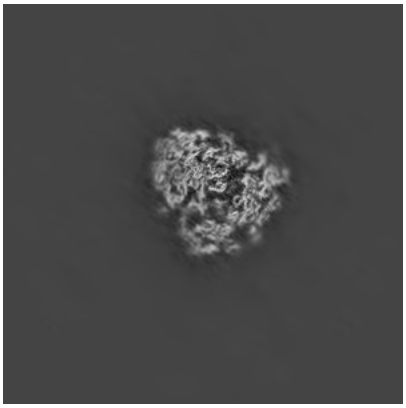
6.3.1 Primary map



X Index: 264



Y Index: 208

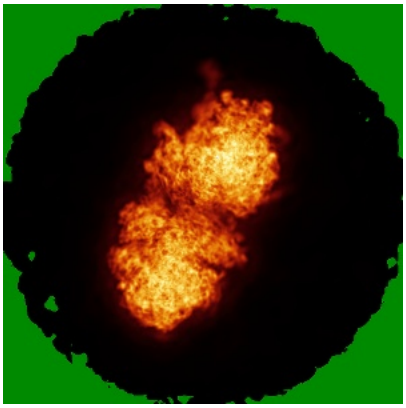


Z Index: 315

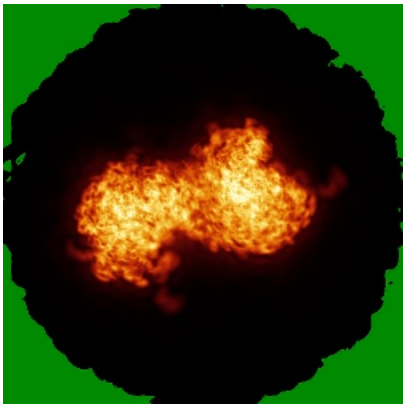
The images above show the largest variance slices of the map in three orthogonal directions.

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

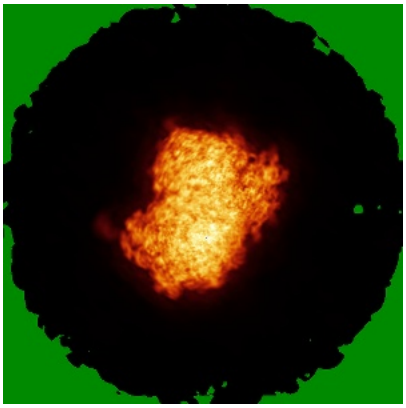
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

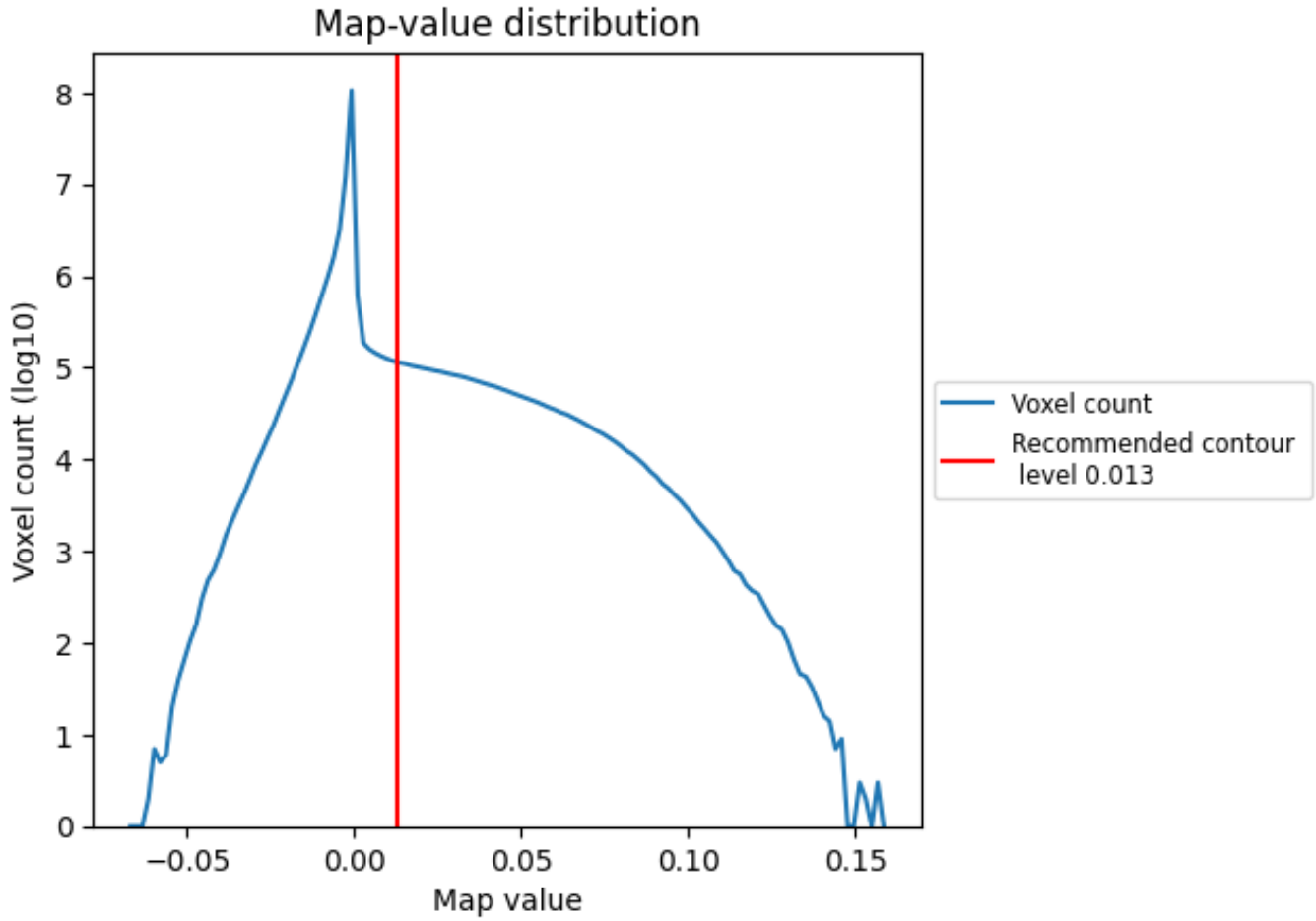
6.6 Mask visualisation (i)

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

7 Map analysis

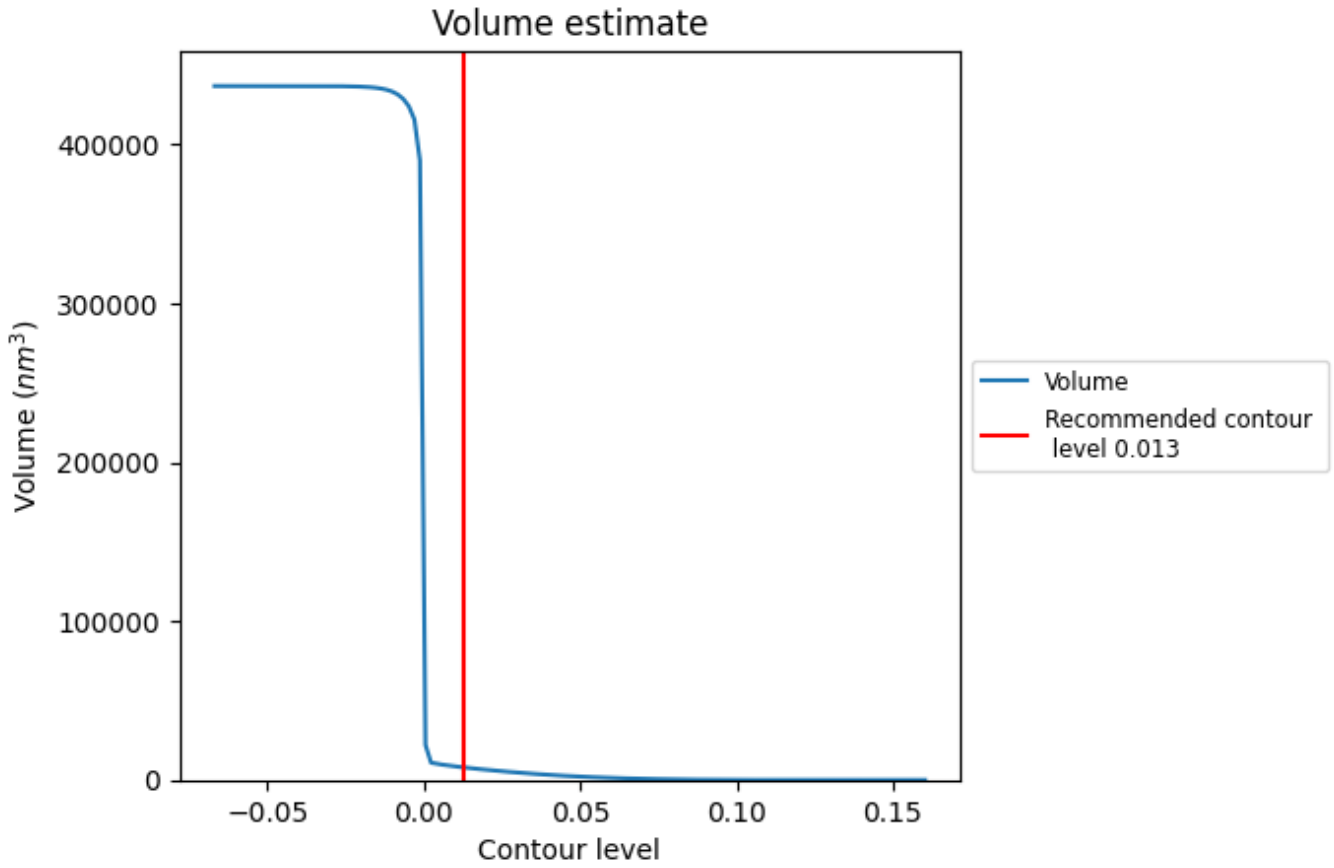
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

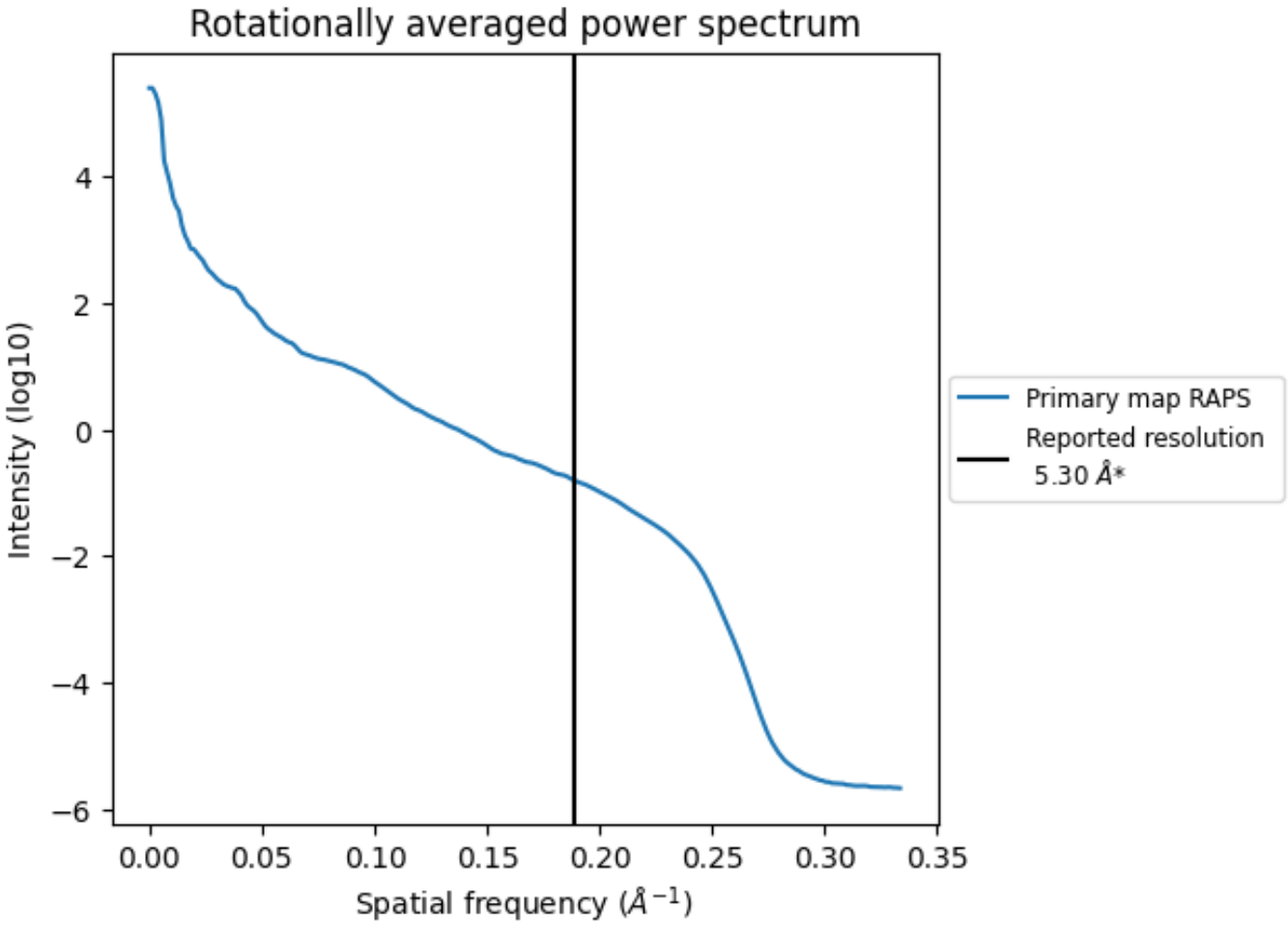
7.2 Volume estimate (i)



The volume at the recommended contour level is 7857 nm^3; this corresponds to an approximate mass of 7097 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

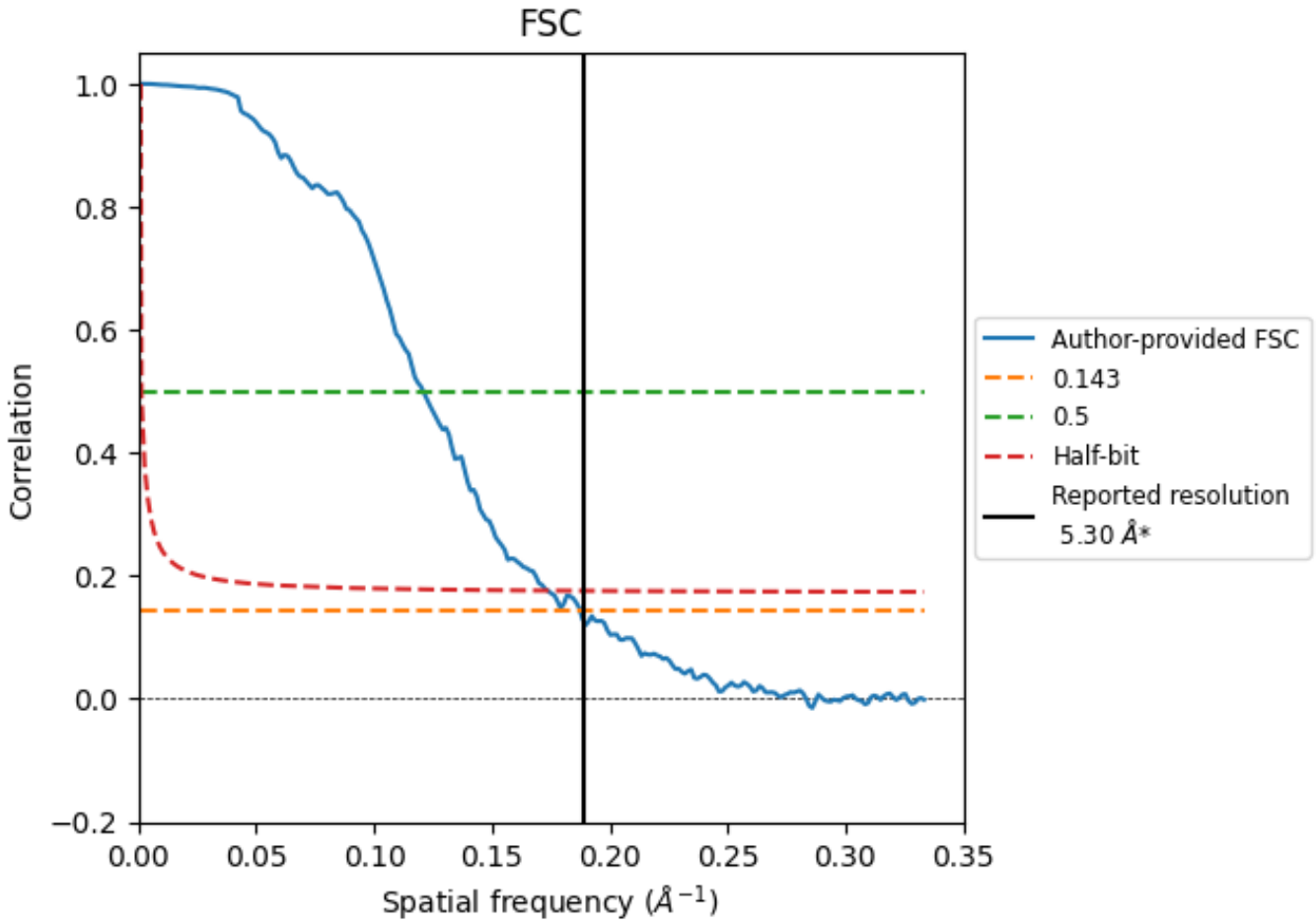


*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.189 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.33	8.27	5.76
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

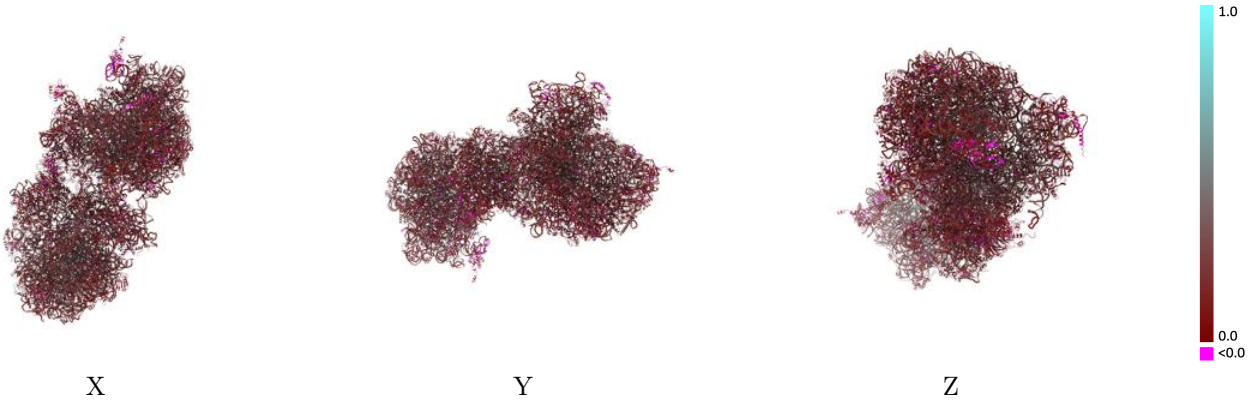
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4427 and PDB model 6I7O. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay

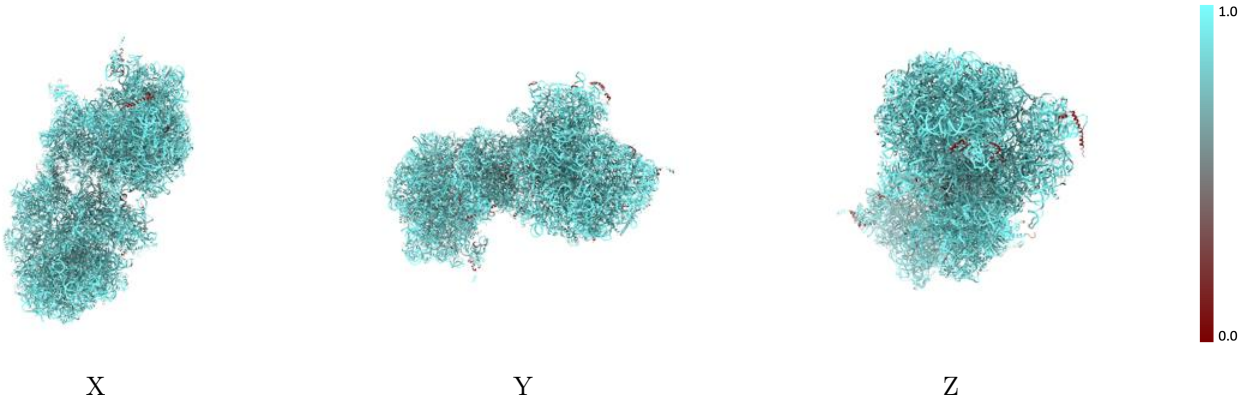
This section was not generated.

9.2 Q-score mapped to coordinate model



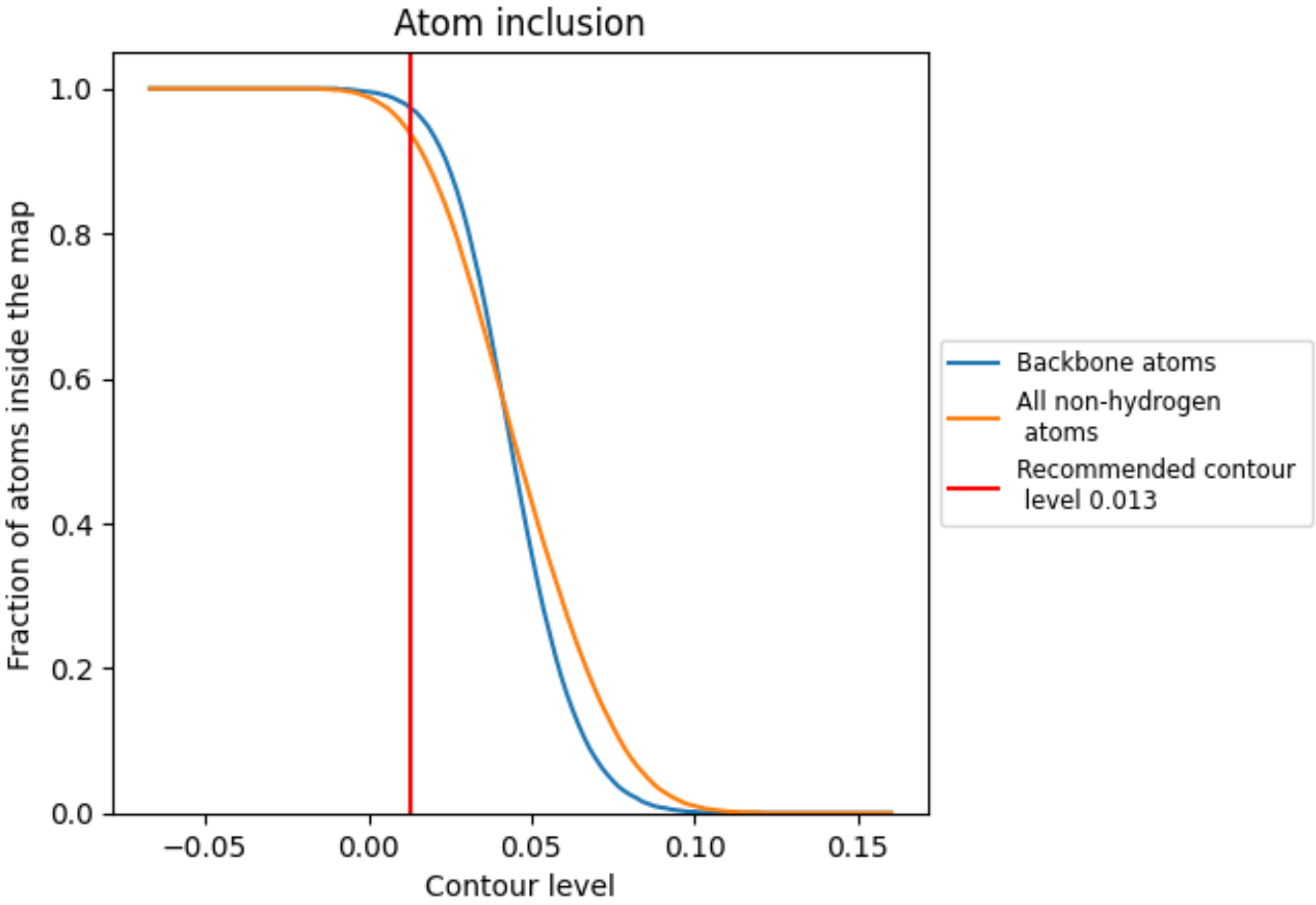
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9370	0.2120
2	0.9820	0.2500
2b	0.9850	0.2320
A	0.8470	0.1750
AA	0.8700	0.1540
AB	0.8720	0.2900
AC	0.8510	0.1560
AD	0.9260	0.1910
AE	0.5140	0.1200
AF	0.9210	0.1960
AG	0.9320	0.1220
AH	0.9030	0.1640
AI	0.8890	0.1510
AJ	0.8990	0.1590
AK	0.9270	0.1610
AL	0.8750	0.1770
AM	0.9450	0.1640
AN	0.9160	0.1560
AO	0.8890	0.2060
AP	0.8570	0.1380
AQ	0.8980	0.1490
AR	0.9290	0.1550
AS	0.7830	0.2540
AT	0.8190	0.2490
AU	0.9070	0.2080
AV	0.8320	0.1460
AW	0.8510	0.2310
AX	0.9320	0.2170
AY	0.8070	0.1830
Ab	0.7970	0.1770
B	0.8210	0.1500
BA	0.9160	0.2310
BB	0.9050	0.1430
BC	0.8770	0.1880
BD	0.8920	0.1600

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Chain	Atom inclusion	Q-score
BE	0.9110	0.1590
BF	0.8760	0.1760
BG	0.8470	0.1680
BH	0.8910	0.1470
BI	0.9330	0.1030
BJ	0.8720	0.1380
BK	0.9130	0.1470
BL	0.9120	0.1530
BM	0.8970	0.1420
BN	0.8130	0.1610
BO	0.9090	0.1530
BP	0.8760	0.1590
BQ	0.9870	0.2460
BR	0.9980	0.1950
BS	0.9920	0.2240
BU	0.6580	0.0420
Bb	0.8800	0.1820
C	0.9350	0.1600
Cb	0.9050	0.1620
D	0.8740	0.1140
Db	0.8500	0.1130
E	0.9220	0.1390
Eb	0.8890	0.1440
F	0.9040	0.1470
Fb	0.9220	0.1600
G	0.8260	0.1810
Gb	0.8500	0.1790
H	0.9490	0.1490
Hb	0.9120	0.1580
I	0.9570	0.1370
Ib	0.9430	0.1440
J	0.9320	0.1600
Jb	0.9050	0.1580
K	0.8840	0.1420
Kb	0.9170	0.1630
L	0.7780	0.1800
Lb	0.8660	0.2060
M	0.9340	0.0610
Mb	0.8870	0.0590
N	0.8330	0.1060
Nb	0.8670	0.1110
O	0.8330	0.1420

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Chain	Atom inclusion	Q-score
Ob	0.9490	0.1530
P	0.8800	0.2200
Pb	0.8930	0.2140
Q	0.7920	0.1990
Qb	0.8580	0.1950
R	0.8910	0.2510
Rb	0.8110	0.2130
S	0.8970	0.1680
Sb	0.8360	0.1390
T	0.9340	0.1510
Tb	0.9170	0.1410
U	0.8860	0.1770
Ub	0.8990	0.1540
V	0.9240	0.1590
Vb	0.9120	0.1280
W	0.8790	0.1960
Wb	0.7770	0.1490
X	0.8490	0.2010
XA	0.9170	0.1720
XB	0.8390	0.1680
XC	0.8990	0.1780
XD	0.9050	0.1380
XE	0.6710	0.1250
XF	0.9260	0.2350
XG	0.9140	0.1420
XH	0.9150	0.1840
XI	0.8990	0.1540
XJ	0.9110	0.1960
XK	0.9310	0.1580
XL	0.8720	0.2280
XM	0.9260	0.1470
XN	0.9190	0.1400
XO	0.7550	0.1230
XP	0.8000	0.2070
XQ	0.9040	0.2060
XR	0.9160	0.2170
XS	0.7170	0.2150
XT	0.8550	0.2290
XU	0.8710	0.1680
XV	0.8740	0.2020
XW	0.8640	0.2600
XX	0.9080	0.2020

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Chain	Atom inclusion	Q-score
XY	0.8120	0.1620
Xb	0.8220	0.1510
Y	0.8350	0.2120
YA	0.9120	0.1540
YB	0.8950	0.1860
YC	0.8530	0.1530
YD	0.8830	0.1580
YE	0.9160	0.1970
YF	0.8770	0.1690
YG	0.8660	0.2150
YH	0.8700	0.1350
YI	0.9390	0.1340
YJ	0.8730	0.1650
YK	0.9210	0.1560
YL	0.9100	0.1380
YM	0.9290	0.1410
YN	0.8580	0.1620
YO	0.8880	0.1650
YP	0.9130	0.1710
YQ	0.9860	0.2550
YR	0.9950	0.2020
YS	0.9950	0.2560
YU	0.6320	0.0430
Yb	0.8810	0.1880
Z	0.8670	0.2080
Zb	0.9000	0.2000
a	0.8520	0.2050
ab	0.8330	0.2050
b	0.8720	0.2150
bb	0.8500	0.1730
c	0.8620	0.2710
cb	0.8200	0.1940
d	0.9140	0.1590
db	0.8430	0.1220
e	0.8770	0.2640
eb	0.8700	0.2550
f	0.8620	0.1950
fb	0.9020	0.1820
g	0.8370	0.1940
gb	0.7080	0.1420
l	0.8640	0.2020
m	0.5120	0.1390

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Chain	Atom inclusion	Q-score
mb	0.9690	0.2520
n	0.9740	0.2370
nb	0.9570	0.2040