



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:20 AM UTC

PDB ID : 6Z1P / pdb_00006z1p
EMDB ID : EMD-11032
Title : Structure of the mitochondrial ribosome from *Tetrahymena thermophila*
Authors : Tobiasson, V.; Amunts, A.
Deposited on : 2020-05-14
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

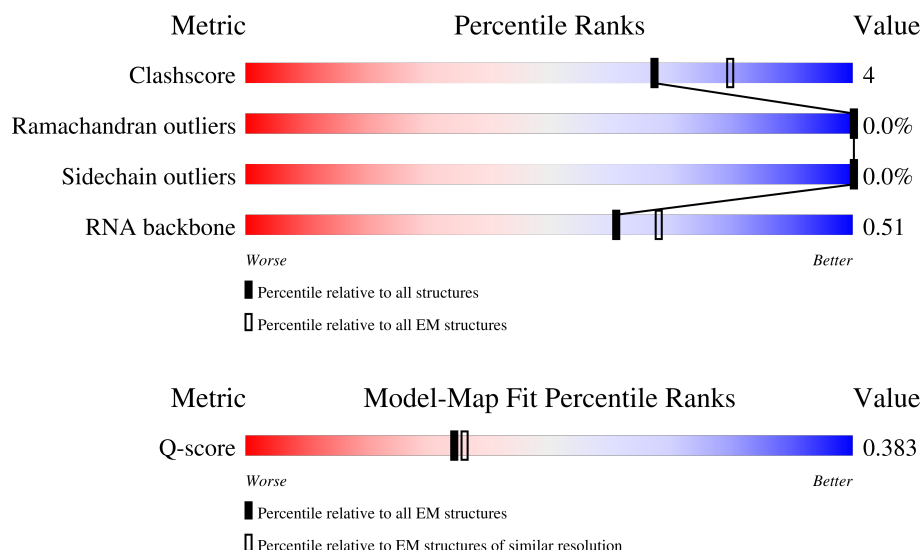
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Aa	278	
2	Ab	2314	
3	Ac	262	

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Mol	Chain	Length	Quality of chain
4	Ad	439	
5	Ae	358	
6	Af	68	
7	Ag	179	
8	Ah	106	
9	Ai	61	
10	Aj	69	
11	Ak	105	
12	Al	223	
13	Am	166	
14	An	158	
15	Ao	391	
16	Ap	119	
17	Aq	305	
18	Ar	143	
19	As	237	
20	At	242	
21	Au	170	
22	Av	235	
23	Aw	364	
24	Ax	138	
25	Ay	234	
26	Az	321	
27	AA	237	
28	AB	289	

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Mol	Chain	Length	Quality of chain
29	AC	307	
30	AD	36	
31	AE	64	
32	AF	164	
33	AG	93	
34	AH	199	
35	AI	155	
36	AJ	179	
37	AK	309	
38	AL	145	
39	AM	184	
40	AN	158	
41	AO	155	
42	AP	386	
43	AQ	109	
44	AR	348	
45	AS	764	
46	AT	299	
47	AU	499	
48	AV	160	
49	Ba	196	
50	Bb	1395	
51	Bc	159	
52	Bd	330	
53	Be	405	

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Mol	Chain	Length	Quality of chain
54	Bf	351	
55	Bg	141	
56	Bh	276	
57	Bi	737	
58	Bj	152	
59	Bk	238	
60	Bl	133	
61	Bm	276	
62	Bn	101	
63	Bo	196	
64	Bp	437	
65	Bq	182	
66	Br	549	
67	Bs	98	
68	Bt	102	
69	Bu	567	
70	Bv	579	
71	Bw	703	
72	Bx	719	
73	By	132	
74	Bz	147	
75	BA	149	
76	BB	112	
77	BC	37	
78	BD	130	

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Mol	Chain	Length	Quality of chain
79	BE	464	
80	BF	23	
81	BG	182	
82	BH	63	
83	BI	1451	
84	BJ	1539	
85	BK	267	
86	BL	310	
87	BM	355	
88	BN	283	
89	BO	142	
90	BP	100	
91	BQ	1032	
92	BR	143	
93	BS	1086	
94	BT	297	
95	BU	439	
96	BV	310	
97	BW	285	
98	BX	151	
99	BY	327	

2 Entry composition

There are 103 unique types of molecules in this entry. The entry contains 518719 atoms, of which 235830 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 LSU rRNA_1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Aa	278	Total	C	H	N	O	P	0	0
			8881	2659	2963	1052	1929	278		

- Molecule 2 is a RNA chain called LSU rRNA_2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Ab	2237	Total	C	H	N	O	P	0	0
			71421	21355	23854	8399	15576	2237		

- Molecule 3 is a protein called Ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Ac	262	Total	C	H	N	O	S	0	0
			4332	1365	2218	385	358	6		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Ad	374	Total	C	H	N	O	S	0	0
			6024	1892	3035	538	546	13		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	Ae	337	Total	C	H	N	O	S	0	0
			5671	1770	2890	505	500	6		

- Molecule 6 is a protein called Ymf69.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Af	68	Total	C	H	N	O	S	0	0
			1232	409	639	91	90	3		

- Molecule 7 is a protein called Ymf60.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Ag	176	Total	C	H	N	O	S	0	0
			3072	997	1555	265	253	2		

- Molecule 8 is a protein called bL7/L12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ah	106	Total	C	H	N	O	0	0
			641	318	111	106	106		

- Molecule 9 is a protein called bL7/12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ai	61	Total	C	H	N	O	0	0
			369	183	64	61	61		

- Molecule 10 is a protein called bL7/12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Aj	69	Total	C	H	N	O	0	0
			419	207	74	69	69		

- Molecule 11 is a protein called Ribosomal protein L7/L12 carboxy-terminal domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	Ak	105	Total	C	H	N	O	S	0	0
			1705	564	831	151	158	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ak	12	LYS	-	expression tag	UNP Q24IM4
Ak	13	UNK	-	expression tag	UNP Q24IM4
Ak	61	ALA	ARG	conflict	UNP Q24IM4

- Molecule 12 is a protein called Ribosomal protein L9, amine-terminal domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Al	53	Total	C	H	N	O	S	0	0
			869	278	439	79	72	1		

- Molecule 13 is a protein called Ymf74.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Am	166	Total	C	H	N	O	S	0	0
			2862	946	1456	223	235	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Am	-8	UNK	-	expression tag	UNP Q951B5
Am	-7	UNK	-	expression tag	UNP Q951B5
Am	-6	UNK	-	expression tag	UNP Q951B5
Am	-5	UNK	-	expression tag	UNP Q951B5
Am	-4	UNK	-	expression tag	UNP Q951B5
Am	-3	UNK	-	expression tag	UNP Q951B5
Am	-2	UNK	-	expression tag	UNP Q951B5
Am	-1	UNK	-	expression tag	UNP Q951B5
Am	0	UNK	-	expression tag	UNP Q951B5

- Molecule 14 is a protein called Ribosomal protein L11, amine-terminal domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	An	158	Total	C	H	N	O	S	0	0
			2562	802	1317	214	219	10		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Ao	330	Total	C	H	N	O	S	0	0
			5591	1788	2820	485	485	13		

- Molecule 16 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Ap	119	Total	C	H	N	O	S	0	0
			2014	625	1058	172	155	4		

- Molecule 17 is a protein called Ribosomal protein L15, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Aq	273	Total	C	H	N	O	S	0	0
			4477	1387	2293	416	376	5		

- Molecule 18 is a protein called Ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Ar	143	Total	C	H	N	O	S	0	0
			2561	813	1329	224	190	5		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	As	236	Total	C	H	N	O	S	0	0
			3953	1227	2015	355	351	5		

- Molecule 20 is a protein called bL19m.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	At	183	Total	C	H	N	O	S	0	0
			3069	987	1531	273	273	5		

- Molecule 21 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	Au	169	Total	C	H	N	O	S	0	0
			2888	904	1469	274	239	2		

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Av	206	Total	C	H	N	O	S	0	0
			3434	1080	1722	307	322	3		

- Molecule 23 is a protein called Ribosomal protein L22/L17e.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Aw	342	Total	C	H	N	O	S	0	0
			5767	1788	2943	514	514	8		

- Molecule 24 is a protein called Ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Ax	132	Total	C	H	N	O	S	0	0
			2257	711	1164	186	191	5		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Ay	190	Total	C	H	N	O	S	0	0
			3124	960	1597	285	281	1		

- Molecule 26 is a protein called bL25m.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Az	237	Total	C	H	N	O	S	0	0
			3934	1246	1990	344	350	4		

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AA	176	Total	C	H	N	O	S	0	0
			2872	907	1425	276	263	1		

- Molecule 28 is a protein called Ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AB	264	Total	C	H	N	O	S	0	0
			4599	1439	2341	410	397	12		

- Molecule 29 is a protein called 39-S ribosomal protein L47.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AC	284	Total	C	H	N	O	S	0	0
			4819	1494	2434	442	446	3		

- Molecule 30 is a protein called bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AD	36	Total	C	H	N	O	S	0	0
			326	108	146	36	36			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AE	57	Total	C	H	N	O	S	0	0
			935	296	483	78	78			

- Molecule 32 is a protein called bL35m.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	AF	115	Total	C	H	N	O	S	0	0
			2028	618	1054	209	145	2		

- Molecule 33 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	AG	38	Total	C	H	N	O	S	0	0
			673	201	357	64	46	5		

- Molecule 34 is a protein called mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	AH	177	Total	C	H	N	O	S	0	0
			2989	942	1496	264	282	5		

- Molecule 35 is a protein called Ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	AI	122	Total	C	H	N	O	S	0	0
			2088	662	1052	190	182	2		

- Molecule 36 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	AJ	178	Total	C	H	N	O	S	0	0
			2961	948	1480	260	267	6		

- Molecule 37 is a protein called mL46.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	AK	244	Total	C	H	N	O	S	0	0
			4093	1340	2017	351	377	8		

- Molecule 38 is a protein called Large subunit ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	AL	145	Total	C	H	N	O	S	0	0
			2406	748	1225	224	203	6		

- Molecule 39 is a protein called mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	AM	126	Total	C	H	N	O	S	0	0
			2085	673	1026	185	198	3		

- Molecule 40 is a protein called mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	AN	96	Total	C	H	N	O	S	0	0
			1629	524	815	140	148	2		

- Molecule 41 is a protein called mL64.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	AO	120	Total	C	H	N	O	S	0	0
			2060	649	1049	191	169	2		

- Molecule 42 is a protein called mL101.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	AP	364	Total	C	H	N	O	S	0	0
			6118	1976	3070	515	546	11		

- Molecule 43 is a protein called mL102.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	AQ	50	Total	C	H	N	O	S	0	0
			863	262	444	85	68	4		

- Molecule 44 is a protein called mL103.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	AR	274	Total	C	H	N	O	S	0	0
			4603	1492	2253	405	447	6		

- Molecule 45 is a protein called mL104.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	AS	728	Total	C	H	N	O	S	0	0
			12114	3916	6045	1028	1105	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	764	GLU	-	expression tag	UNP I7LTP6

- Molecule 46 is a protein called Signal peptide-binding domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	AT	166	Total	C	H	N	O	S	0	0
			2811	875	1434	247	252	3		

- Molecule 47 is a protein called mL106.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	AU	479	Total	C	H	N	O	S	0	0
			7927	2508	4014	662	735	8		

- Molecule 48 is a protein called Iron-binding zinc finger CDGSH type protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	AV	129	Total	C	H	N	O	S	0	0
			2068	666	1030	170	193	9		

- Molecule 49 is a RNA chain called SSU rRNA_1.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	Ba	196	Total	C	H	N	O	P	0	0
			6269	1875	2097	750	1351	196		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ba	14	A	-	expression tag	GB 15011465
Ba	15	A	-	expression tag	GB 15011465
Ba	16	A	-	expression tag	GB 15011465
Ba	17	A	-	expression tag	GB 15011465
Ba	18	U	-	expression tag	GB 15011465
Ba	19	A	-	expression tag	GB 15011465
Ba	20	A	-	expression tag	GB 15011465
Ba	21	A	-	expression tag	GB 15011465
Ba	22	A	-	expression tag	GB 15011465
Ba	23	A	-	expression tag	GB 15011465
Ba	24	A	-	expression tag	GB 15011465

- Molecule 50 is a RNA chain called SSU rRNA_2.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	Bb	1385	Total	C	H	N	O	P	0	0
			44233	13212	14779	5192	9665	1385		

- Molecule 51 is a protein called Ymf73.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	Bc	159	Total	C	H	N	O	S	0	0
			2838	925	1465	217	224	7		

- Molecule 52 is a protein called Ymf64.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	Bd	330	Total	C	H	N	O	S	0	0
			5839	1868	3013	477	468	13		

- Molecule 53 is a protein called Ymf76.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	Be	405	Total	C	H	N	O	S	0	0
			7533	2416	3929	645	537	6		

- Molecule 54 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Bf	337	Total	C	H	N	O	S	0	0
			5491	1745	2735	483	515	13		

- Molecule 55 is a protein called Ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Bg	136	Total	C	H	N	O	S	0	0
			2204	681	1124	197	200	2		

- Molecule 56 is a protein called Ymf63.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Bh	256	Total	C	H	N	O	S	0	0
			4454	1459	2250	350	386	9		

- Molecule 57 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	Bi	626	Total	C	H	N	O	S	0	0
			10472	3325	5228	916	990	13		

- Molecule 58 is a protein called Ymf59.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Bj	152	Total	C	H	N	O	S	0	0
			2652	870	1348	217	214	3		

- Molecule 59 is a protein called Ymf61.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Bk	226	Total	C	H	N	O	S	0	0
			4012	1310	2055	325	321	1		

- Molecule 60 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	Bl	129	Total	C	H	N	O	S	0	0
			2199	656	1154	226	159	4		

- Molecule 61 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	Bm	224	Total	C	H	N	O	S	0	0
			3877	1268	1946	328	330	5		

- Molecule 62 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	Bn	101	Total	C	H	N	O	S	0	0
			1804	565	939	161	134	5		

- Molecule 63 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	Bo	179	Total	C	H	N	O	S	0	0
			3003	944	1515	273	264	7		

- Molecule 64 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	Bp	412	Total	C	H	N	O	S	0	0
			6956	2214	3499	611	624	8		

- Molecule 65 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	Bq	176	Total	C	H	N	O	S	0	0
			2959	927	1505	257	265	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bq	181	VAL	-	expression tag	UNP I7M6C7
Bq	182	ALA	-	expression tag	UNP I7M6C7
Bq	183	ALA	-	expression tag	UNP I7M6C7

- Molecule 66 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	Br	523	Total	C	H	N	O	S	0	0
			8589	2689	4310	755	829	6		

- Molecule 67 is a protein called Ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	Bs	87	Total	C	H	N	O	S	0	0
			1508	479	786	123	118	2		

- Molecule 68 is a protein called bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	Bt	102	Total	C	H	N	O	S	0	0
			1760	555	891	169	141	4		

- Molecule 69 is a protein called mS23.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	Bu	559	Total	C	H	N	O	S	0	0
			7883	2656	3630	777	804	16		

- Molecule 70 is a protein called mS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	Bv	465	Total	C	H	N	O	S	0	0
			7896	2484	3977	686	736	13		

- Molecule 71 is a protein called Ribosomal death-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	Bw	662	Total	C	H	N	O	S	0	0
			10999	3589	5447	937	1004	22		

- Molecule 72 is a protein called mS31.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	Bx	530	Total	C	H	N	O	S	0	0
			8568	2781	4175	731	865	16		

- Molecule 73 is a protein called mS33.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	By	107	Total	C	H	N	O	S	0	0
			1772	556	903	155	152	6		

- Molecule 74 is a protein called mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	Bz	123	Total	C	H	N	O		0	0
			1999	644	1000	176	179			

- Molecule 75 is a protein called Ribosomal subunit protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	BA	138	Total	C	H	N	O	S	0	0
			2335	743	1167	205	212	8		

- Molecule 76 is a protein called mS37.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	BB	110	Total	C	H	N	O	S	0	0
			1864	596	930	167	165	6		

- Molecule 77 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	BC	37	Total	C	H	N	O	0	0
			226	111	41	37	37		

- Molecule 78 is a protein called IGR motif protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	BD	107	Total	C	H	N	O	S	0	0
			1791	569	908	152	158	4		

- Molecule 79 is a protein called mS45.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	BE	447	Total	C	H	N	O	S	0	0
			7339	2342	3615	630	739	13		

- Molecule 80 is a protein called mS75.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	BF	23	Total	C	H	N	O	0	0
			147	69	32	23	23		

- Molecule 81 is a protein called mS76.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	BG	164	Total	C	H	N	O	S	0	0
			2704	863	1329	237	270	5		

- Molecule 82 is a protein called mS77.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	BH	63	Total	C	H	N	O	0	0
			382	189	67	63	63		

- Molecule 83 is a protein called Enoyl-CoA hydratase/isomerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	BI	1413	Total	C	H	N	O	S	0	0
			23519	7509	11719	1995	2263	33		

- Molecule 84 is a protein called mS78.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	BJ	1515	Total	C	H	N	O	S	0	0
			24865	7913	12419	2110	2396	27		

- Molecule 85 is a protein called mS79.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	BK	267	Total	C	H	N	O	S	0	0
			4236	1356	2106	366	401	7		

- Molecule 86 is a protein called SelR domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	BL	181	Total	C	H	N	O	S	0	0
			2962	954	1461	267	272	8		

- Molecule 87 is a protein called mS81.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	BM	284	Total	C	H	N	O	S	0	0
			4692	1522	2321	404	436	9		

- Molecule 88 is a protein called mS82.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	BN	274	Total	C	H	N	O	S	0	0
			4557	1481	2253	389	424	10		

- Molecule 89 is a protein called PARP alpha-helical domain-containing protein,mS83.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	BO	142	Total	C	H	N	O	S	0	0
			1225	511	397	151	164	2		

- Molecule 90 is a protein called mS84,mS84.

Mol	Chain	Residues	Atoms						AltConf	Trace
90	BP	100	Total	C	H	N	O		0	0
			1259	428	567	127	137			

- Molecule 91 is a protein called mS85.

Mol	Chain	Residues	Atoms						AltConf	Trace
91	BQ	622	Total	C	H	N	O	S	0	0
			10266	3281	5095	853	1025	12		

- Molecule 92 is a protein called Iron donor protein CyaY.

Mol	Chain	Residues	Atoms						AltConf	Trace
92	BR	143	Total	C	H	N	O	S	0	0
			2361	746	1179	210	223	3		

- Molecule 93 is a protein called mS87.

Mol	Chain	Residues	Atoms						AltConf	Trace
93	BS	433	Total	C	H	N	O	S	0	0
			7221	2298	3602	611	697	13		

- Molecule 94 is a protein called mS88.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	BT	297	Total	C	H	N	O		
			1815	891	330	297	297	0	0

- Molecule 95 is a protein called mS89.

Mol	Chain	Residues	Atoms						AltConf	Trace
95	BU	309	Total	C	H	N	O	S	0	0
			5164	1667	2568	441	481	7		

- Molecule 96 is a protein called mS90.

Mol	Chain	Residues	Atoms						AltConf	Trace
96	BV	310	Total	C	H	N	O	S	0	0
			4185	1427	1924	405	426	3		

- Molecule 97 is a protein called mS91.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	BW	285	Total	C	H	N	O		
			1731	855	306	285	285	0	0

- Molecule 98 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
98	BX	133	Total	C	H	N	O	S	0	0
			2351	776	1195	190	182	8		

- Molecule 99 is a protein called mS93.

Mol	Chain	Residues	Atoms						AltConf	Trace
99	BY	327	Total	C	H	N	O	S	0	0
			5119	1667	2528	446	472	6		

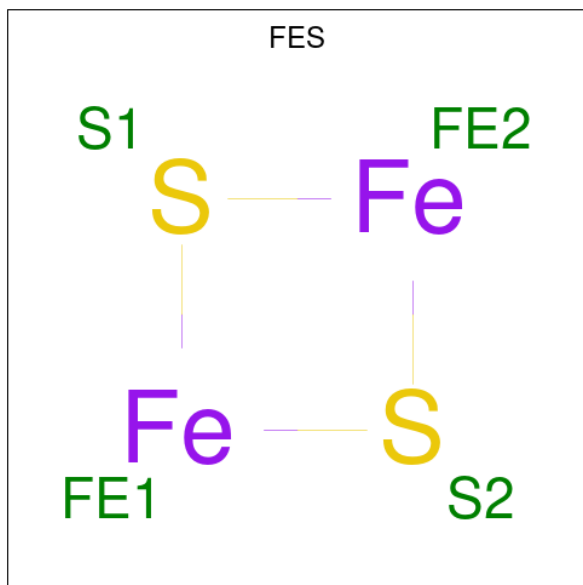
- Molecule 100 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
100	Aa	28	Total	Mg	0
			28	28	
100	Ab	270	Total	Mg	0
			270	270	
100	Ad	1	Total	Mg	0
			1	1	
100	Ae	1	Total	Mg	0
			1	1	
100	Aq	1	Total	Mg	0
			1	1	
100	AB	1	Total	Mg	0
			1	1	
100	AF	1	Total	Mg	0
			1	1	
100	AQ	1	Total	Mg	0
			1	1	
100	Ba	10	Total	Mg	0
			10	10	
100	Bb	76	Total	Mg	0
			76	76	
100	Bi	1	Total	Mg	0
			1	1	
100	Bw	1	Total	Mg	0
			1	1	
100	Bz	1	Total	Mg	0
			1	1	

- Molecule 101 is ZINC ION (CCD ID: ZN) (formula: Zn).

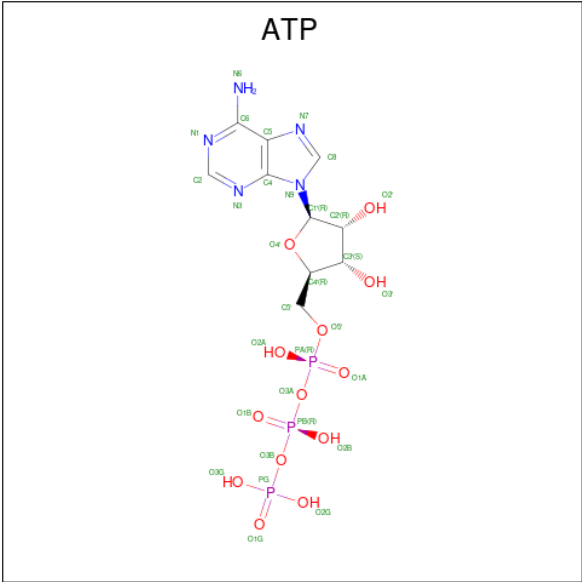
Mol	Chain	Residues	Atoms		AltConf
101	AG	1	Total	Zn	0
			1	1	
101	BL	1	Total	Zn	0
			1	1	

- Molecule 102 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
102	AV	1	Total	Fe	S	0
			4	2	2	
102	AV	1	Total	Fe	S	0
			4	2	2	

- Molecule 103 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).

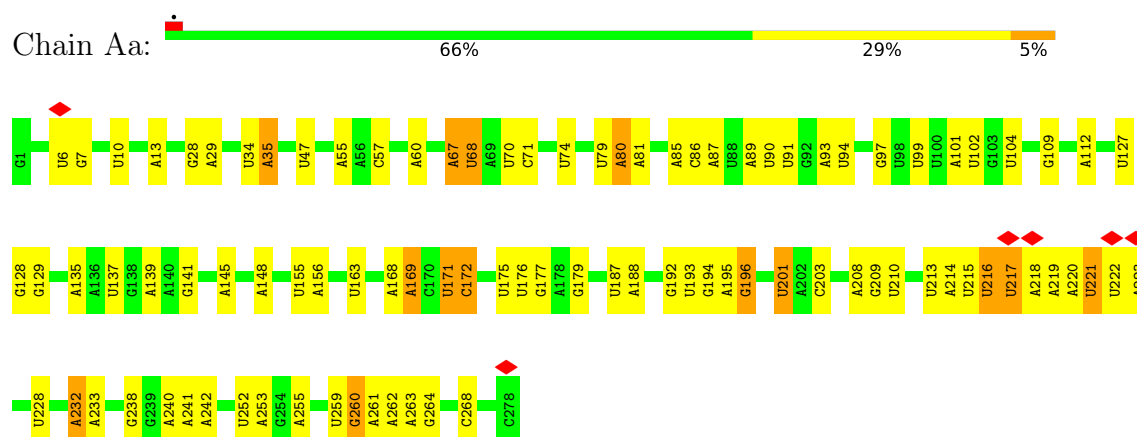


Mol	Chain	Residues	Atoms						AltConf
103	Bw	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	

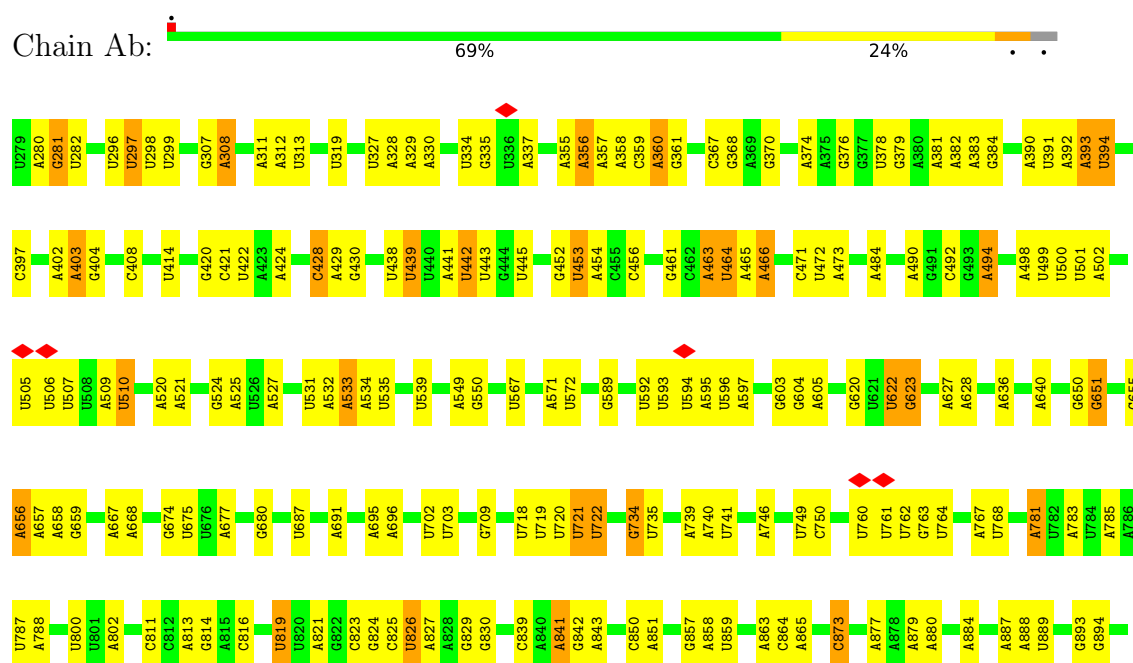
3 Residue-property plots

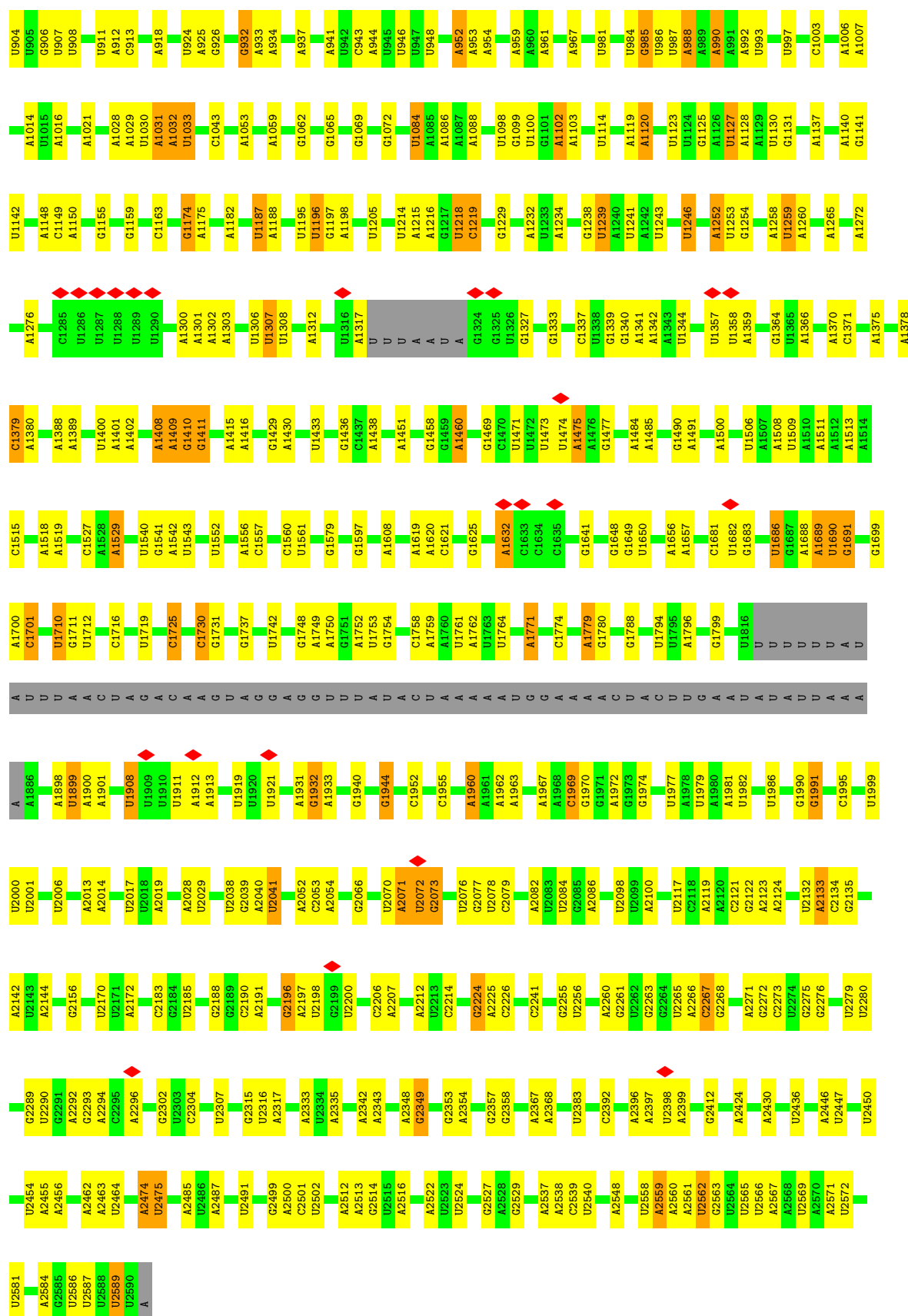
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: LSU rRNA_1



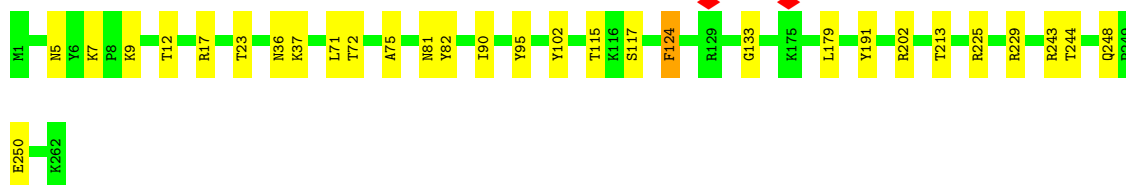
• Molecule 2: LSU rRNA_2





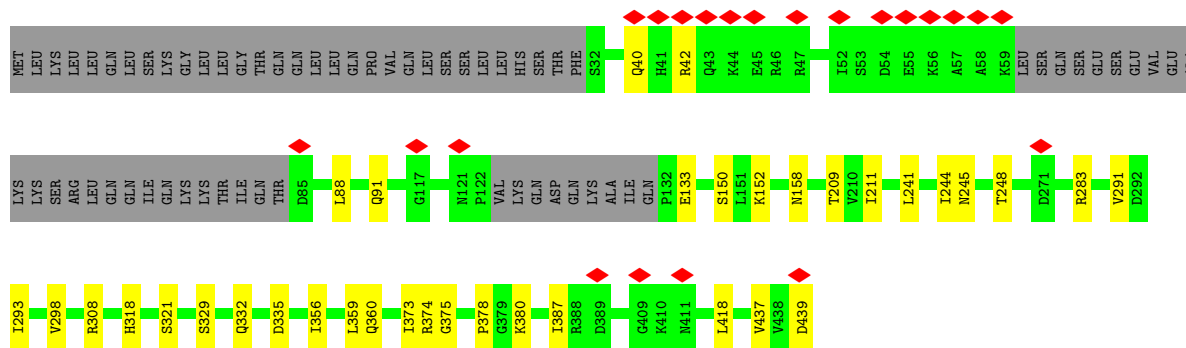
- Molecule 3: Ribosomal protein L2

Chain Ac:  89% 11%



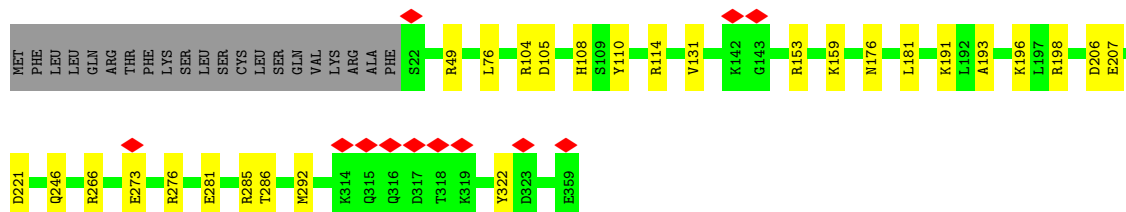
- Molecule 4: 50S ribosomal protein L3

Chain Ad:  5% 77% 8% 15%



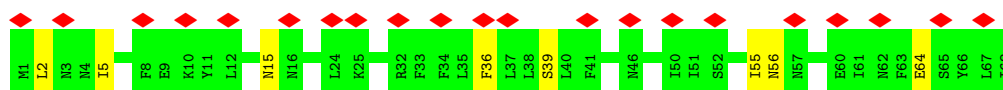
- Molecule 5: 50S ribosomal protein L4

Chain Ae:  86% 8% 6%



- Molecule 6: Ymf69

Chain Af:  31% 88% 12%

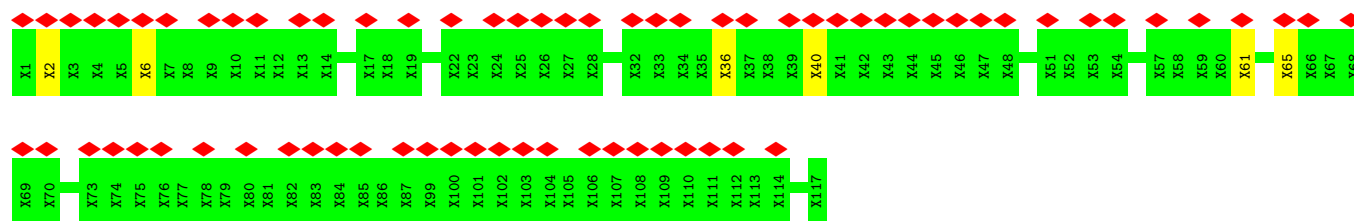


- Molecule 7: Ymf60

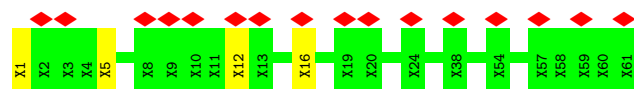
Chain Ag:  85% 13%



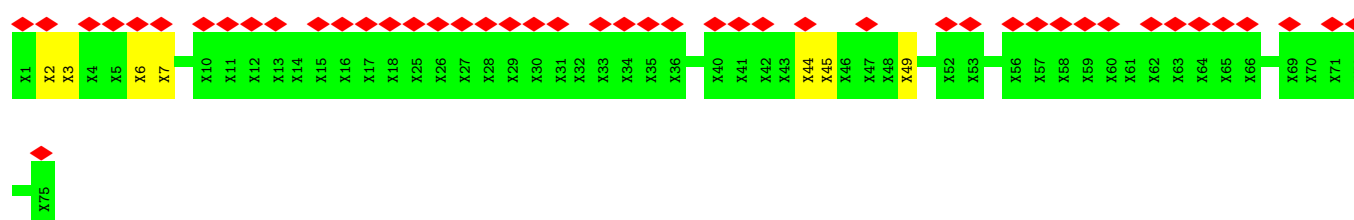
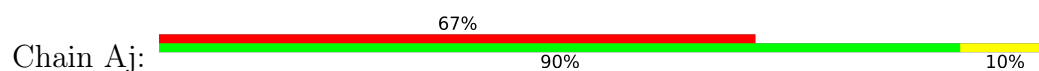
- Molecule 8: bL7/L12m



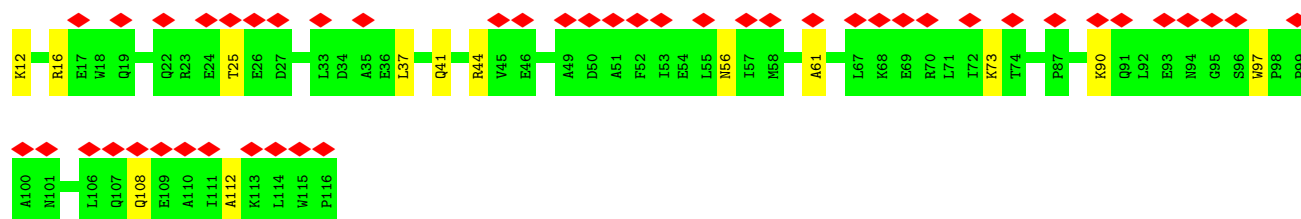
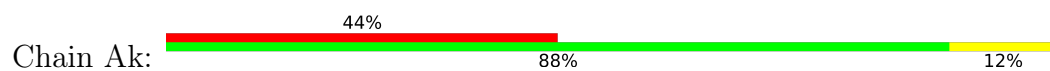
- Molecule 9: bL7/12m



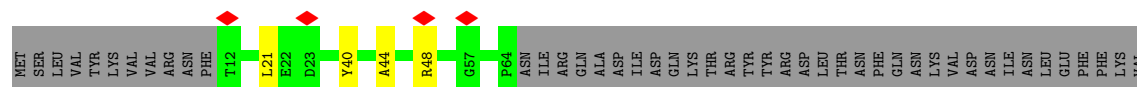
- Molecule 10: bL7/12m



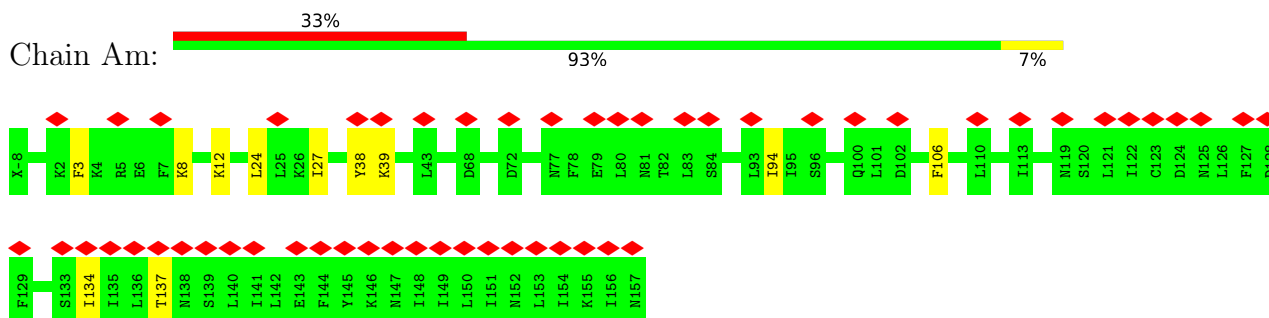
- Molecule 11: Ribosomal protein L7/L12 carboxy-terminal domain protein



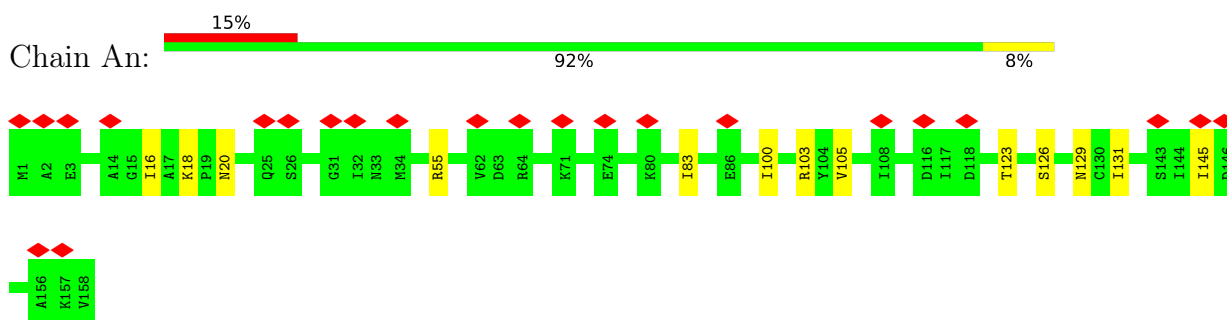
- Molecule 12: Ribosomal protein L9, amine-terminal domain protein



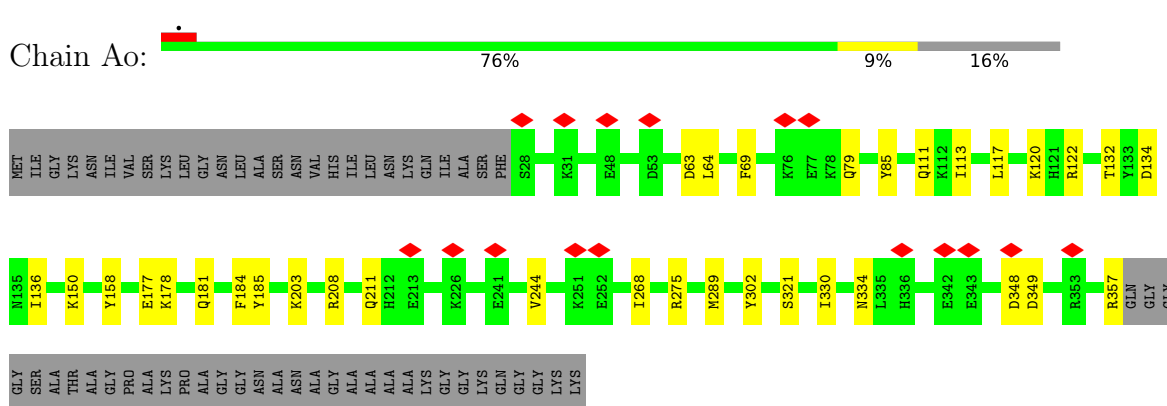
- Molecule 13: Ymf74



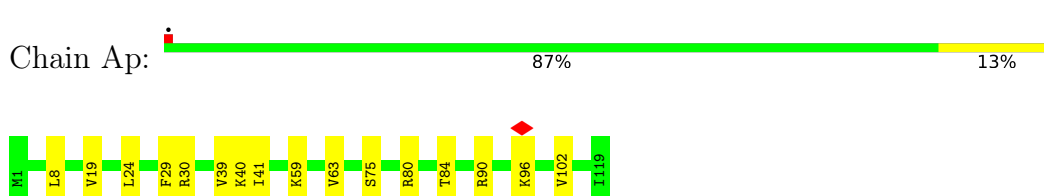
- Molecule 14: Ribosomal protein L11, amine-terminal domain protein



- Molecule 15: 50S ribosomal protein L13

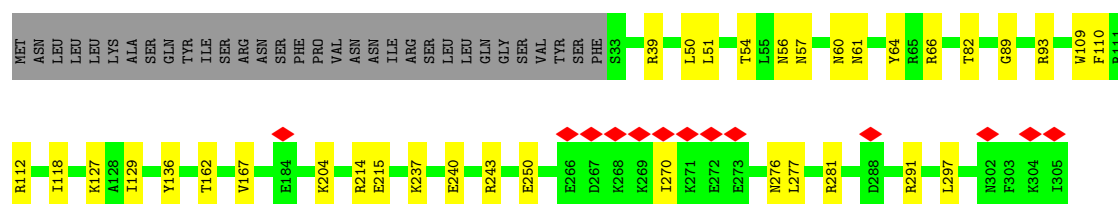


- Molecule 16: Ribosomal protein L14



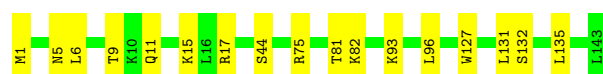
- Molecule 17: Ribosomal protein L15, putative

Chain Aq:  78% 11% 10%



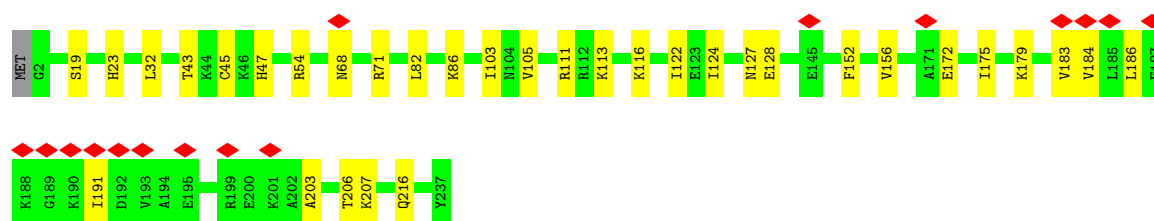
- Molecule 18: Ribosomal protein L16

Chain Ar:  88% 12%



- Molecule 19: 50S ribosomal protein L17

Chain As:  7% 86% 14%



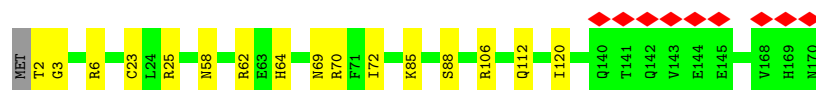
- Molecule 20: bL19m

Chain At:  72% 24%



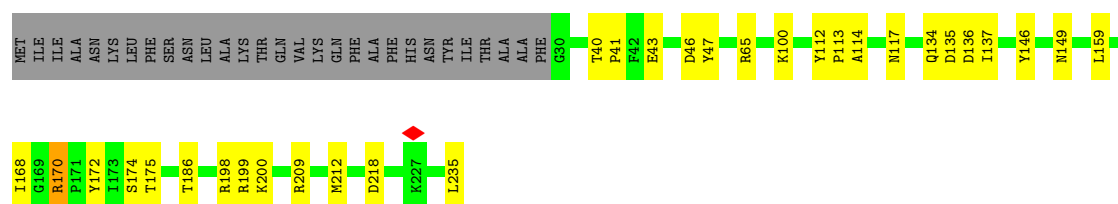
- Molecule 21: 50S ribosomal protein L20

Chain Au:  5% 90% 9%

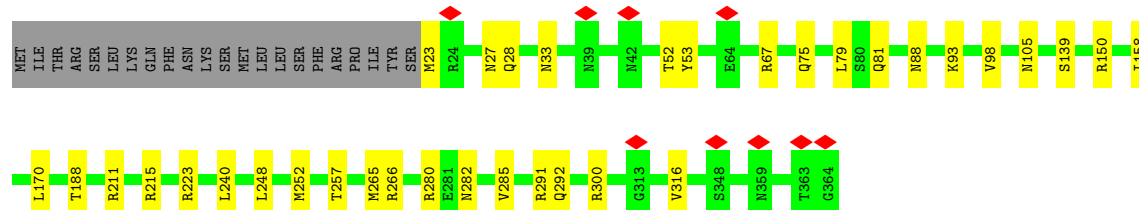
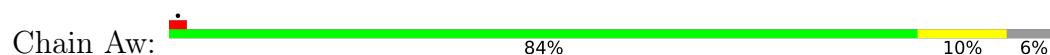


- Molecule 22: 50S ribosomal protein L21

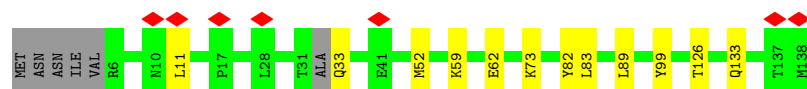
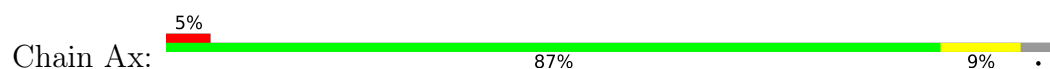
Chain Av:  74% 13% 12%



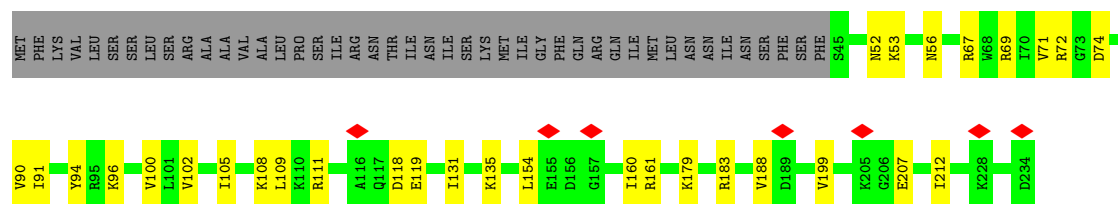
• Molecule 23: Ribosomal protein L22/L17e



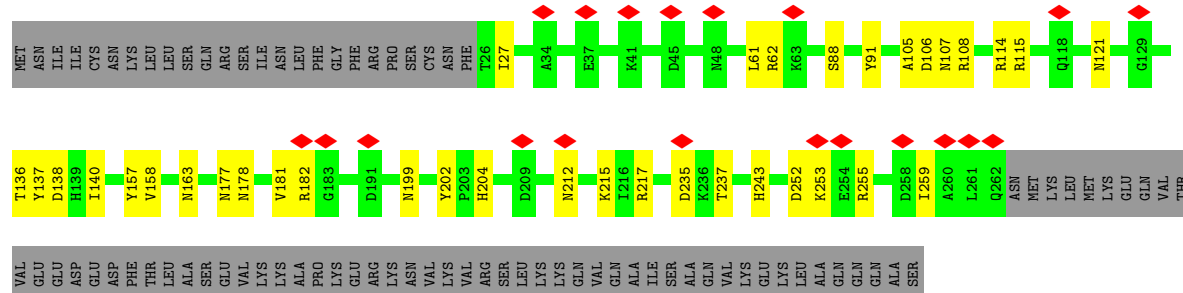
• Molecule 24: Ribosomal protein L23, putative



• Molecule 25: 50S ribosomal protein L24

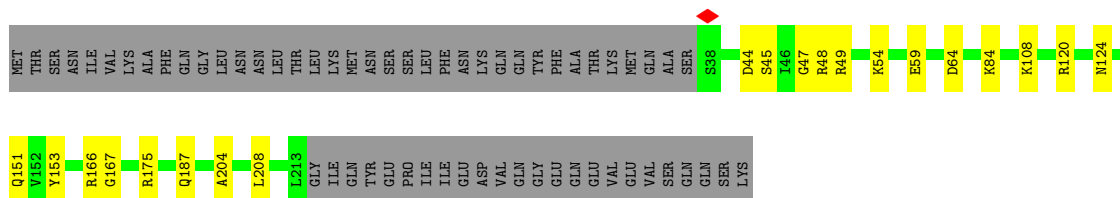


• Molecule 26: bL25m



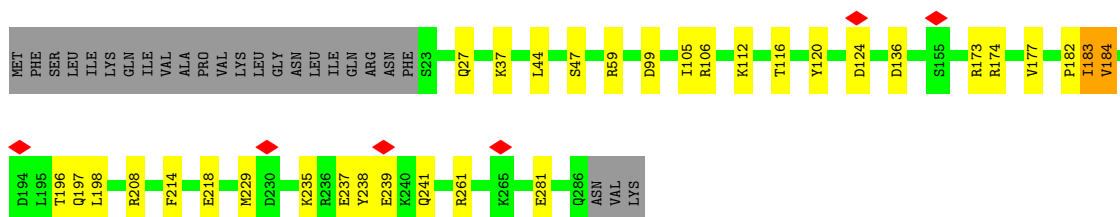
- Molecule 27: 50S ribosomal protein L27

Chain AA:  66% 8% 26%



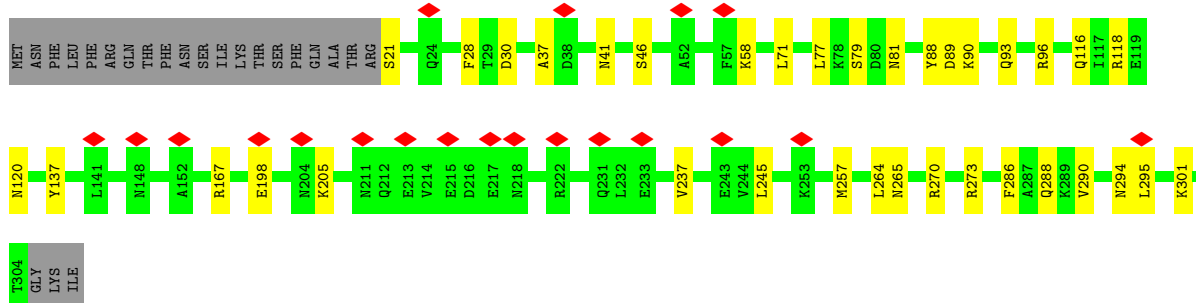
- Molecule 28: Ribosomal protein L28

Chain AB:  80% 11% 9%

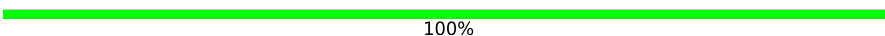


- Molecule 29: 39-S ribosomal protein L47

Chain AC:  7% 81% 12% 7%



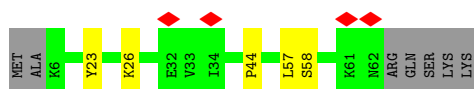
- Molecule 30: bL32m

Chain AD:  100%

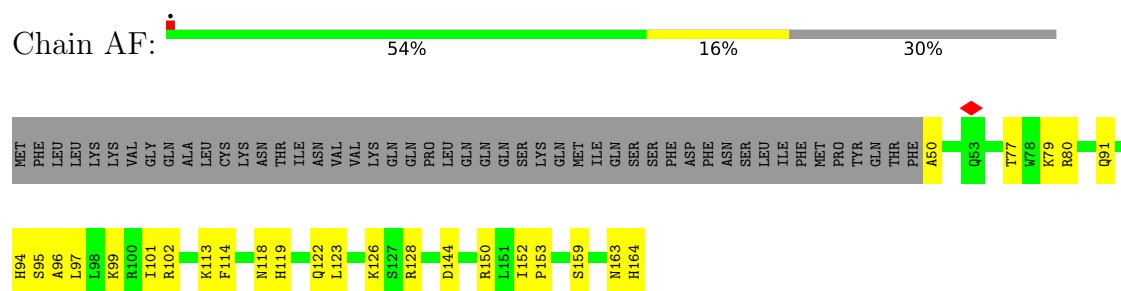
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L33

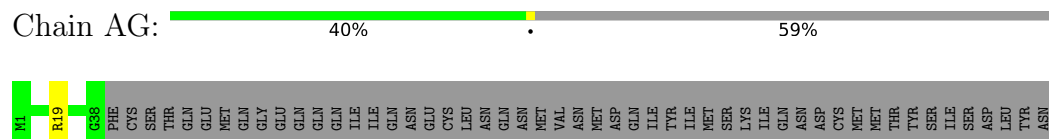
Chain AE:  6% 81% 8% 11%



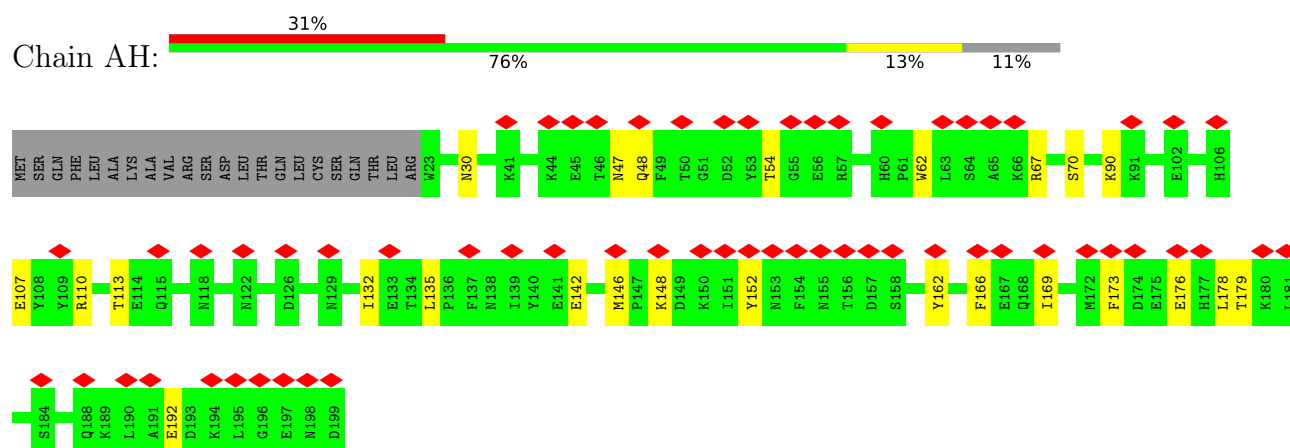
- Molecule 32: bL35m



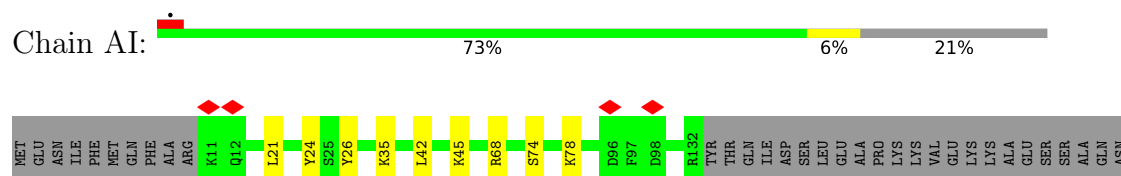
- Molecule 33: Ribosomal protein



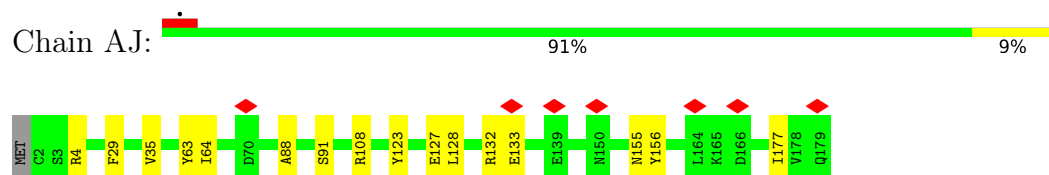
- Molecule 34: mL40



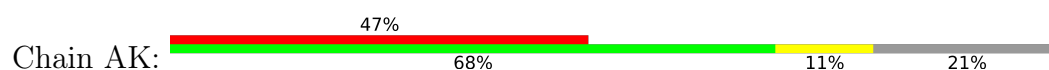
- Molecule 35: Ribosomal protein L27

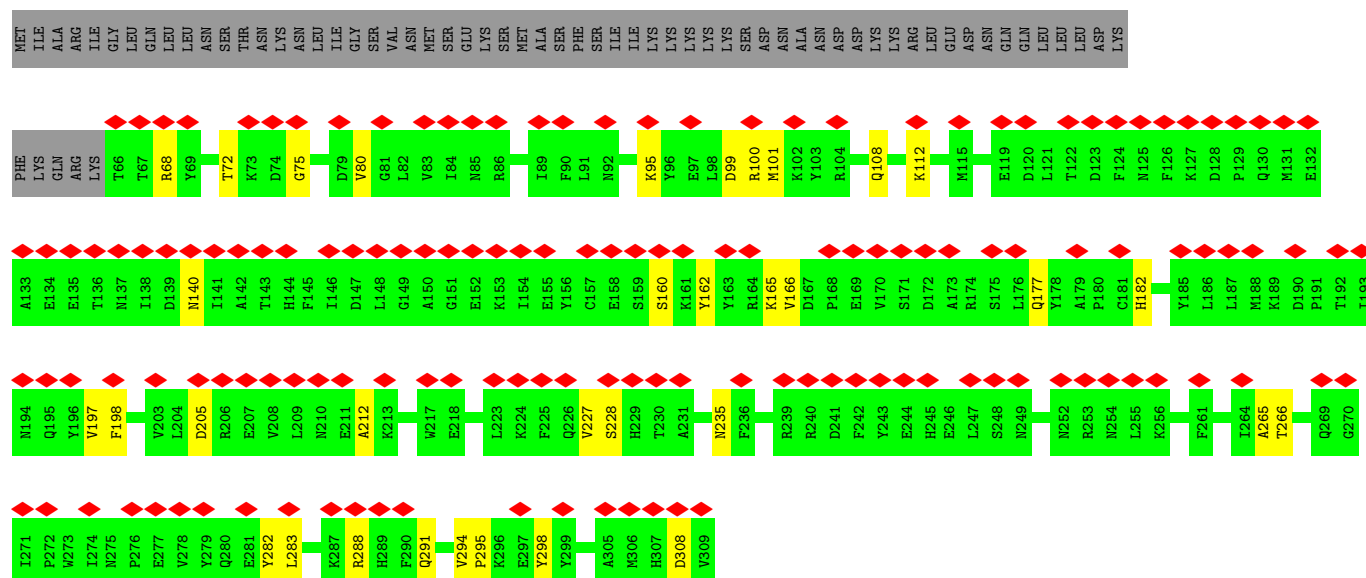


- Molecule 36: Ribosomal protein L51/S25/CI-B8 domain protein



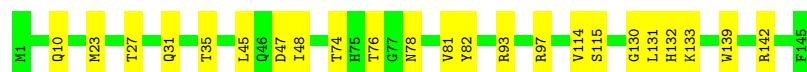
- Molecule 37: mL46





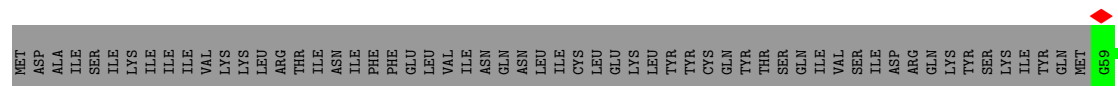
• Molecule 38: Large subunit ribosomal protein

Chain AL: 84% 16%



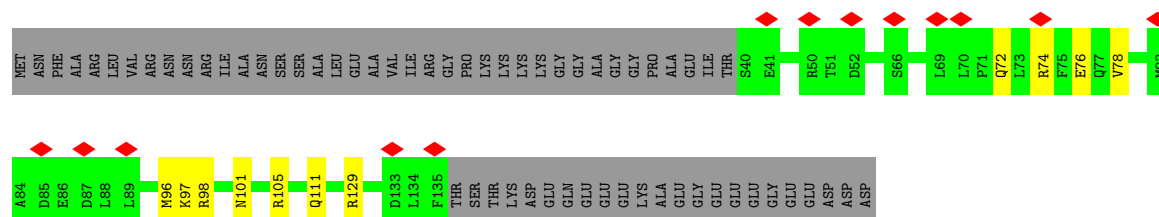
• Molecule 39: mL53

Chain AM: 60% 8% 32%



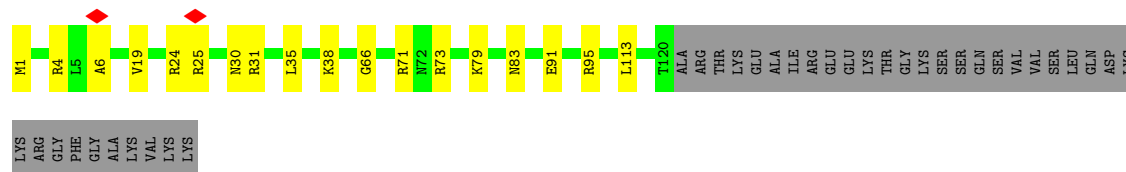
• Molecule 40: mL54

Chain AN: 8% 54% 7% 39%

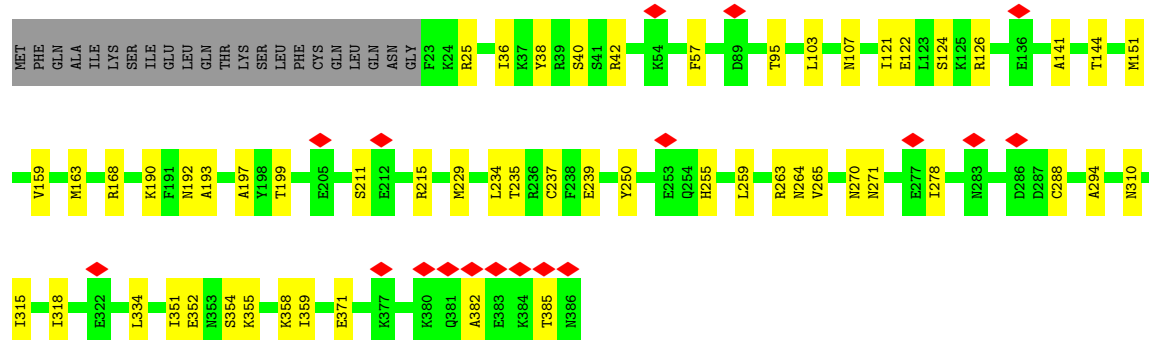
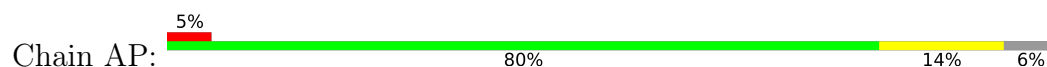


• Molecule 41: mL64

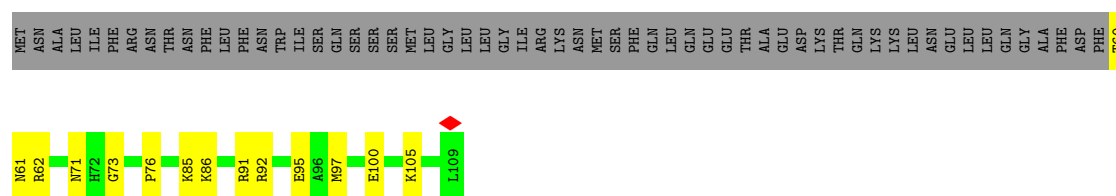
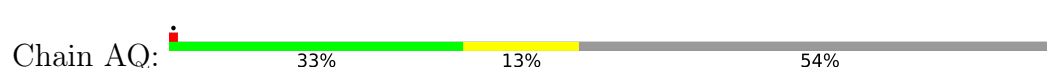
Chain AO: 66% 12% 23%



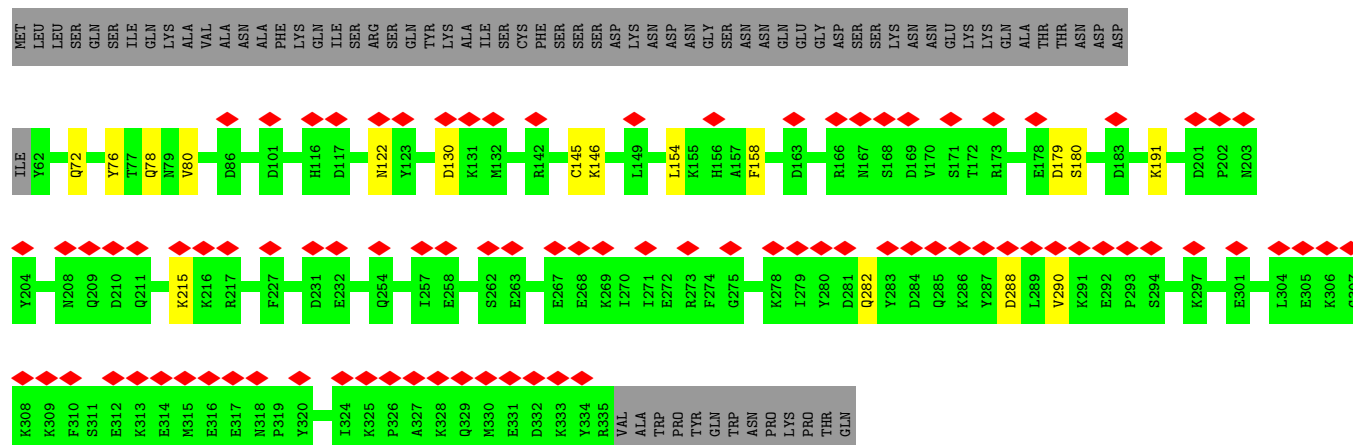
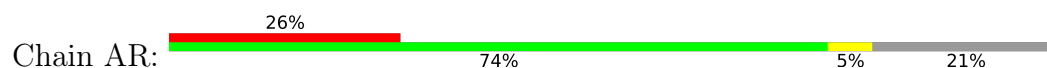
• Molecule 42: mL101



• Molecule 43: mL102

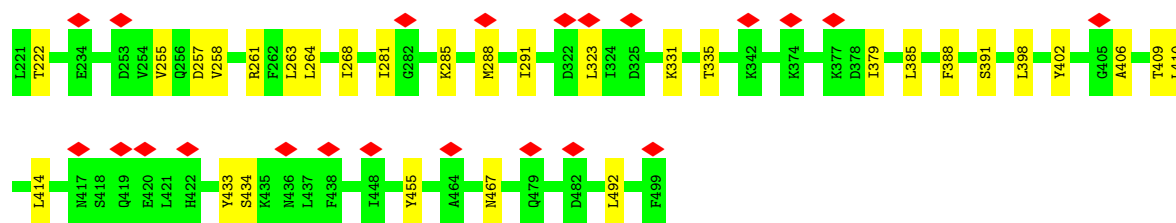


• Molecule 44: mL103

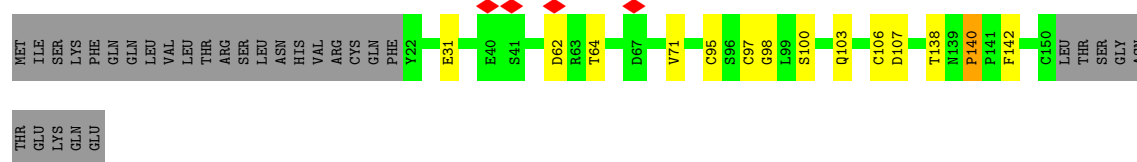
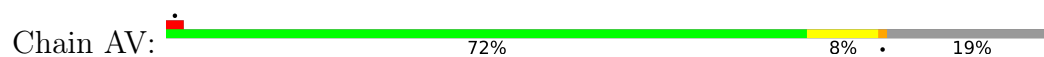


• Molecule 45: mL104





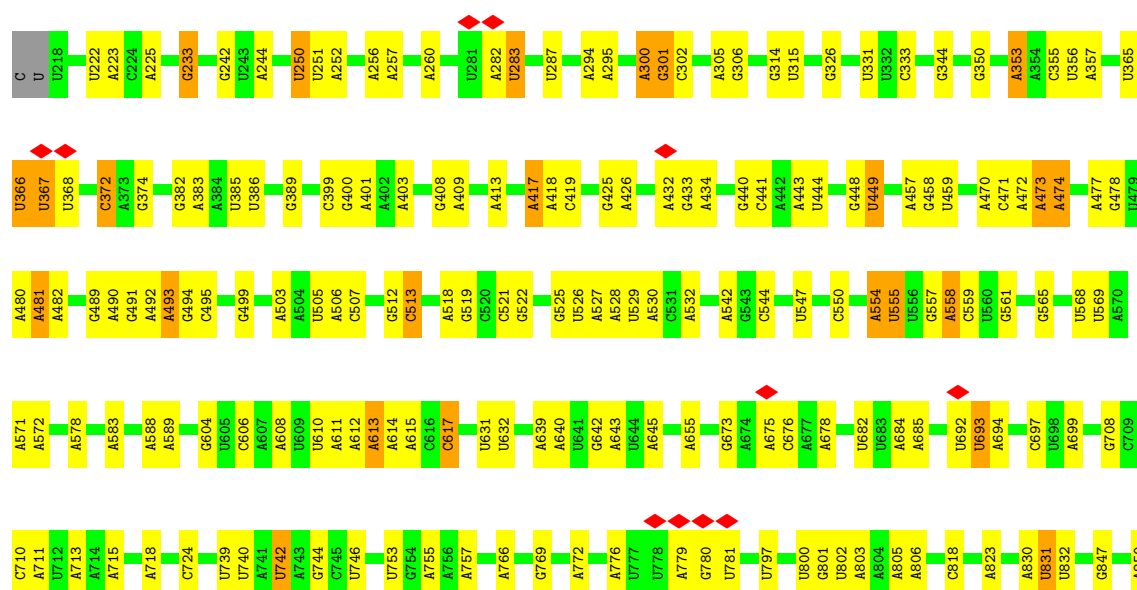
- Molecule 48: Iron-binding zinc finger CDGSH type protein

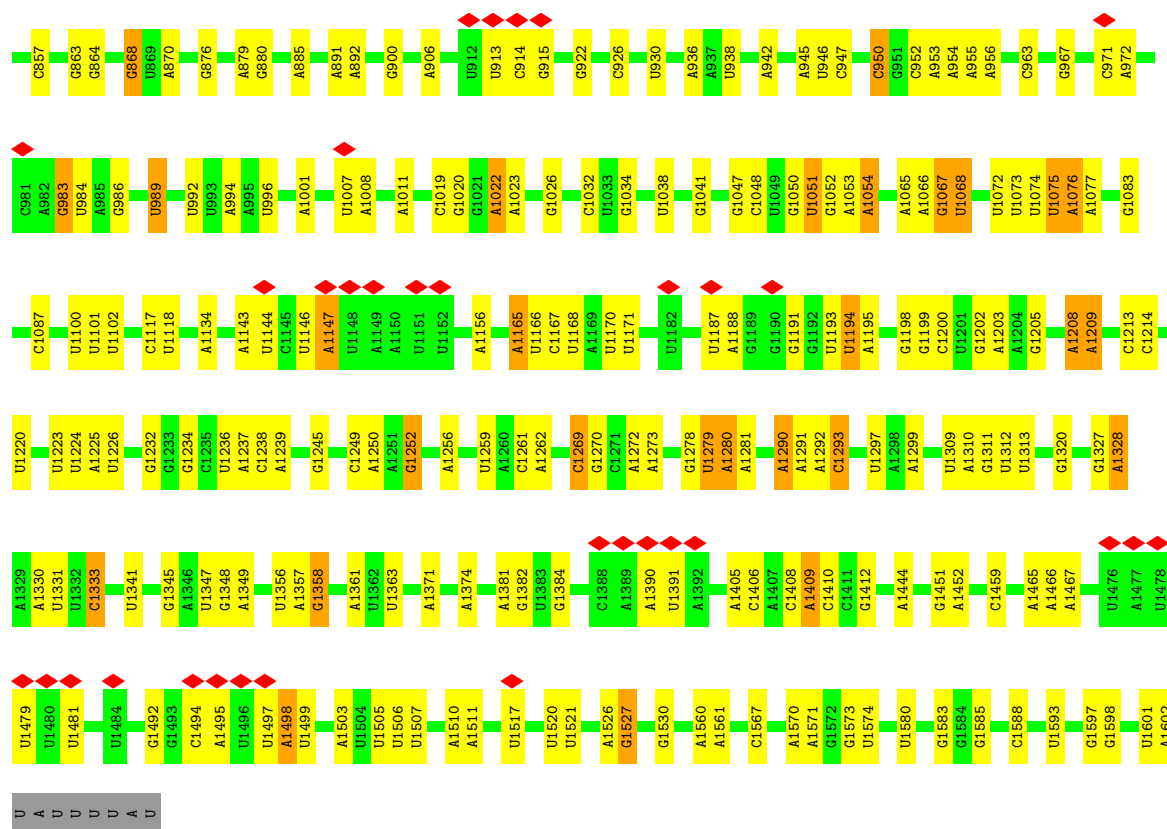


- Molecule 49: SSU rRNA_1

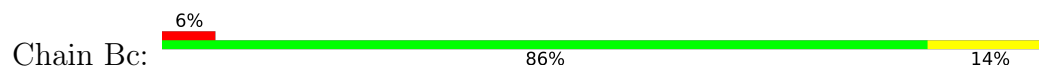


- Molecule 50: SSU rRNA_2

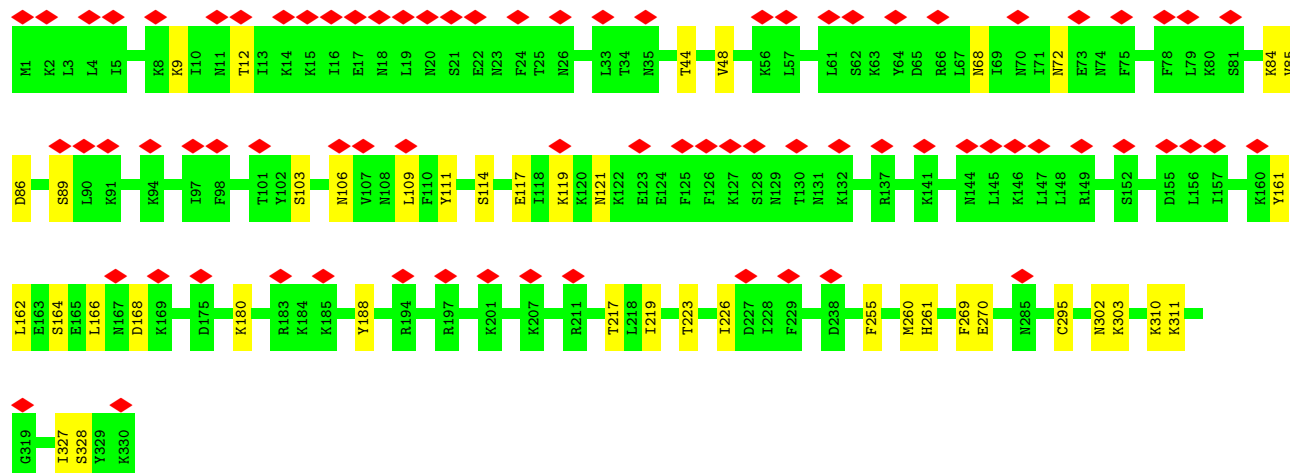
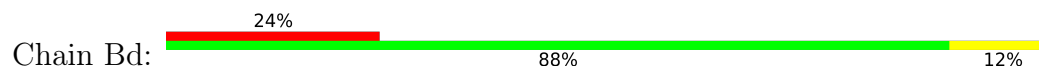




• Molecule 51: Ymf73

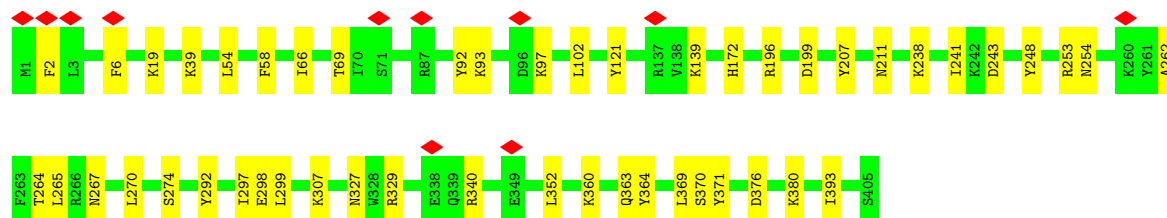


• Molecule 52: Ymf64



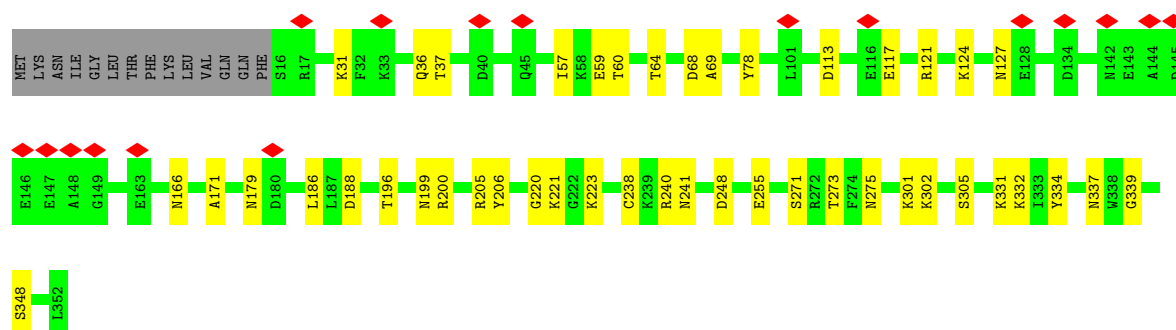
- Molecule 53: Ymf76

Chain Be:  88% 12%



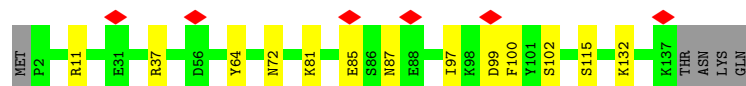
- Molecule 54: 30S ribosomal protein S5

Chain Bf:  5% 83% 13%



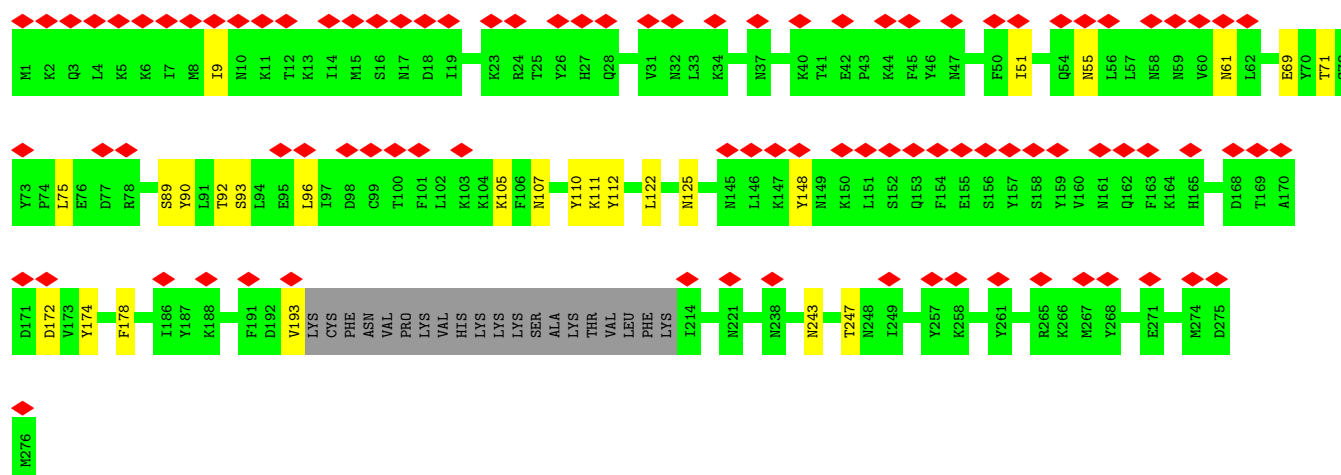
- Molecule 55: Ribosomal protein S6

Chain Bg:  87% 9%

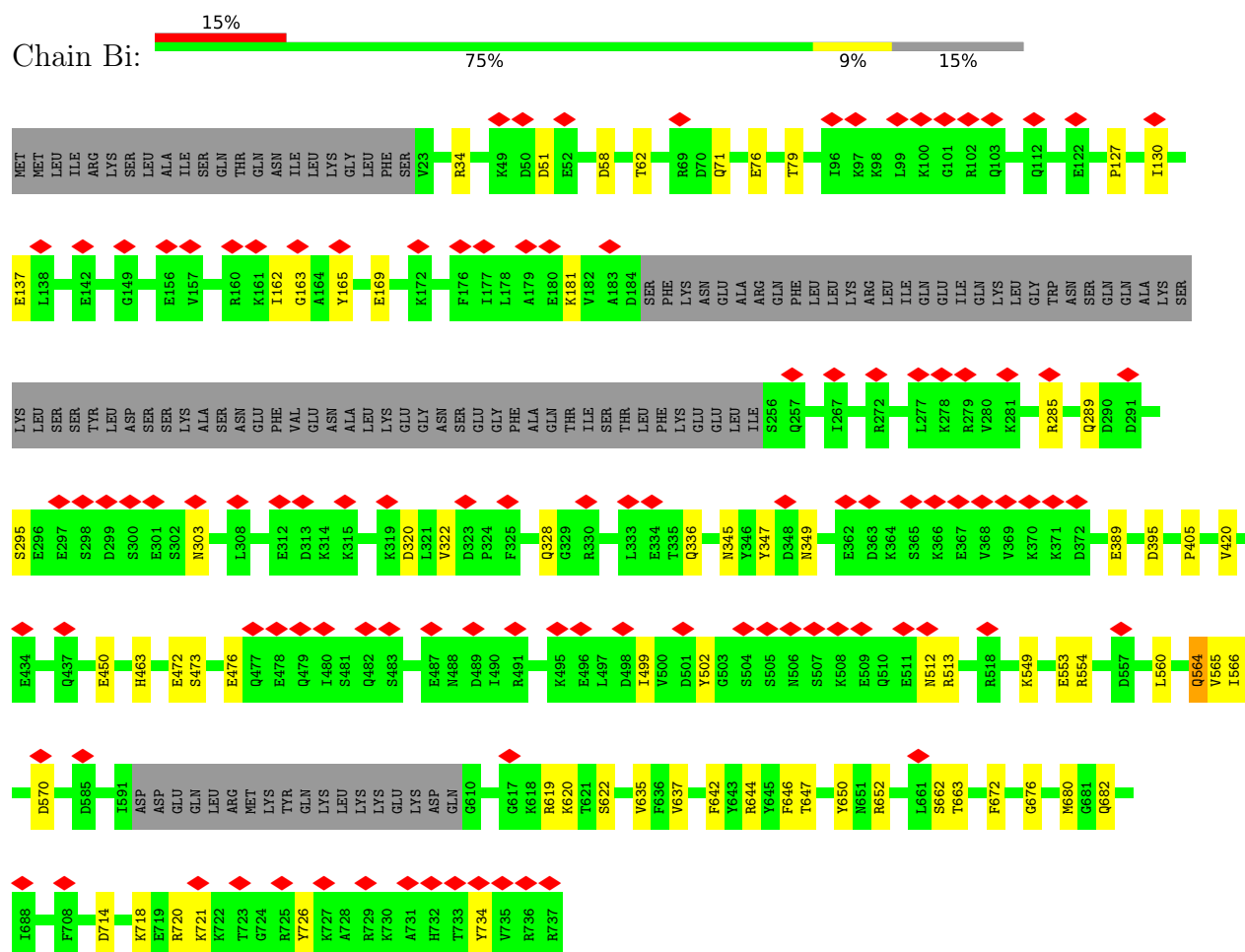


- Molecule 56: Ymf63

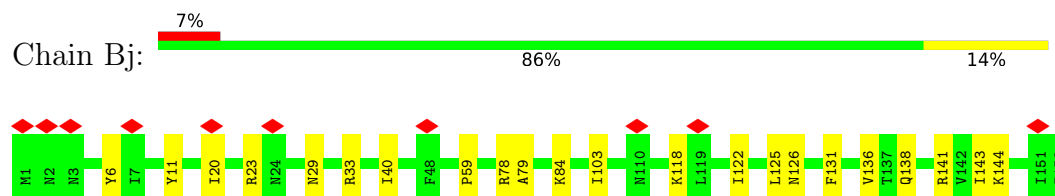
Chain Bh:  34% 83% 9% 7%



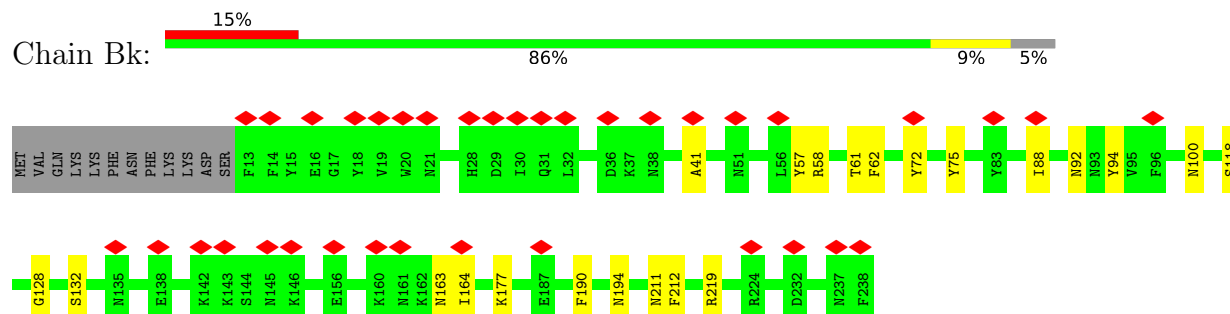
- Molecule 57: Ribosomal protein S9



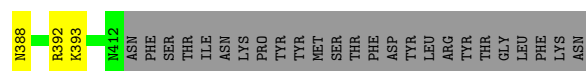
- Molecule 58: Ymf59



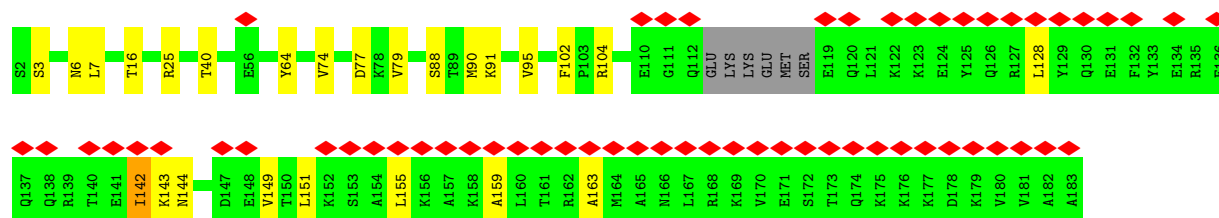
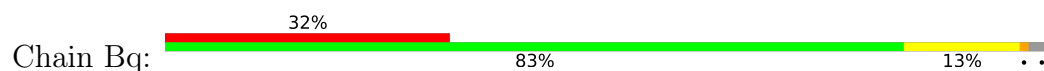
- Molecule 59: Ymf61



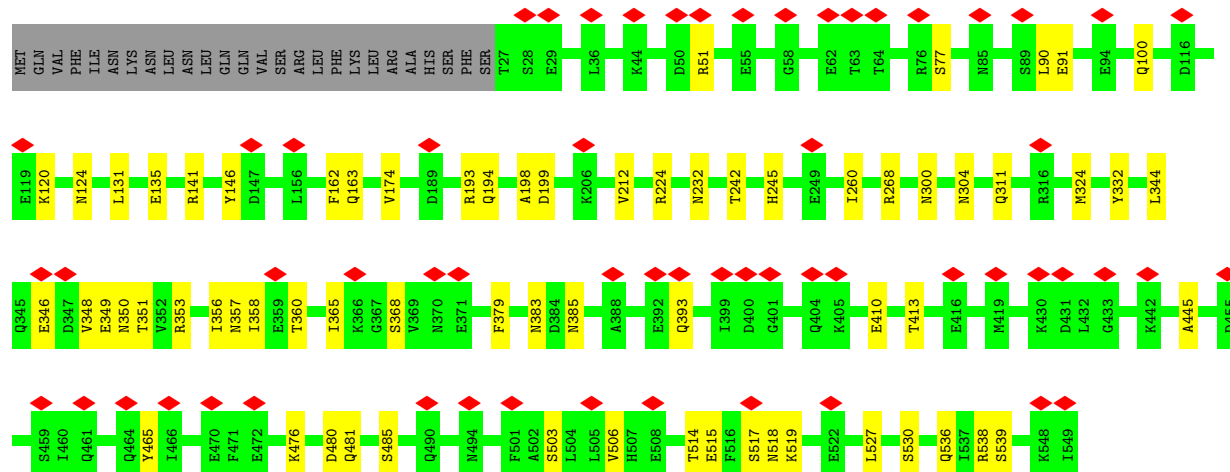
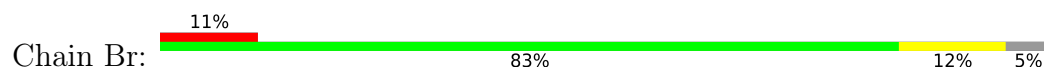
- Molecule 60: Ribosomal protein S12



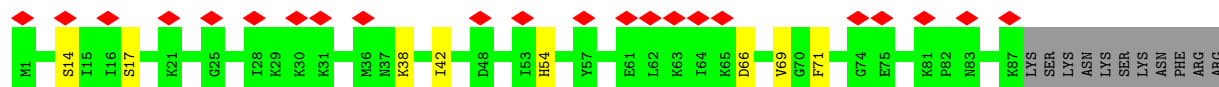
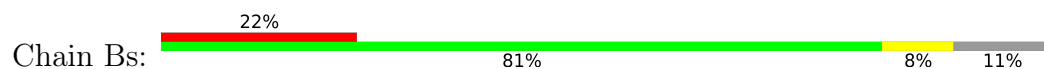
- Molecule 65: 30S ribosomal protein S17



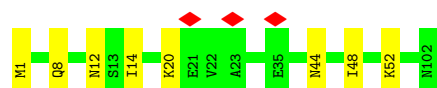
- Molecule 66: Ribosomal protein S18



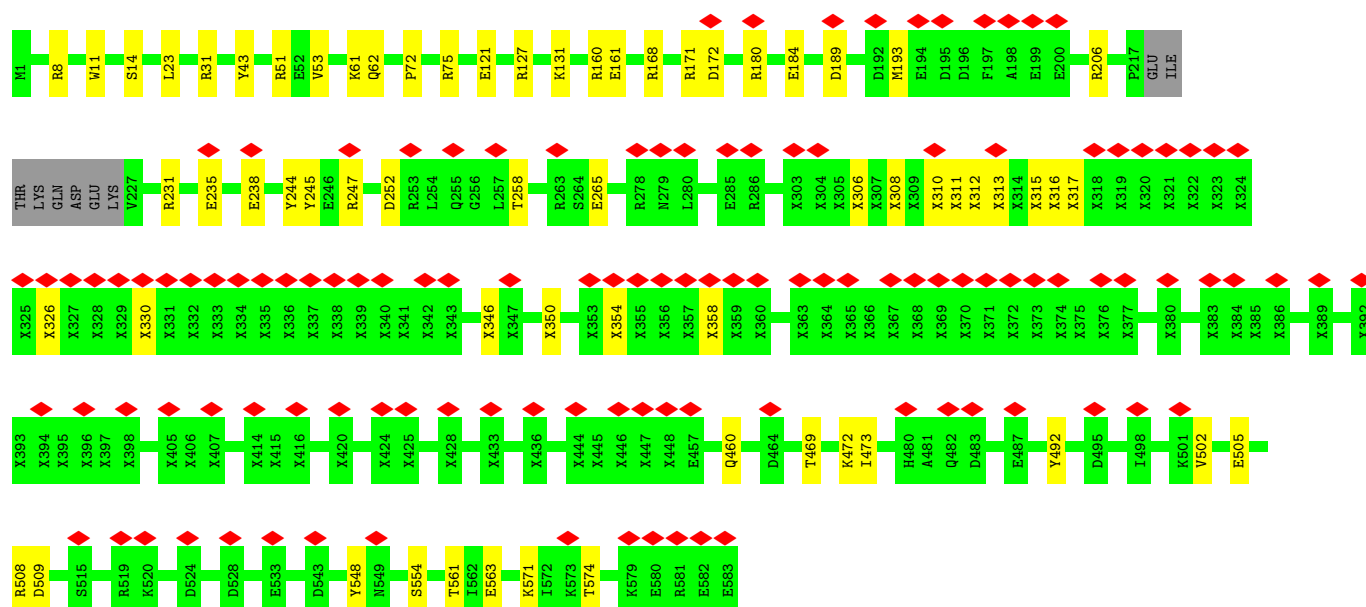
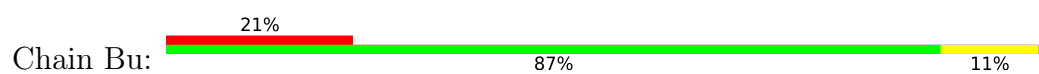
- Molecule 67: Ribosomal protein S19



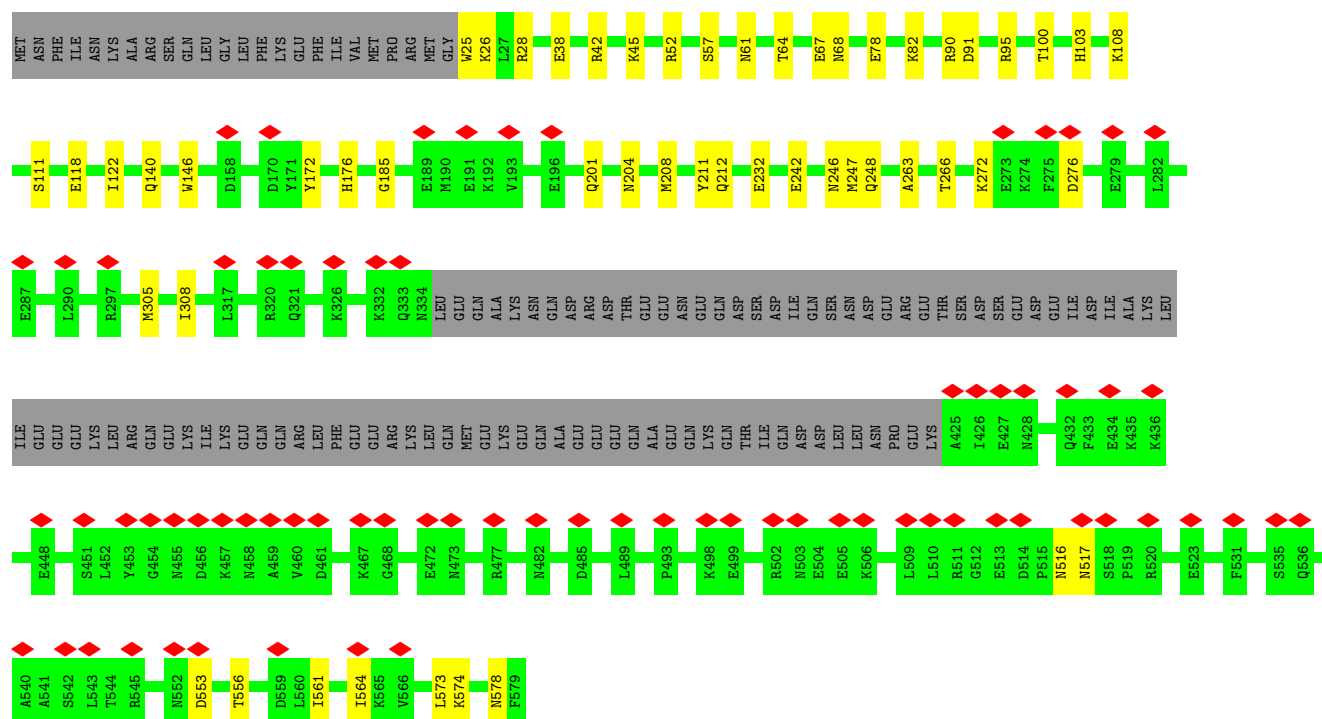
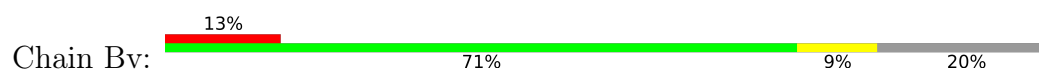
- Molecule 68: bS21m



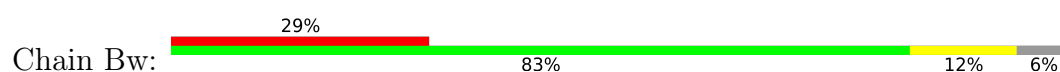
- Molecule 69: mS23

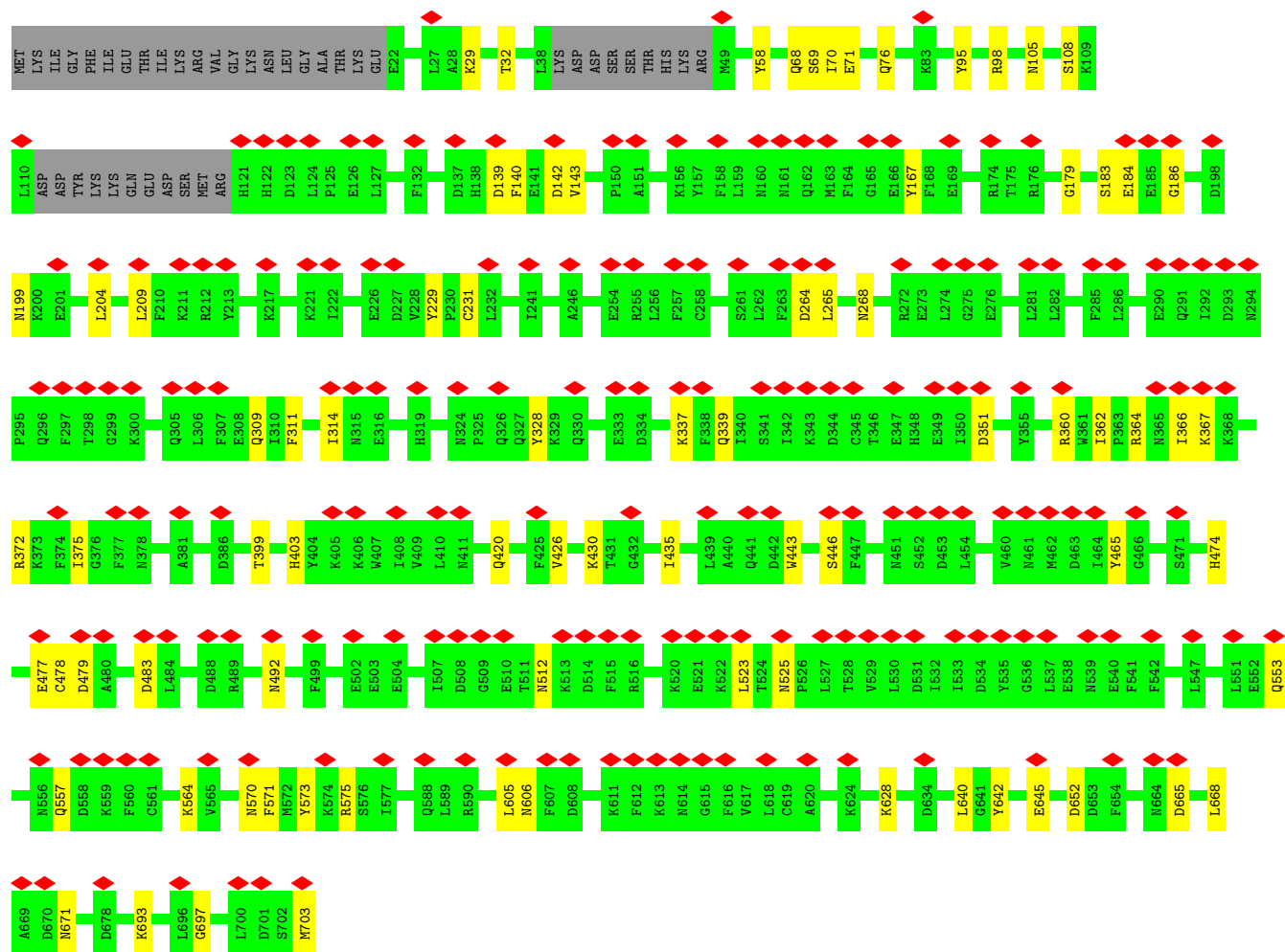


• Molecule 70: mS26

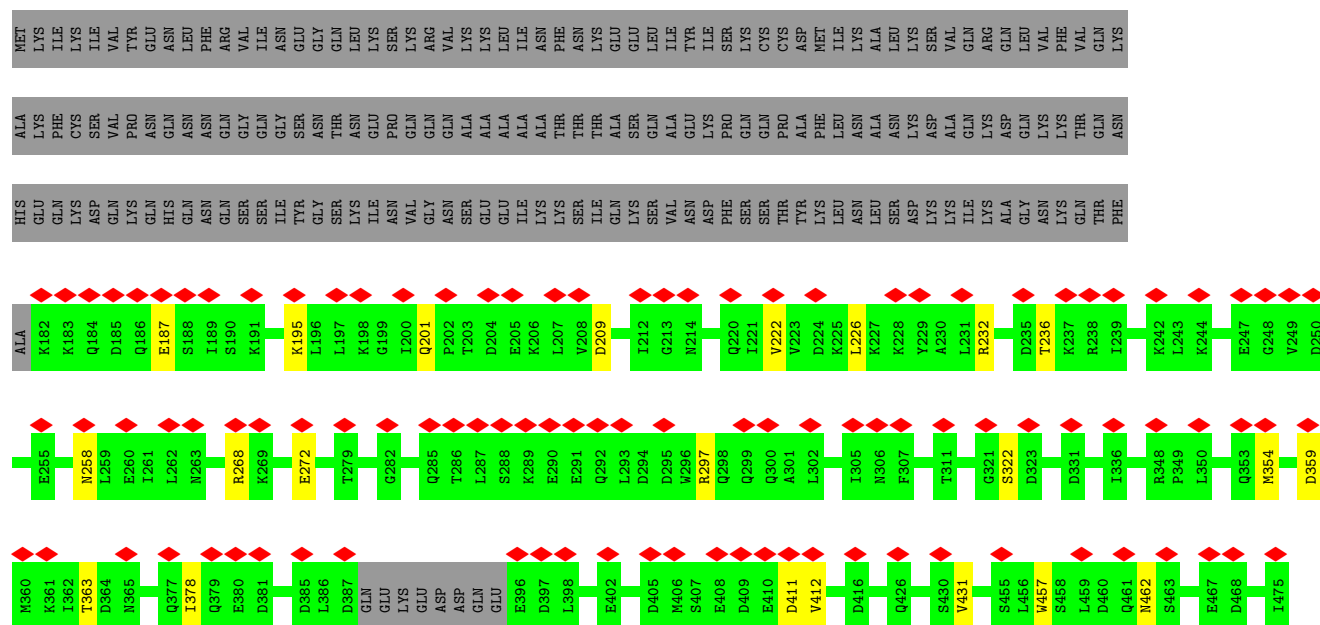


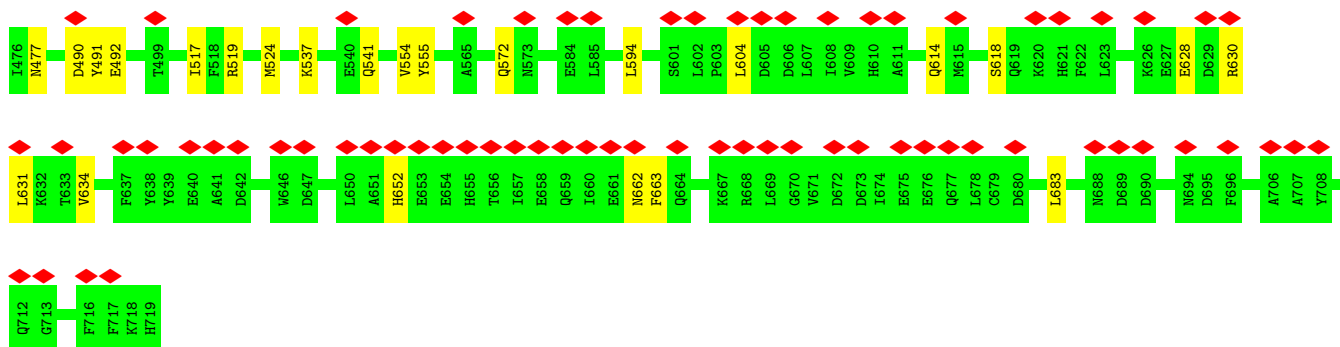
• Molecule 71: Ribosomal death-associated protein



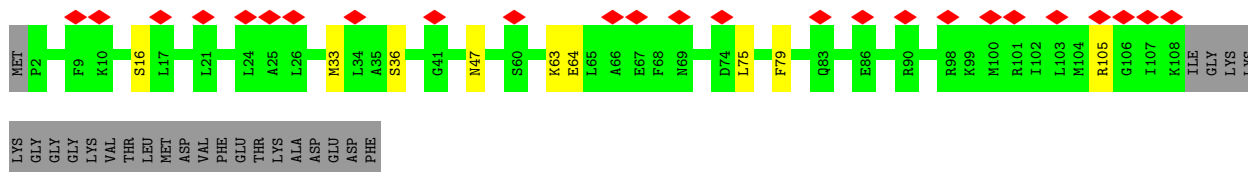
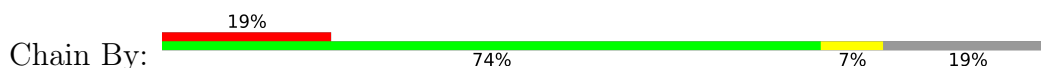


• Molecule 72: mS31

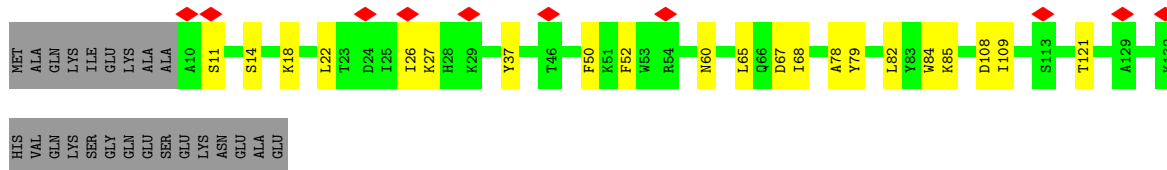




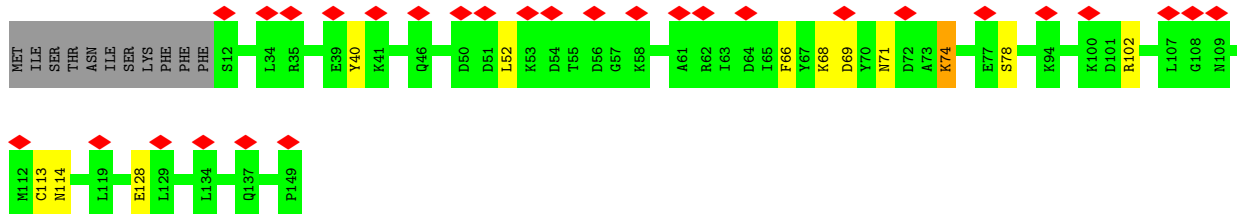
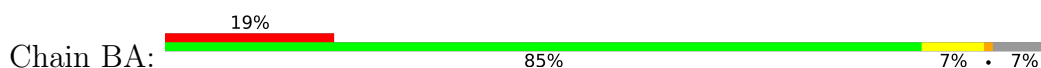
• Molecule 73: mS33



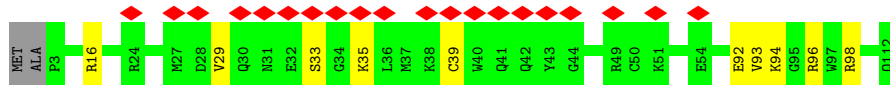
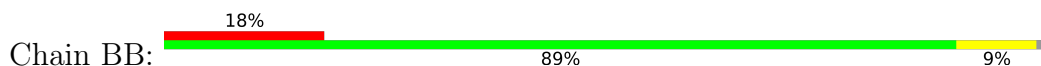
• Molecule 74: mS34



• Molecule 75: Ribosomal subunit protein



• Molecule 76: mS37



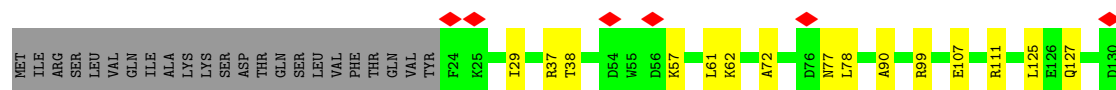
• Molecule 77: mS38

Chain BC:  100%

There are no outlier residues recorded for this chain.

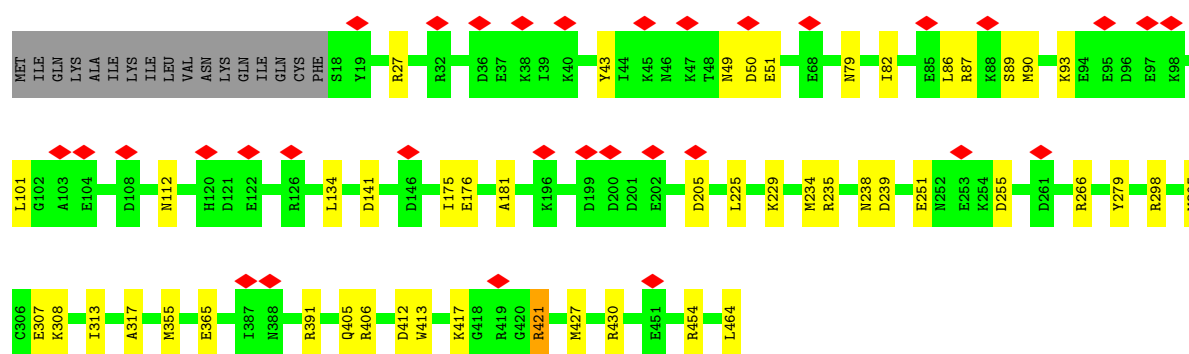
- Molecule 78: IGR motif protein

Chain BD:  5% 71% 12% 18%



- Molecule 79: mS45

Chain BE:  7% 86% 10%



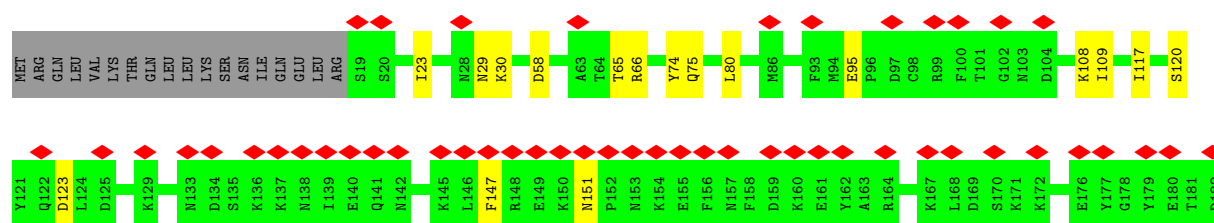
- Molecule 80: mS75

Chain BF:  96%



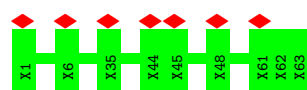
- Molecule 81: mS76

Chain BG:  27% 81% 9% 10%



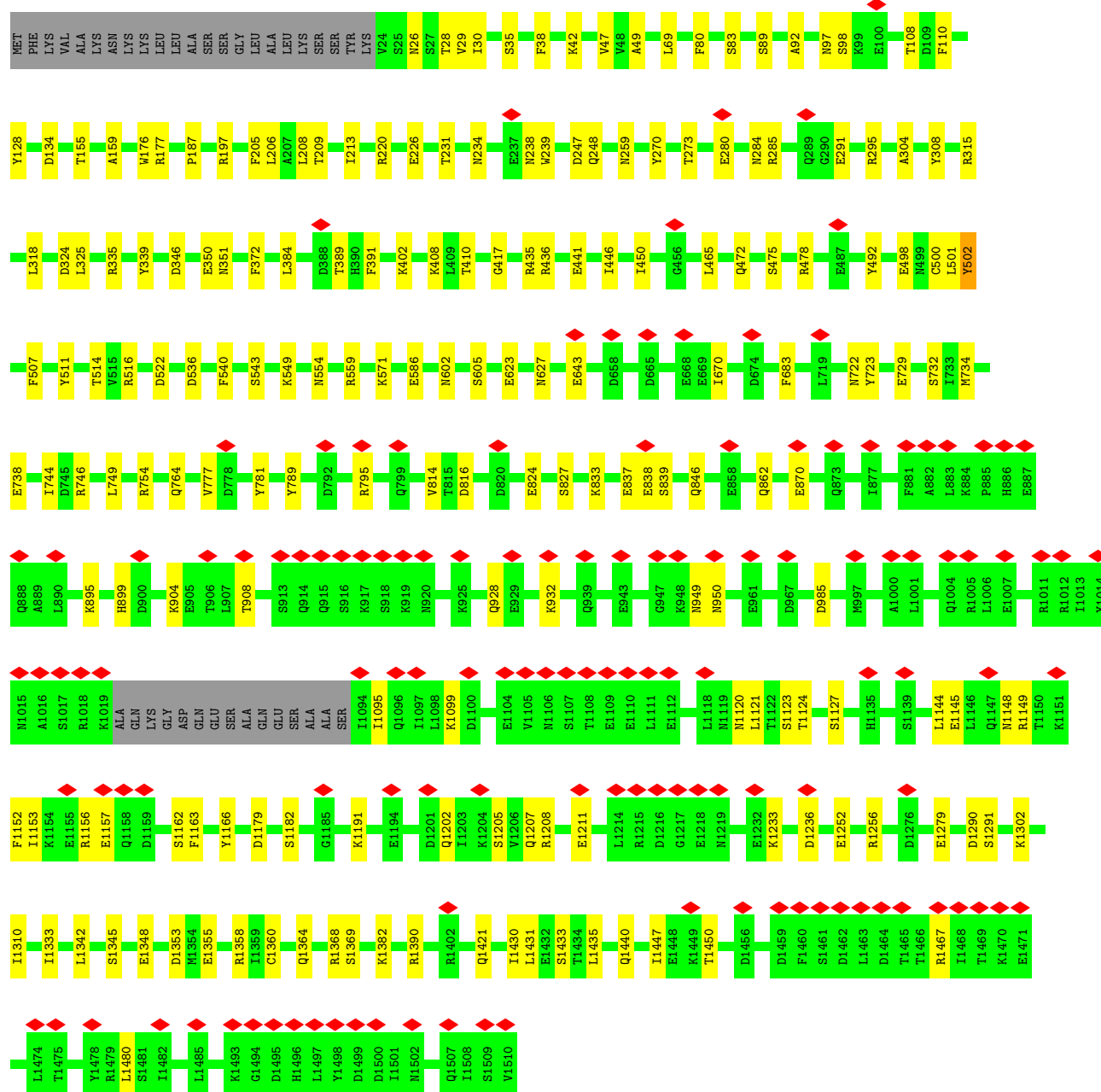
- Molecule 82: mS77

Chain BH:  11% 100%



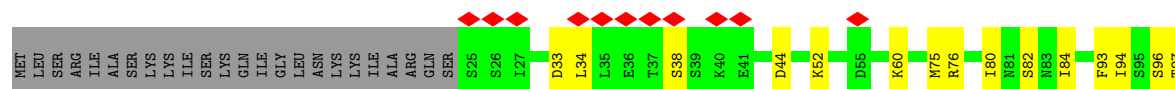
• Molecule 83: Enoyl-CoA hydratase/isomerase

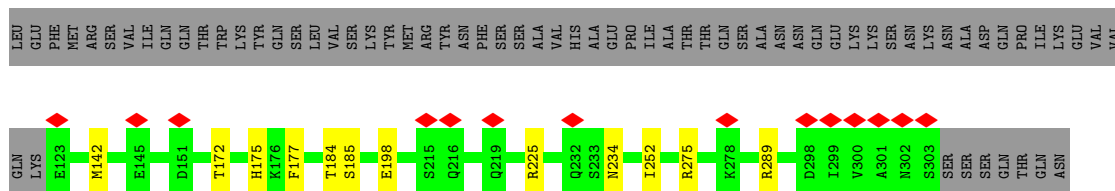
Chain BI: 



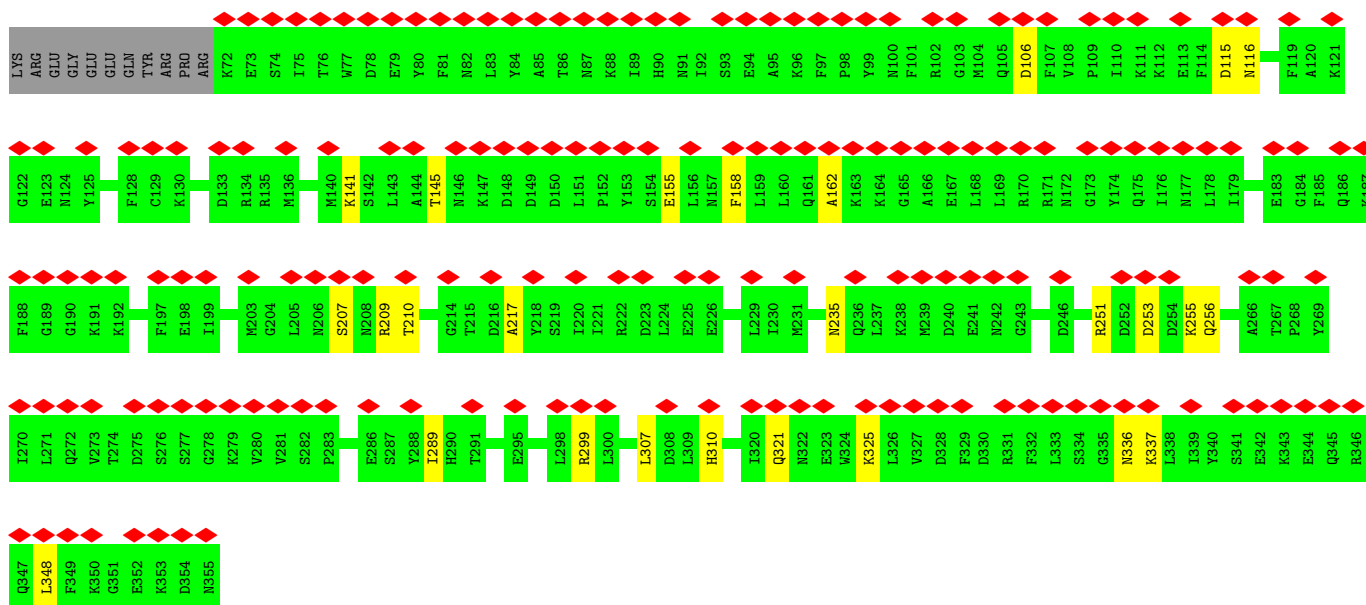
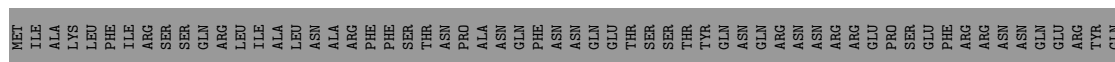
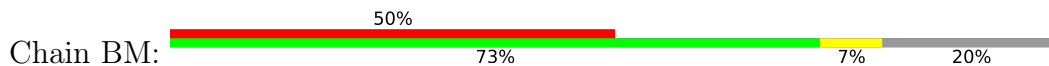
• Molecule 84: mS78

Chain BJ: 

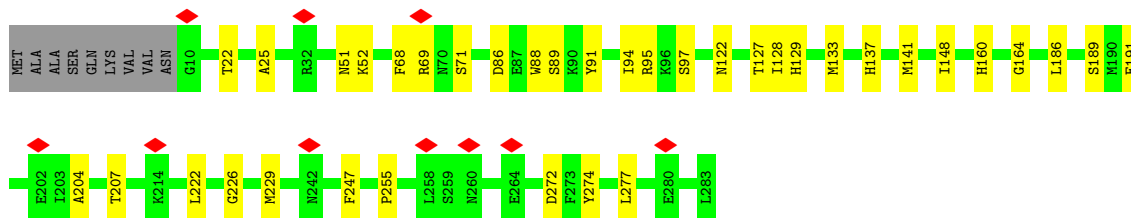
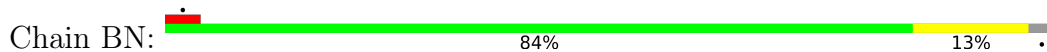




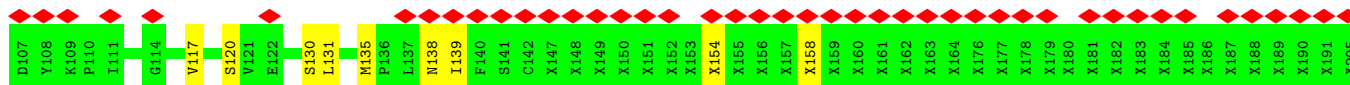
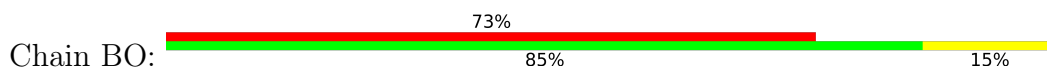
• Molecule 87: mS81



• Molecule 88: mS82

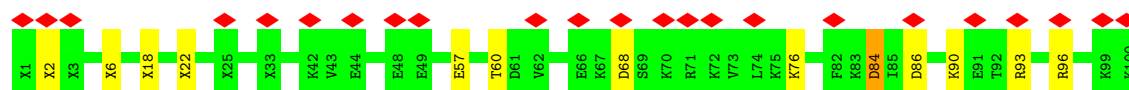
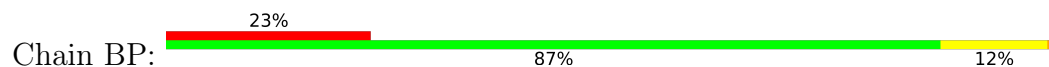


• Molecule 89: PARP alpha-helical domain-containing protein,mS83

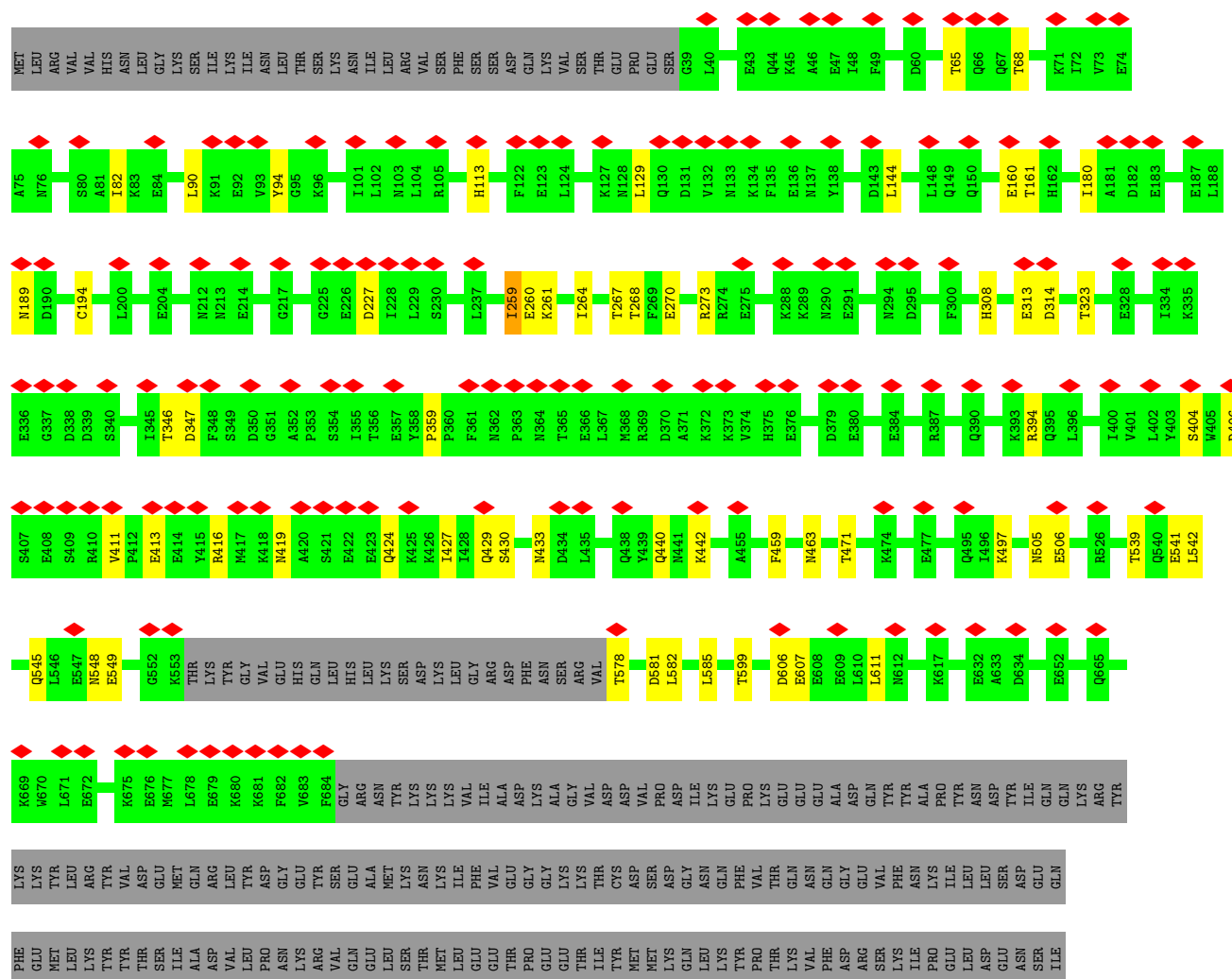




• Molecule 90: mS84,mS84

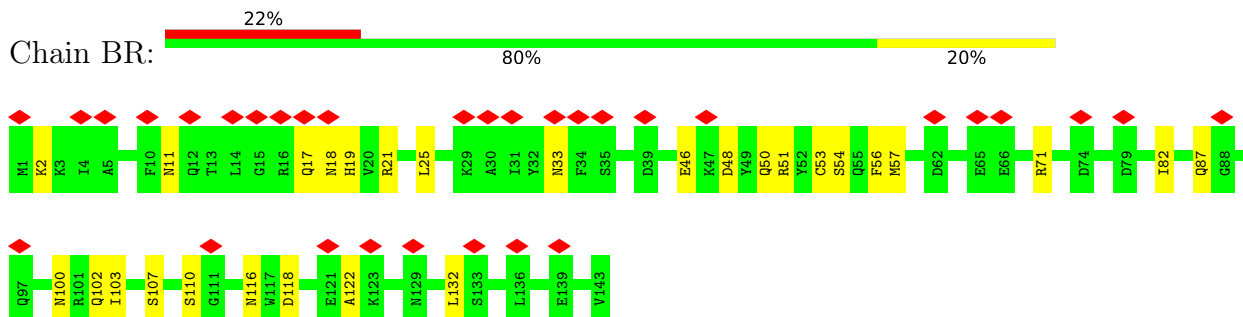


• Molecule 91: mS85



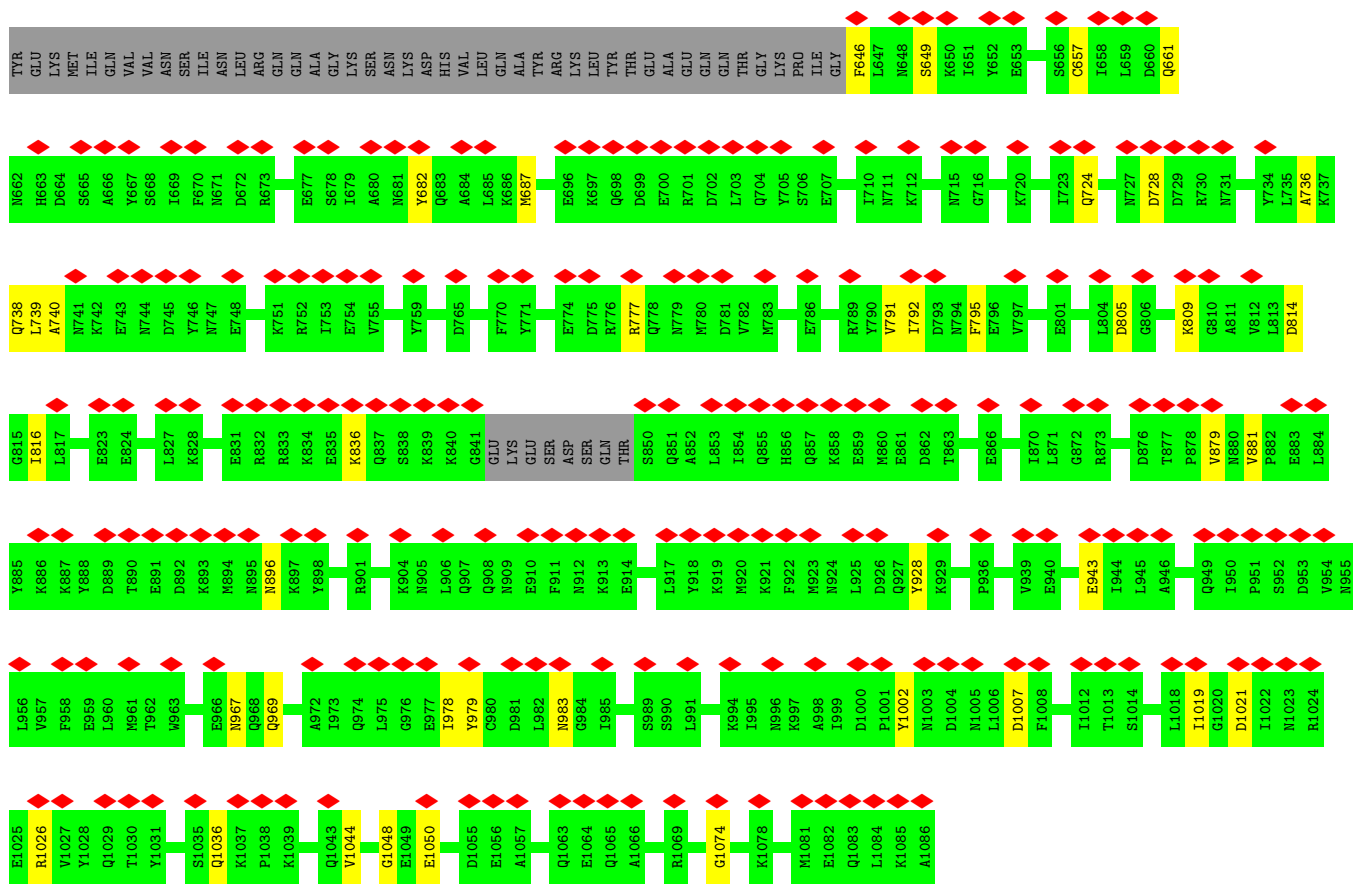
[illegible]

- Molecule 92: Iron donor protein CyaY

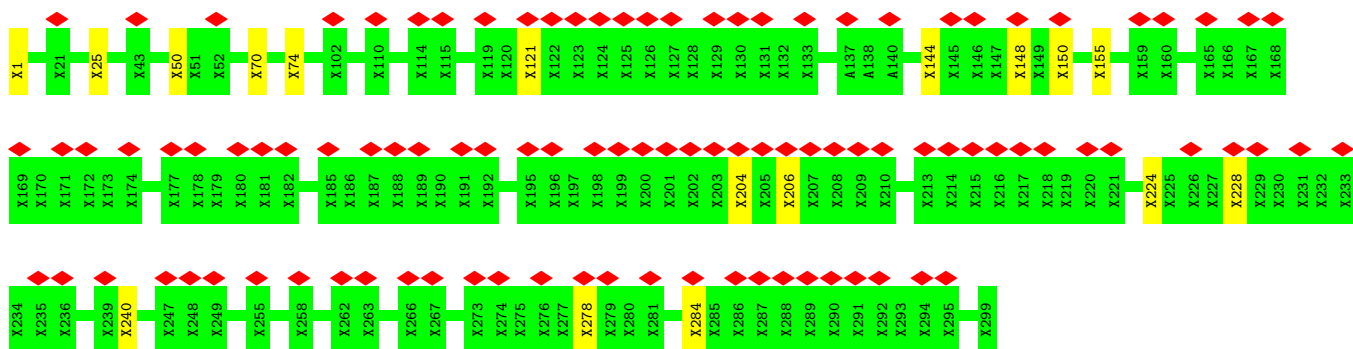


- Molecule 93: mS87

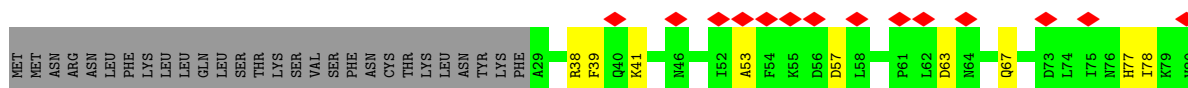
[illegible]

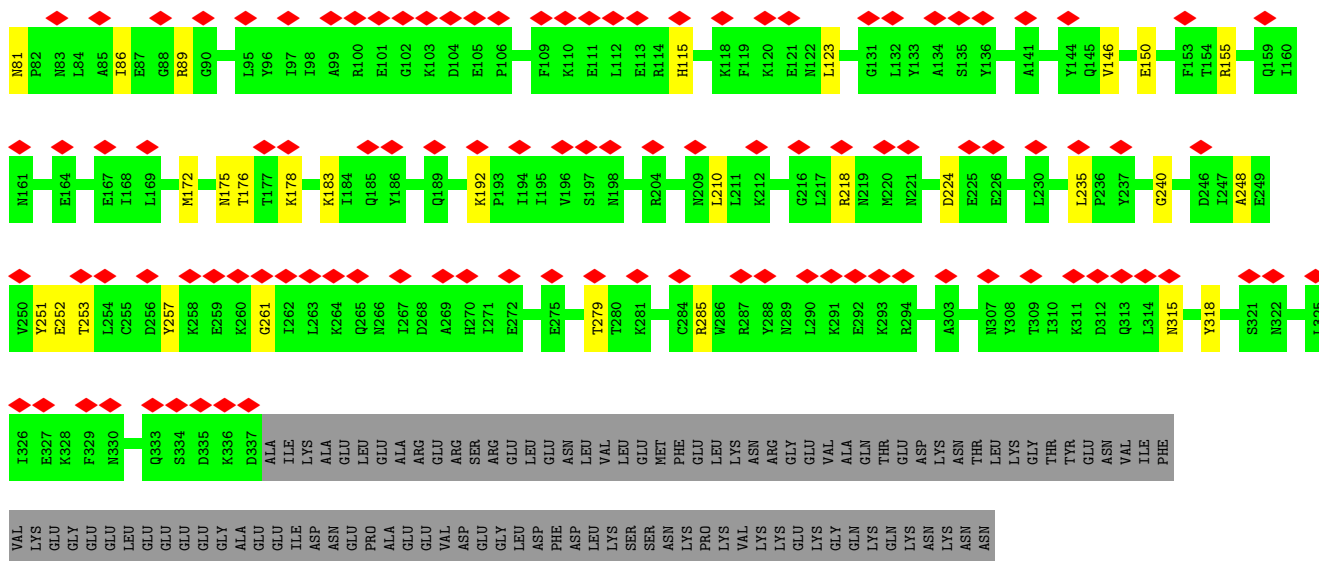


• Molecule 94: mS88

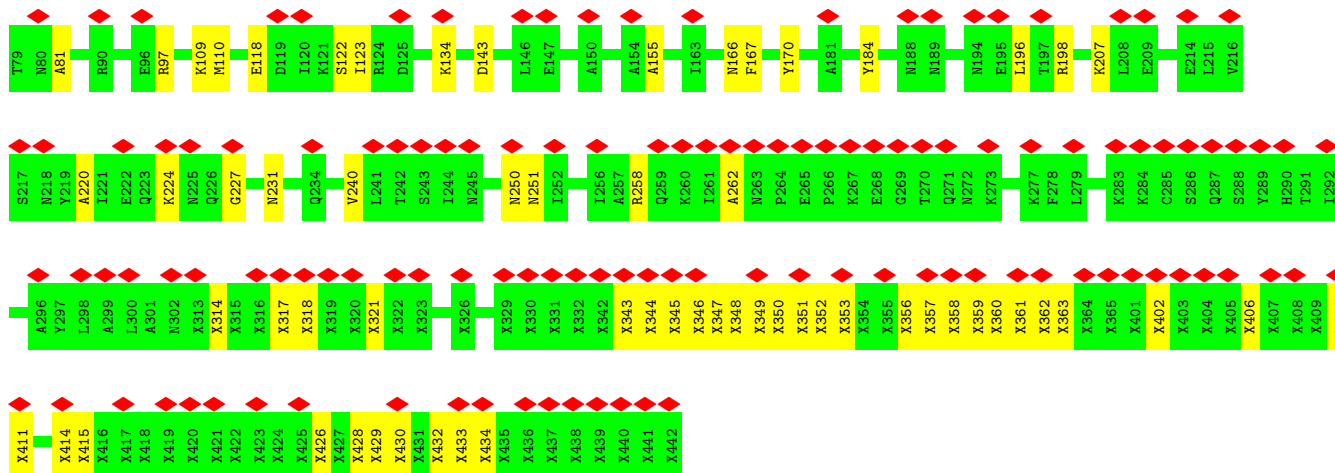
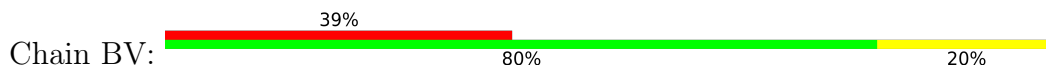


• Molecule 95: mS89

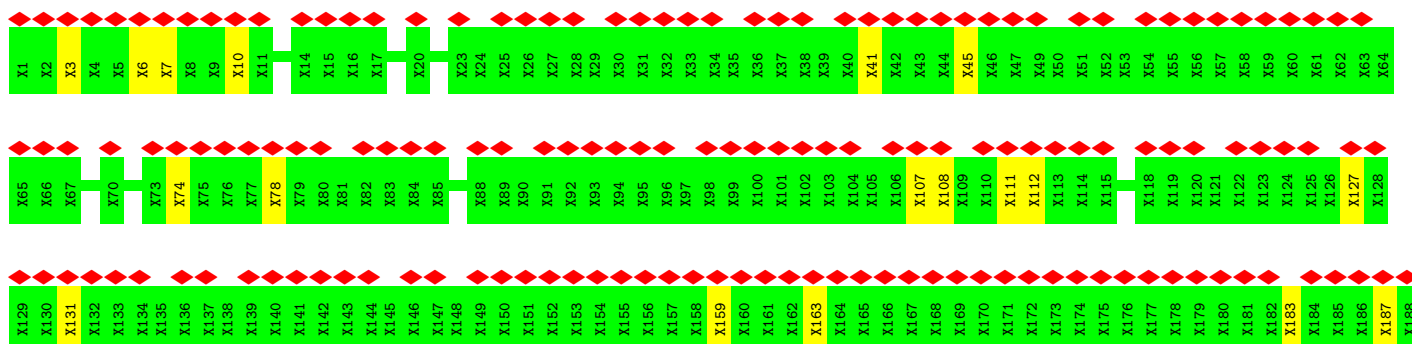
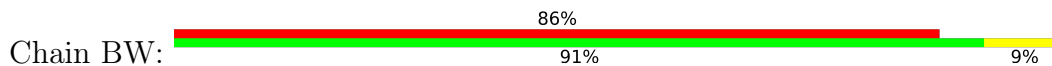


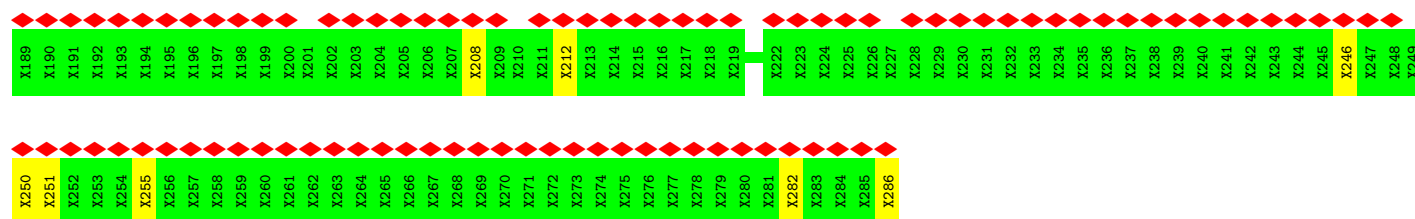


• Molecule 96: mS90

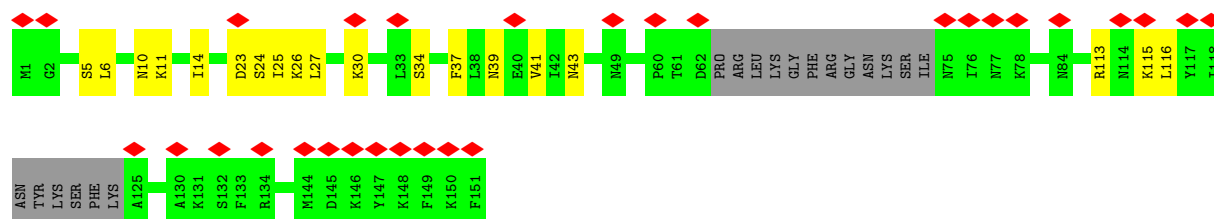
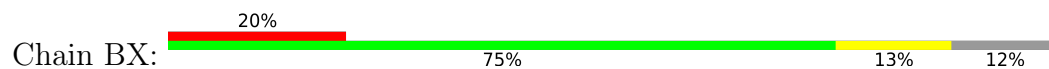


• Molecule 97: mS91

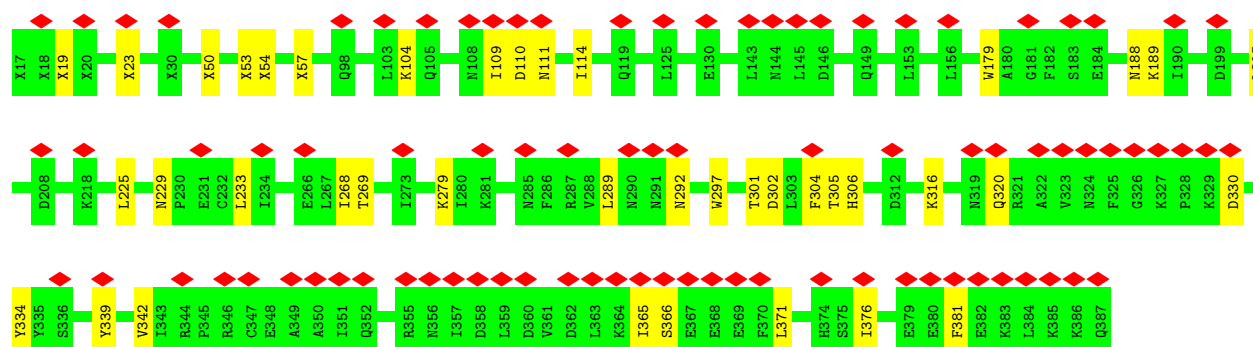
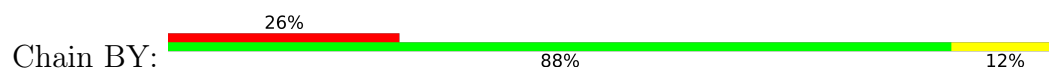




• Molecule 98: Ribosomal protein S3



• Molecule 99: mS93



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	99300	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	92000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	588.5, 588.5, 588.5	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Aa	0.33	0/6630	0.38	0/10321
2	Ab	0.35	0/53260	0.38	0/82922
3	Ac	0.45	0/2161	0.54	2/2897 (0.1%)
4	Ad	0.43	0/3051	0.49	0/4097
5	Ae	0.44	0/2836	0.48	0/3817
6	Af	0.30	0/608	0.41	0/811
7	Ag	0.42	0/1553	0.48	0/2081
11	Ak	0.30	0/890	0.47	0/1205
12	Al	0.37	0/440	0.52	0/596
13	Am	0.36	0/1389	0.45	0/1861
14	An	0.35	0/1268	0.44	0/1709
15	Ao	0.43	0/2842	0.46	0/3820
16	Ap	0.45	0/975	0.54	0/1303
17	Aq	0.45	0/2232	0.50	0/2998
18	Ar	0.45	0/1261	0.53	0/1682
19	As	0.40	0/1964	0.49	0/2620
20	At	0.44	0/1579	0.52	0/2128
21	Au	0.48	0/1449	0.54	0/1949
22	Av	0.44	0/1744	0.56	2/2350 (0.1%)
23	Aw	0.41	0/2866	0.48	0/3840
24	Ax	0.39	0/1115	0.46	0/1498
25	Ay	0.39	0/1548	0.49	0/2068
26	Az	0.39	0/1984	0.50	0/2680
27	AA	0.41	0/1482	0.49	0/2003
28	AB	0.42	0/2304	0.50	0/3082
29	AC	0.40	0/2416	0.47	0/3227
31	AE	0.40	0/459	0.51	0/612
32	AF	0.45	0/997	0.50	0/1321
33	AG	0.46	0/320	0.48	0/418
34	AH	0.30	0/1520	0.39	0/2038
35	AI	0.40	0/1059	0.46	0/1416
36	AJ	0.44	0/1513	0.47	0/2031

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	AK	0.25	0/2136	0.45	0/2895
38	AL	0.46	0/1208	0.47	0/1630
39	AM	0.43	0/1083	0.42	0/1458
40	AN	0.39	0/833	0.49	0/1129
41	AO	0.44	0/1037	0.52	0/1403
42	AP	0.40	0/3125	0.44	0/4220
43	AQ	0.52	0/428	0.56	0/567
44	AR	0.31	0/2415	0.43	0/3250
45	AS	0.34	0/6212	0.44	0/8373
46	AT	0.28	0/1398	0.39	0/1867
47	AU	0.35	0/3979	0.41	0/5353
48	AV	0.45	0/1067	0.48	0/1439
49	Ba	0.25	0/4674	0.33	0/7275
50	Bb	0.25	0/32970	0.33	0/51341
51	Bc	0.39	0/1403	0.48	0/1880
52	Bd	0.27	0/2883	0.41	0/3843
53	Be	0.38	0/3693	0.46	0/4907
54	Bf	0.37	0/2814	0.45	0/3788
55	Bg	0.33	0/1095	0.48	0/1471
56	Bh	0.23	0/2259	0.40	0/3043
57	Bi	0.30	0/5344	0.43	0/7174
58	Bj	0.35	0/1339	0.50	0/1801
59	Bk	0.28	0/2006	0.43	0/2685
60	Bl	0.34	0/1062	0.57	0/1415
61	Bm	0.29	0/1983	0.43	0/2661
62	Bn	0.37	0/881	0.47	0/1168
63	Bo	0.34	0/1519	0.48	0/2038
64	Bp	0.33	0/3537	0.45	0/4761
65	Bq	0.33	0/1480	0.45	0/1982
66	Br	0.31	0/4353	0.43	0/5860
67	Bs	0.34	0/739	0.48	0/983
68	Bt	0.34	0/891	0.41	0/1195
69	Bu	0.30	0/3548	0.43	0/4746
70	Bv	0.29	0/3981	0.38	0/5335
71	Bw	0.32	1/5700 (0.0%)	0.43	0/7694
72	Bx	0.27	0/4504	0.39	0/6108
73	By	0.30	0/887	0.35	0/1185
74	Bz	0.28	0/1025	0.43	0/1388
75	BA	0.33	0/1193	0.48	1/1601 (0.1%)
76	BB	0.30	0/959	0.39	0/1290
78	BD	0.30	0/903	0.40	0/1214
79	BE	0.35	0/3795	0.44	0/5084
81	BG	0.27	0/1402	0.41	0/1878

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
83	BI	0.34	0/12014	0.43	0/16144
84	BJ	0.33	0/12675	0.39	0/17091
85	BK	0.34	0/2176	0.45	0/2937
86	BL	0.32	0/1542	0.41	0/2078
87	BM	0.24	0/2428	0.38	0/3263
88	BN	0.31	0/2359	0.41	0/3168
89	BO	0.26	0/306	0.41	0/414
90	BP	0.34	0/489	0.55	0/647
91	BQ	0.26	0/5264	0.40	0/7086
92	BR	0.27	0/1204	0.38	0/1623
93	BS	0.22	0/3682	0.37	0/4953
94	BT	0.12	0/19	0.27	0/25
95	BU	0.29	0/2655	0.40	0/3578
96	BV	0.22	0/1868	0.36	0/2523
98	BX	0.32	0/1189	0.44	0/1591
99	BY	0.21	0/2465	0.42	0/3331
All	All	0.34	1/289793 (0.0%)	0.41	5/410231 (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
3	Ac	0	1
15	Ao	0	1
19	As	0	1
20	At	0	1
22	Av	0	1
26	Az	0	2
28	AB	0	2
36	AJ	0	1
47	AU	0	1
48	AV	0	1
53	Be	0	1
56	Bh	0	1
57	Bi	0	1
63	Bo	0	1
65	Bq	0	1
71	Bw	0	1
75	BA	0	1
83	BI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
84	BJ	0	2
90	BP	0	1
91	BQ	0	1
All	All	0	24

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	Bw	525	ASN	C-O	5.25	1.26	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	BA	66	PHE	CA-CB-CG	5.55	119.35	113.80
22	Av	112	TYR	CA-C-N	5.48	140.16	127.00
22	Av	112	TYR	C-N-CA	5.48	140.16	127.00
3	Ac	124	PHE	CB-CA-C	5.45	119.51	111.06
3	Ac	124	PHE	CA-C-O	-5.31	113.30	120.15

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Ac	124	PHE	Mainchain
15	Ao	211	GLN	Peptide
19	As	124	ILE	Peptide
20	At	46	TRP	Peptide
22	Av	170	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	5918	2963	2963	37	0
2	Ab	47567	23854	23854	228	0
3	Ac	2114	2218	2221	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ad	2989	3035	3034	23	0
5	Ae	2781	2890	2889	21	0
6	Af	593	639	642	7	0
7	Ag	1517	1555	1555	17	0
8	Ah	530	111	117	3	0
9	Ai	305	64	64	2	0
10	Aj	345	74	76	4	0
11	Ak	874	831	876	9	0
12	Al	430	439	439	4	0
13	Am	1406	1456	1458	7	0
14	An	1245	1317	1317	8	0
15	Ao	2771	2820	2820	25	0
16	Ap	956	1058	1058	13	0
17	Aq	2184	2293	2293	32	0
18	Ar	1232	1329	1329	15	0
19	As	1938	2015	2015	20	0
20	At	1538	1531	1533	7	0
21	Au	1419	1469	1469	12	0
22	Av	1712	1722	1722	21	0
23	Aw	2824	2943	2943	31	0
24	Ax	1093	1164	1164	13	0
25	Ay	1527	1597	1597	24	0
26	Az	1944	1990	1990	25	0
27	AA	1447	1425	1425	15	0
28	AB	2258	2341	2341	26	0
29	AC	2385	2434	2434	27	0
30	AD	180	146	40	0	0
31	AE	452	483	483	4	0
32	AF	974	1054	1054	26	0
33	AG	316	357	357	1	0
34	AH	1493	1496	1496	18	0
35	AI	1036	1052	1052	5	0
36	AJ	1481	1480	1480	12	0
37	AK	2076	2017	2017	24	0
38	AL	1181	1225	1225	17	0
39	AM	1059	1026	1026	10	0
40	AN	814	815	815	10	0
41	AO	1011	1049	1049	15	0
42	AP	3048	3070	3070	38	0
43	AQ	419	444	444	14	0
44	AR	2350	2253	2253	13	0
45	AS	6069	6045	6043	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	AT	1377	1434	1434	4	0
47	AU	3913	4014	4015	30	0
48	AV	1038	1030	1030	9	0
49	Ba	4172	2097	2097	30	0
50	Bb	29454	14779	14779	159	0
51	Bc	1373	1465	1465	16	0
52	Bd	2826	3013	3015	28	0
53	Be	3604	3929	3929	37	0
54	Bf	2756	2735	2735	37	0
55	Bg	1080	1124	1124	9	0
56	Bh	2204	2250	2248	19	0
57	Bi	5244	5228	5228	51	0
58	Bj	1304	1348	1348	18	0
59	Bk	1957	2055	2056	13	0
60	Bl	1045	1154	1154	15	0
61	Bm	1931	1946	1946	14	0
62	Bn	865	939	939	14	0
63	Bo	1488	1515	1515	10	0
64	Bp	3457	3499	3499	45	0
65	Bq	1454	1505	1505	20	0
66	Br	4279	4310	4310	49	0
67	Bs	722	786	786	5	0
68	Bt	869	891	891	7	0
69	Bu	4253	3630	3634	47	0
70	Bv	3919	3977	3977	40	0
71	Bw	5552	5447	5444	51	0
72	Bx	4393	4175	4177	35	0
73	By	869	903	903	6	0
74	Bz	999	1000	1000	17	0
75	BA	1168	1167	1167	9	0
76	BB	934	930	930	7	0
77	BC	185	41	42	0	0
78	BD	883	908	908	11	0
79	BE	3724	3615	3615	45	0
80	BF	115	32	27	1	0
81	BG	1375	1329	1329	13	0
82	BH	315	67	68	0	0
83	BI	11800	11719	11719	132	0
84	BJ	12446	12419	12418	124	0
85	BK	2130	2106	2106	25	0
86	BL	1501	1461	1462	7	0
87	BM	2371	2321	2322	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	BN	2304	2253	2252	24	0
89	BO	828	397	406	12	0
90	BP	692	567	568	12	0
91	BQ	5171	5095	5094	44	0
92	BR	1182	1179	1179	19	0
93	BS	3619	3602	3602	25	0
94	BT	1485	330	340	12	0
95	BU	2596	2568	2567	25	0
96	BV	2261	1924	1929	39	0
97	BW	1425	306	328	13	0
98	BX	1156	1195	1195	15	0
99	BY	2591	2528	2531	24	0
100	AB	1	0	0	0	0
100	AF	1	0	0	0	0
100	AQ	1	0	0	0	0
100	Aa	28	0	0	0	0
100	Ab	270	0	0	0	0
100	Ad	1	0	0	0	0
100	Ae	1	0	0	0	0
100	Aq	1	0	0	0	0
100	Ba	10	0	0	0	0
100	Bb	76	0	0	0	0
100	Bi	1	0	0	0	0
100	Bw	1	0	0	0	0
100	Bz	1	0	0	0	0
101	AG	1	0	0	0	0
101	BL	1	0	0	0	0
102	AV	8	0	0	0	0
103	Bw	31	4	12	0	0
All	All	282889	235830	235841	1862	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 4.

The worst 5 of 1862 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)
34:AH:178:LEU:HD13	37:AK:101:MET:HE3	1.45	0.95
22:Av:149:ASN:OD1	27:AA:175:ARG:NH1	2.09	0.84
2:Ab:1120:A:OP1	17:Aq:64:TYR:OH	1.95	0.83
50:Bb:952:C:OP2	62:Bn:72:ASN:ND2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:1955:C:OP1	27:AA:48:ARG:NH1	2.12	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ac	260/262 (99%)	244 (94%)	16 (6%)	0	100	100
4	Ad	368/439 (84%)	344 (94%)	24 (6%)	0	100	100
5	Ae	335/358 (94%)	319 (95%)	16 (5%)	0	100	100
6	Af	66/68 (97%)	63 (96%)	3 (4%)	0	100	100
7	Ag	174/179 (97%)	165 (95%)	9 (5%)	0	100	100
11	Ak	102/105 (97%)	96 (94%)	6 (6%)	0	100	100
12	Al	51/223 (23%)	49 (96%)	2 (4%)	0	100	100
13	Am	156/166 (94%)	145 (93%)	11 (7%)	0	100	100
14	An	156/158 (99%)	150 (96%)	6 (4%)	0	100	100
15	Ao	328/391 (84%)	309 (94%)	19 (6%)	0	100	100
16	Ap	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
17	Aq	271/305 (89%)	251 (93%)	20 (7%)	0	100	100
18	Ar	141/143 (99%)	126 (89%)	15 (11%)	0	100	100
19	As	234/237 (99%)	215 (92%)	19 (8%)	0	100	100
20	At	181/242 (75%)	170 (94%)	10 (6%)	1 (1%)	21	52
21	Au	167/170 (98%)	161 (96%)	6 (4%)	0	100	100
22	Av	204/235 (87%)	193 (95%)	9 (4%)	2 (1%)	12	43
23	Aw	340/364 (93%)	323 (95%)	17 (5%)	0	100	100
24	Ax	130/138 (94%)	124 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Ay	188/234 (80%)	180 (96%)	8 (4%)	0	100	100
26	Az	235/321 (73%)	223 (95%)	11 (5%)	1 (0%)	30	60
27	AA	174/237 (73%)	162 (93%)	12 (7%)	0	100	100
28	AB	262/289 (91%)	247 (94%)	14 (5%)	1 (0%)	30	60
29	AC	282/307 (92%)	269 (95%)	13 (5%)	0	100	100
31	AE	55/64 (86%)	51 (93%)	4 (7%)	0	100	100
32	AF	113/164 (69%)	110 (97%)	3 (3%)	0	100	100
33	AG	36/93 (39%)	35 (97%)	1 (3%)	0	100	100
34	AH	175/199 (88%)	169 (97%)	6 (3%)	0	100	100
35	AI	120/155 (77%)	113 (94%)	7 (6%)	0	100	100
36	AJ	176/179 (98%)	165 (94%)	11 (6%)	0	100	100
37	AK	242/309 (78%)	230 (95%)	12 (5%)	0	100	100
38	AL	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
39	AM	124/184 (67%)	121 (98%)	3 (2%)	0	100	100
40	AN	94/158 (60%)	91 (97%)	3 (3%)	0	100	100
41	AO	118/155 (76%)	117 (99%)	1 (1%)	0	100	100
42	AP	362/386 (94%)	351 (97%)	11 (3%)	0	100	100
43	AQ	48/109 (44%)	41 (85%)	7 (15%)	0	100	100
44	AR	272/348 (78%)	256 (94%)	16 (6%)	0	100	100
45	AS	724/764 (95%)	696 (96%)	28 (4%)	0	100	100
46	AT	164/299 (55%)	155 (94%)	9 (6%)	0	100	100
47	AU	477/499 (96%)	454 (95%)	23 (5%)	0	100	100
48	AV	127/160 (79%)	116 (91%)	11 (9%)	0	100	100
51	Bc	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
52	Bd	328/330 (99%)	316 (96%)	12 (4%)	0	100	100
53	Be	403/405 (100%)	387 (96%)	16 (4%)	0	100	100
54	Bf	335/351 (95%)	314 (94%)	21 (6%)	0	100	100
55	Bg	134/141 (95%)	124 (92%)	10 (8%)	0	100	100
56	Bh	254/276 (92%)	237 (93%)	17 (7%)	0	100	100
57	Bi	620/737 (84%)	593 (96%)	26 (4%)	1 (0%)	43	72
58	Bj	150/152 (99%)	143 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	Bk	224/238 (94%)	208 (93%)	16 (7%)	0	100	100
60	Bl	127/133 (96%)	115 (91%)	12 (9%)	0	100	100
61	Bm	218/276 (79%)	205 (94%)	13 (6%)	0	100	100
62	Bn	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
63	Bo	177/196 (90%)	170 (96%)	7 (4%)	0	100	100
64	Bp	410/437 (94%)	386 (94%)	24 (6%)	0	100	100
65	Bq	172/182 (94%)	164 (95%)	7 (4%)	1 (1%)	21	52
66	Br	521/549 (95%)	498 (96%)	23 (4%)	0	100	100
67	Bs	85/98 (87%)	78 (92%)	7 (8%)	0	100	100
68	Bt	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
69	Bu	400/567 (70%)	385 (96%)	15 (4%)	0	100	100
70	Bv	461/579 (80%)	450 (98%)	11 (2%)	0	100	100
71	Bw	656/703 (93%)	630 (96%)	26 (4%)	0	100	100
72	Bx	526/719 (73%)	505 (96%)	21 (4%)	0	100	100
73	By	105/132 (80%)	104 (99%)	1 (1%)	0	100	100
74	Bz	121/147 (82%)	111 (92%)	10 (8%)	0	100	100
75	BA	136/149 (91%)	127 (93%)	9 (7%)	0	100	100
76	BB	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
78	BD	105/130 (81%)	100 (95%)	5 (5%)	0	100	100
79	BE	445/464 (96%)	418 (94%)	27 (6%)	0	100	100
81	BG	162/182 (89%)	156 (96%)	6 (4%)	0	100	100
83	BI	1409/1451 (97%)	1337 (95%)	72 (5%)	0	100	100
84	BJ	1513/1539 (98%)	1438 (95%)	75 (5%)	0	100	100
85	BK	265/267 (99%)	253 (96%)	12 (4%)	0	100	100
86	BL	179/310 (58%)	170 (95%)	9 (5%)	0	100	100
87	BM	282/355 (79%)	265 (94%)	17 (6%)	0	100	100
88	BN	272/283 (96%)	257 (94%)	15 (6%)	0	100	100
89	BO	34/142 (24%)	30 (88%)	4 (12%)	0	100	100
90	BP	58/100 (58%)	49 (84%)	9 (16%)	0	100	100
91	BQ	618/1032 (60%)	578 (94%)	40 (6%)	0	100	100
92	BR	141/143 (99%)	136 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
93	BS	429/1086 (40%)	416 (97%)	13 (3%)	0	100	100
94	BT	4/297 (1%)	4 (100%)	0	0	100	100
95	BU	307/439 (70%)	298 (97%)	9 (3%)	0	100	100
96	BV	222/310 (72%)	210 (95%)	12 (5%)	0	100	100
98	BX	127/151 (84%)	121 (95%)	6 (5%)	0	100	100
99	BY	290/327 (89%)	279 (96%)	11 (4%)	0	100	100
All	All	22381/27039 (83%)	21256 (95%)	1118 (5%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	At	46	TRP
22	Av	114	ALA
26	Az	138	ASP
57	Bi	565	VAL
65	Bq	143	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ac	235/235 (100%)	235 (100%)	0	100	100
4	Ad	330/391 (84%)	330 (100%)	0	100	100
5	Ae	306/326 (94%)	306 (100%)	0	100	100
6	Af	68/68 (100%)	68 (100%)	0	100	100
7	Ag	170/172 (99%)	170 (100%)	0	100	100
11	Ak	93/93 (100%)	93 (100%)	0	100	100
12	Al	46/203 (23%)	46 (100%)	0	100	100
13	Am	156/156 (100%)	156 (100%)	0	100	100
14	An	138/138 (100%)	138 (100%)	0	100	100
15	Ao	309/345 (90%)	309 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Ap	110/110 (100%)	110 (100%)	0	100	100
17	Aq	239/269 (89%)	239 (100%)	0	100	100
18	Ar	135/135 (100%)	135 (100%)	0	100	100
19	As	208/209 (100%)	208 (100%)	0	100	100
20	At	168/224 (75%)	168 (100%)	0	100	100
21	Au	150/151 (99%)	150 (100%)	0	100	100
22	Av	187/211 (89%)	187 (100%)	0	100	100
23	Aw	309/331 (93%)	309 (100%)	0	100	100
24	Ax	125/130 (96%)	125 (100%)	0	100	100
25	Ay	168/208 (81%)	168 (100%)	0	100	100
26	Az	218/295 (74%)	218 (100%)	0	100	100
27	AA	157/212 (74%)	157 (100%)	0	100	100
28	AB	255/278 (92%)	255 (100%)	0	100	100
29	AC	256/277 (92%)	256 (100%)	0	100	100
31	AE	49/55 (89%)	49 (100%)	0	100	100
32	AF	103/150 (69%)	103 (100%)	0	100	100
33	AG	35/89 (39%)	35 (100%)	0	100	100
34	AH	164/184 (89%)	164 (100%)	0	100	100
35	AI	115/144 (80%)	115 (100%)	0	100	100
36	AJ	164/165 (99%)	164 (100%)	0	100	100
37	AK	226/286 (79%)	226 (100%)	0	100	100
38	AL	132/132 (100%)	132 (100%)	0	100	100
39	AM	113/170 (66%)	113 (100%)	0	100	100
40	AN	91/139 (66%)	91 (100%)	0	100	100
41	AO	109/138 (79%)	109 (100%)	0	100	100
42	AP	339/359 (94%)	339 (100%)	0	100	100
43	AQ	45/98 (46%)	45 (100%)	0	100	100
44	AR	258/324 (80%)	258 (100%)	0	100	100
45	AS	657/691 (95%)	657 (100%)	0	100	100
46	AT	151/273 (55%)	151 (100%)	0	100	100
47	AU	443/461 (96%)	442 (100%)	1 (0%)	87	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	AV	119/149 (80%)	119 (100%)	0	100	100
51	Bc	158/158 (100%)	158 (100%)	0	100	100
52	Bd	319/319 (100%)	319 (100%)	0	100	100
53	Be	396/396 (100%)	396 (100%)	0	100	100
54	Bf	304/317 (96%)	304 (100%)	0	100	100
55	Bg	117/122 (96%)	117 (100%)	0	100	100
56	Bh	249/269 (93%)	249 (100%)	0	100	100
57	Bi	582/683 (85%)	582 (100%)	0	100	100
58	Bj	148/148 (100%)	148 (100%)	0	100	100
59	Bk	216/228 (95%)	216 (100%)	0	100	100
60	Bl	113/116 (97%)	113 (100%)	0	100	100
61	Bm	209/258 (81%)	209 (100%)	0	100	100
62	Bn	94/94 (100%)	94 (100%)	0	100	100
63	Bo	161/177 (91%)	161 (100%)	0	100	100
64	Bp	382/406 (94%)	382 (100%)	0	100	100
65	Bq	161/167 (96%)	161 (100%)	0	100	100
66	Br	481/506 (95%)	481 (100%)	0	100	100
67	Bs	82/93 (88%)	82 (100%)	0	100	100
68	Bt	93/93 (100%)	93 (100%)	0	100	100
69	Bu	378/386 (98%)	378 (100%)	0	100	100
70	Bv	433/540 (80%)	433 (100%)	0	100	100
71	Bw	609/647 (94%)	609 (100%)	0	100	100
72	Bx	491/660 (74%)	491 (100%)	0	100	100
73	By	96/116 (83%)	96 (100%)	0	100	100
74	Bz	107/126 (85%)	107 (100%)	0	100	100
75	BA	130/141 (92%)	130 (100%)	0	100	100
76	BB	101/102 (99%)	101 (100%)	0	100	100
78	BD	98/120 (82%)	98 (100%)	0	100	100
79	BE	404/420 (96%)	403 (100%)	1 (0%)	87	86
81	BG	153/171 (90%)	153 (100%)	0	100	100
83	BI	1306/1335 (98%)	1306 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	BJ	1405/1426 (98%)	1405 (100%)	0	100	100
85	BK	235/235 (100%)	235 (100%)	0	100	100
86	BL	168/291 (58%)	168 (100%)	0	100	100
87	BM	256/322 (80%)	256 (100%)	0	100	100
88	BN	249/256 (97%)	249 (100%)	0	100	100
89	BO	35/35 (100%)	35 (100%)	0	100	100
90	BP	57/57 (100%)	57 (100%)	0	100	100
91	BQ	582/958 (61%)	582 (100%)	0	100	100
92	BR	133/133 (100%)	133 (100%)	0	100	100
93	BS	399/1002 (40%)	399 (100%)	0	100	100
95	BU	285/403 (71%)	285 (100%)	0	100	100
96	BV	197/197 (100%)	197 (100%)	0	100	100
98	BX	126/142 (89%)	126 (100%)	0	100	100
99	BY	280/280 (100%)	280 (100%)	0	100	100
All	All	20827/24225 (86%)	20825 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	AU	189	ASN
79	BE	421	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
83	BI	976	ASN
93	BS	1010	ASN
84	BJ	335	GLN
86	BL	134	HIS
99	BY	245	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	277/278 (99%)	64 (23%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Ab	2234/2314 (96%)	447 (20%)	0
49	Ba	195/196 (99%)	43 (22%)	0
50	Bb	1384/1395 (99%)	256 (18%)	0
All	All	4090/4183 (97%)	810 (19%)	0

5 of 810 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	6	U
1	Aa	7	G
1	Aa	13	A
1	Aa	35	A
1	Aa	47	U

There are no RNA pucker outliers to report.

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 398 ligands modelled in this entry, 395 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
102	FES	AV	202	48	0,4,4	-	-	-		
102	FES	AV	201	48	0,4,4	-	-	-		
103	ATP	Bw	801	100	32,33,33	1.37	4 (12%)	48,52,52	1.93	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
102	FES	AV	201	48	-	-	0/1/1/1
102	FES	AV	202	48	-	-	0/1/1/1
103	ATP	Bw	801	100	-	6/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
103	Bw	801	ATP	C5-C4	4.23	1.46	1.39
103	Bw	801	ATP	C5-C6	2.54	1.48	1.41
103	Bw	801	ATP	C5-N7	-2.45	1.34	1.39
103	Bw	801	ATP	C8-N7	2.43	1.36	1.31

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
103	Bw	801	ATP	C5-C4-N3	-5.80	118.72	126.72
103	Bw	801	ATP	N3-C4-N9	4.30	134.48	127.17
103	Bw	801	ATP	C2-N3-C4	3.95	121.48	111.83
103	Bw	801	ATP	C4-C5-N7	-3.80	106.23	110.58
103	Bw	801	ATP	N3-C2-N1	-3.73	122.93	128.58

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

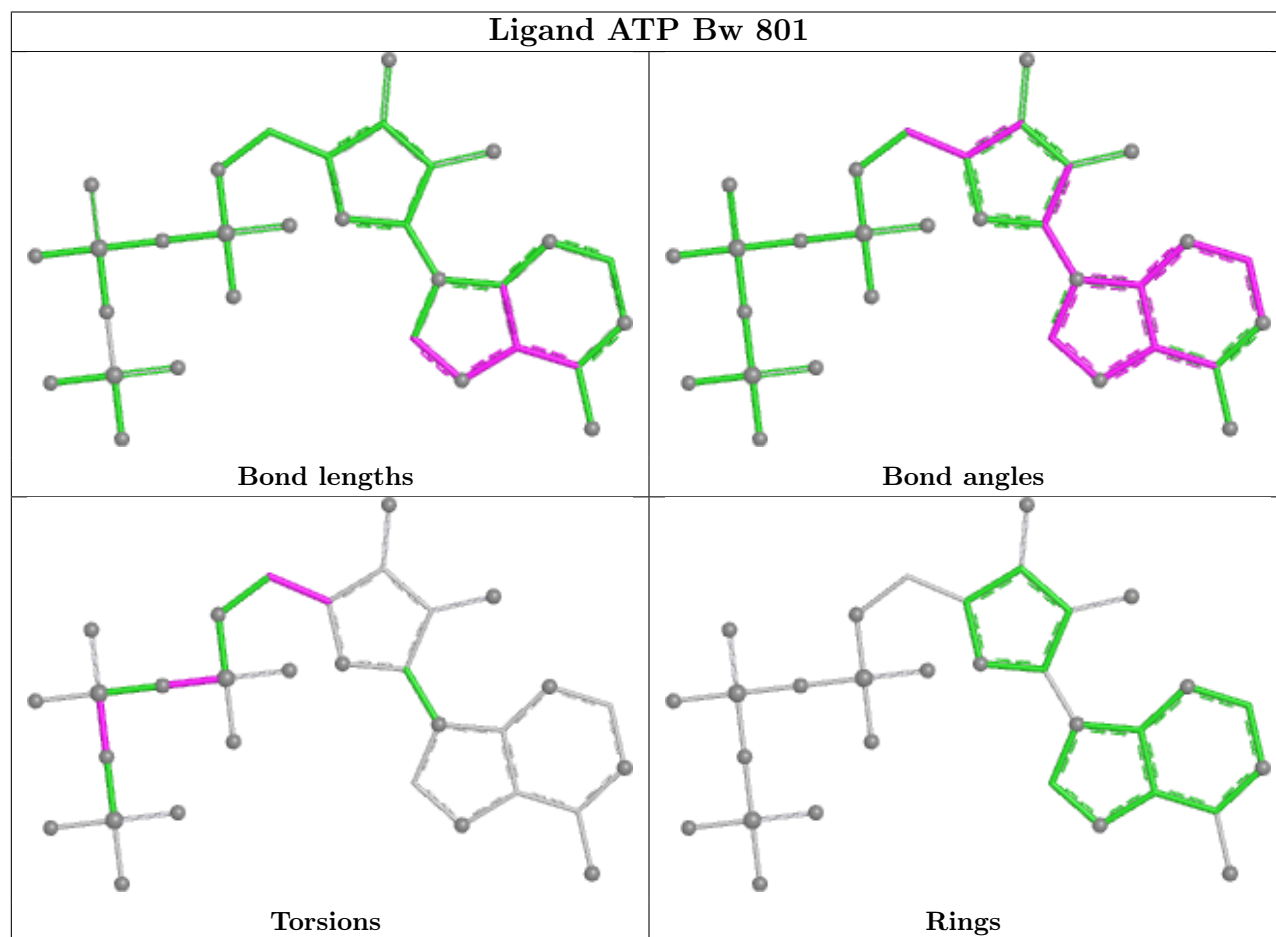
Mol	Chain	Res	Type	Atoms
103	Bw	801	ATP	O4'-C4'-C5'-O5'
103	Bw	801	ATP	C3'-C4'-C5'-O5'
103	Bw	801	ATP	PG-O3B-PB-O1B
103	Bw	801	ATP	PB-O3A-PA-O2A
103	Bw	801	ATP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
97	BW	18

Continued on next page...

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Mol	Chain	Number of breaks
89	BO	8
99	BY	4
96	BV	4
69	Bu	2
10	Aj	1
8	Ah	1
94	BT	1

The worst 5 of 39 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BO	142:CYS	C	147:UNK	N	25.16
1	BW	47:UNK	C	49:UNK	N	20.28
1	Bu	448:UNK	C	457:GLU	N	19.30
1	BW	201:UNK	C	202:UNK	N	19.15
1	BW	83:UNK	C	84:UNK	N	18.63

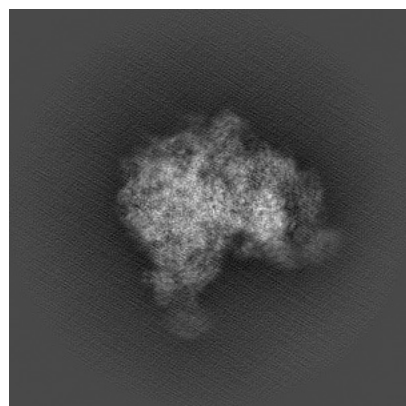
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11032. These allow visual inspection of the internal detail of the map and identification of artifacts.

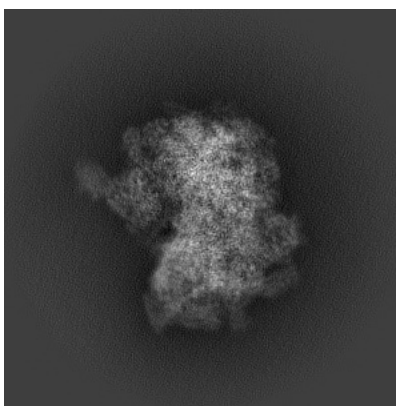
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

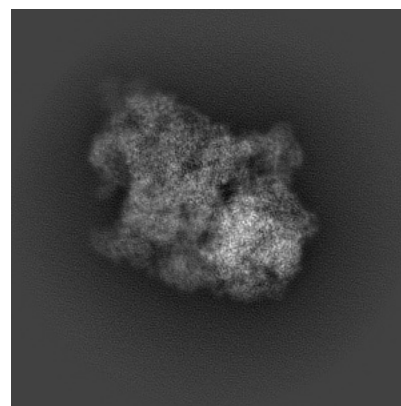
6.1.1 Primary map



X

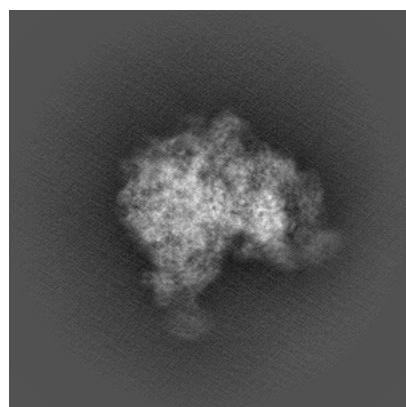


Y

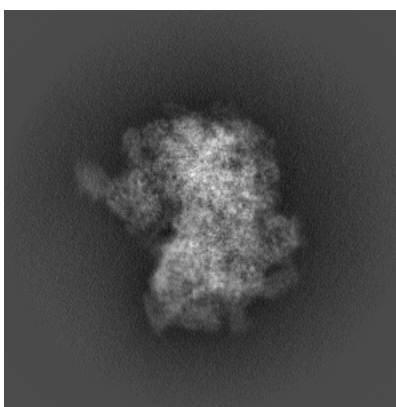


Z

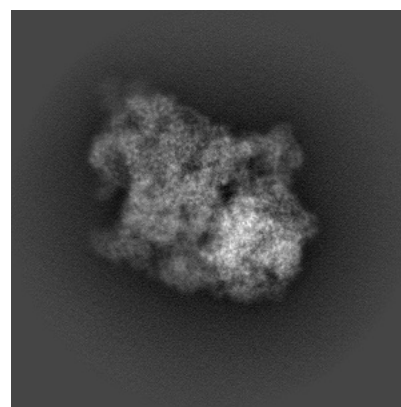
6.1.2 Raw map



X



Y

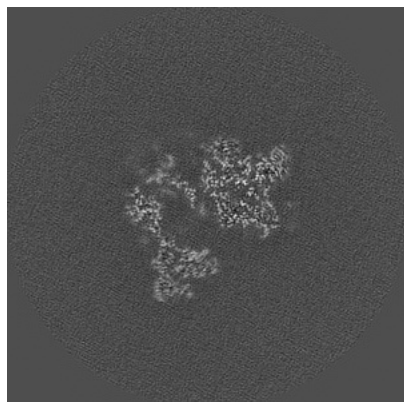


Z

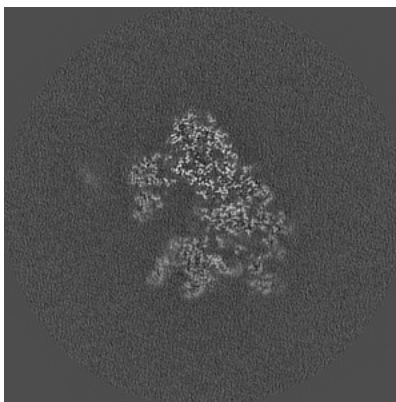
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

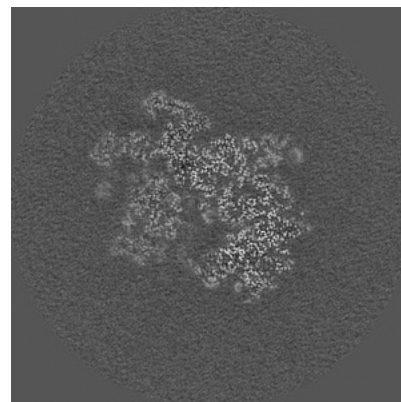
6.2.1 Primary map



X Index: 275

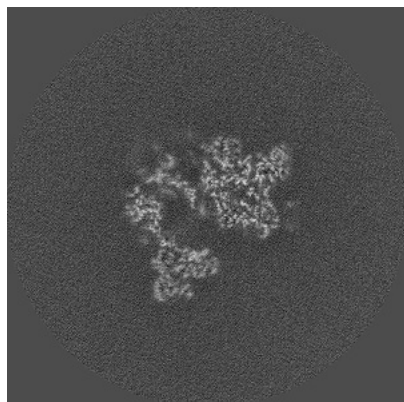


Y Index: 275

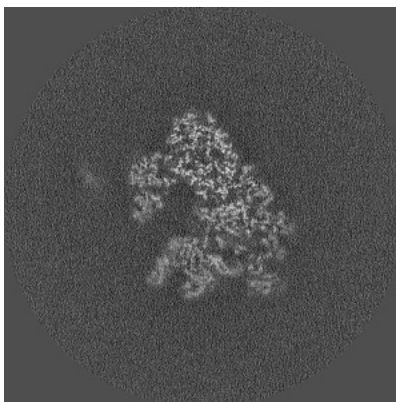


Z Index: 275

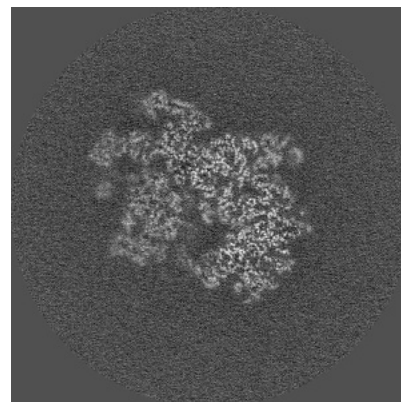
6.2.2 Raw map



X Index: 275



Y Index: 275

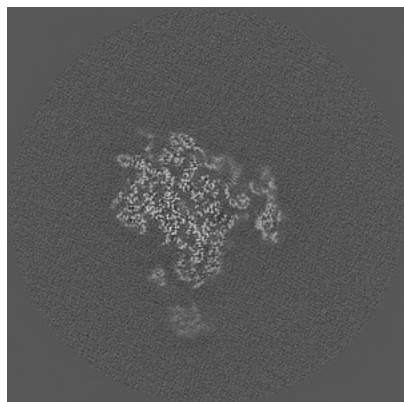


Z Index: 275

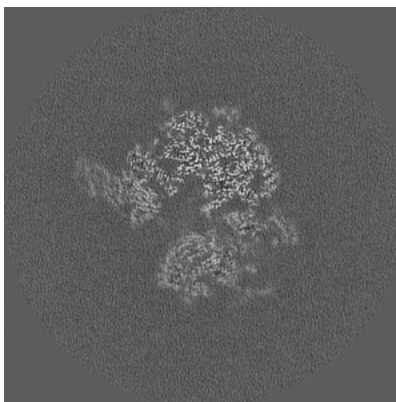
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

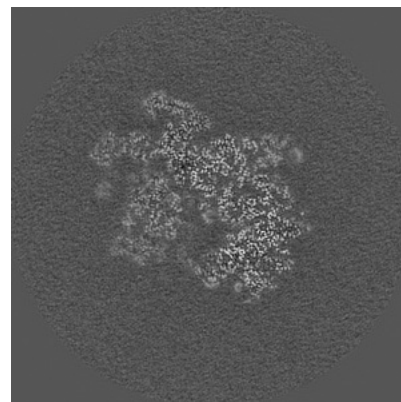
6.3.1 Primary map



X Index: 325

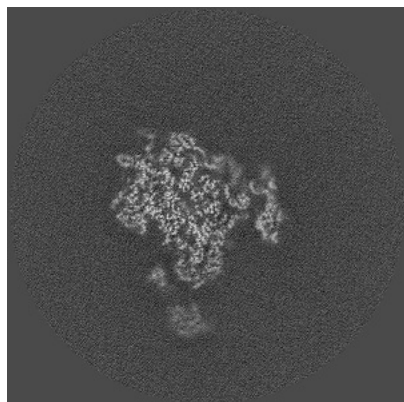


Y Index: 255

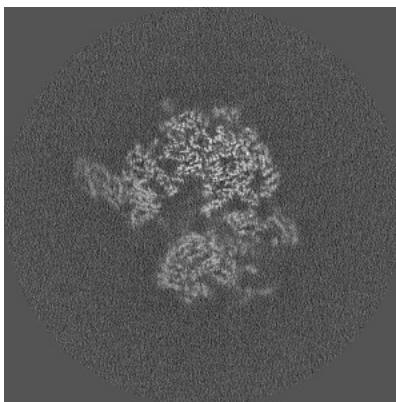


Z Index: 275

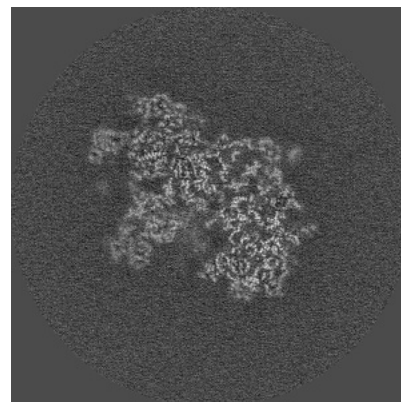
6.3.2 Raw map



X Index: 325



Y Index: 255

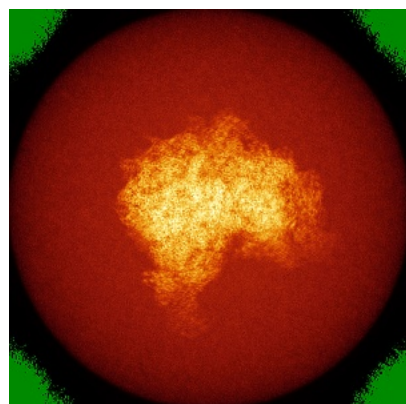


Z Index: 285

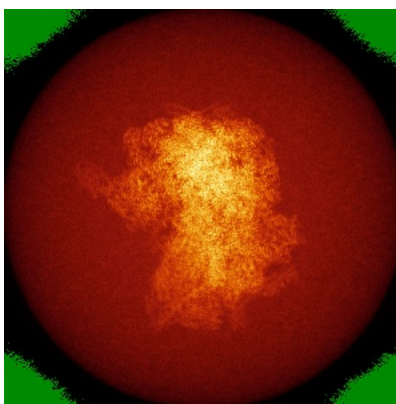
The images above show the largest variance slices of the map in three orthogonal directions.

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

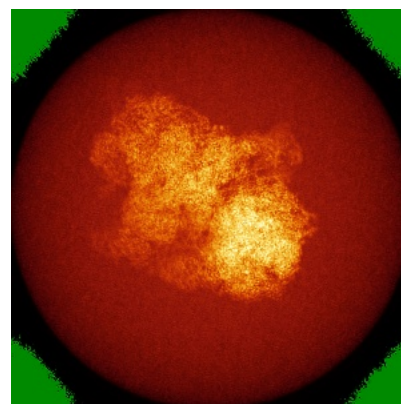
6.4.1 Primary map



X

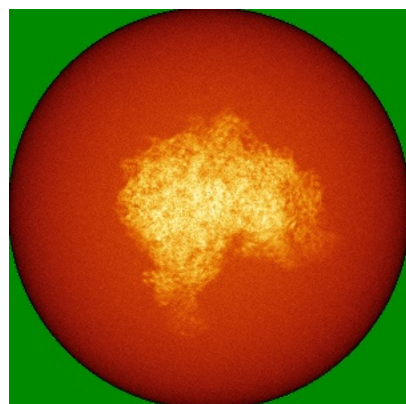


Y

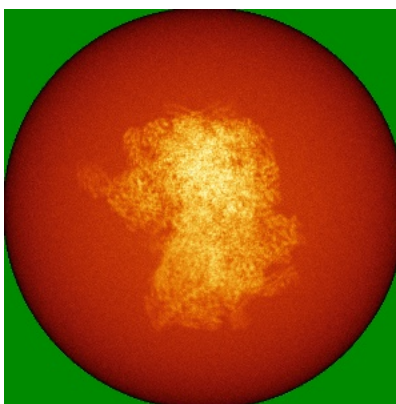


Z

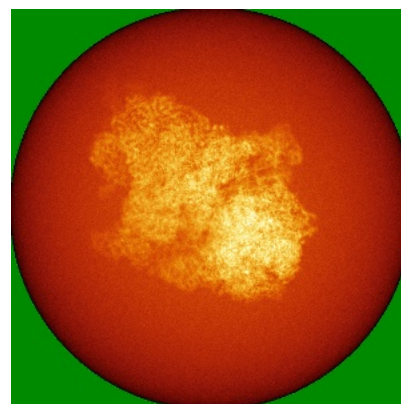
6.4.2 Raw map



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](#)

This section was not generated.

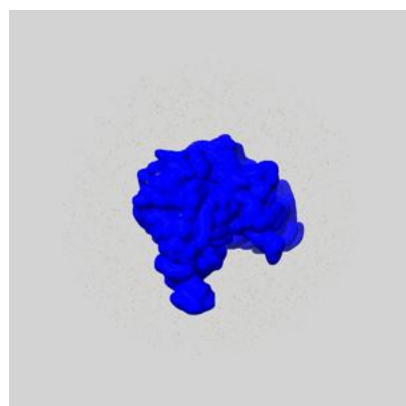
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

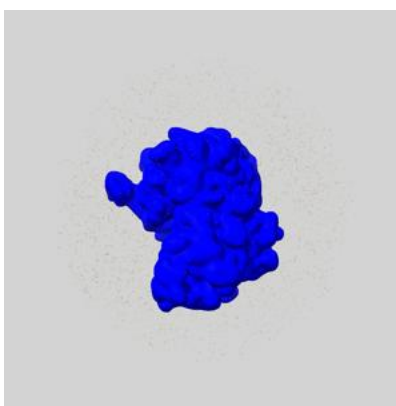
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

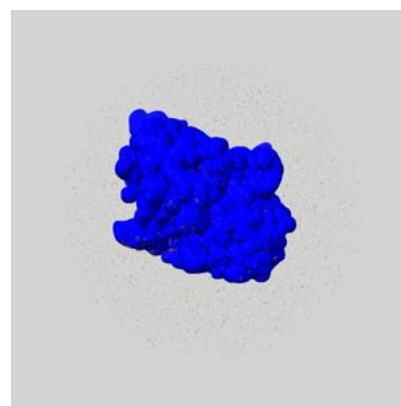
6.6.1 emd_11032_msk_1.map [i](#)



X



Y

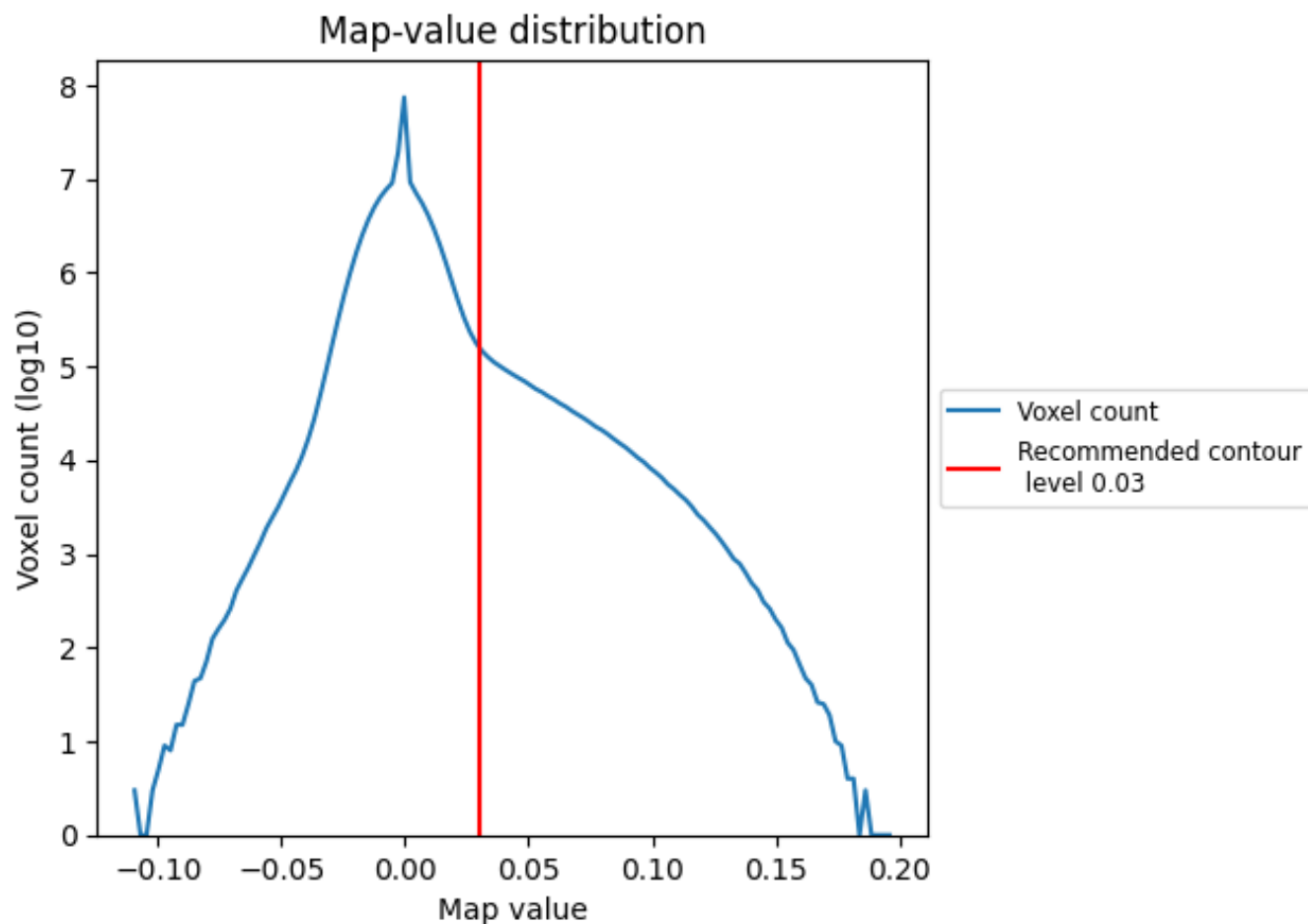


Z

7 Map analysis [i](#)

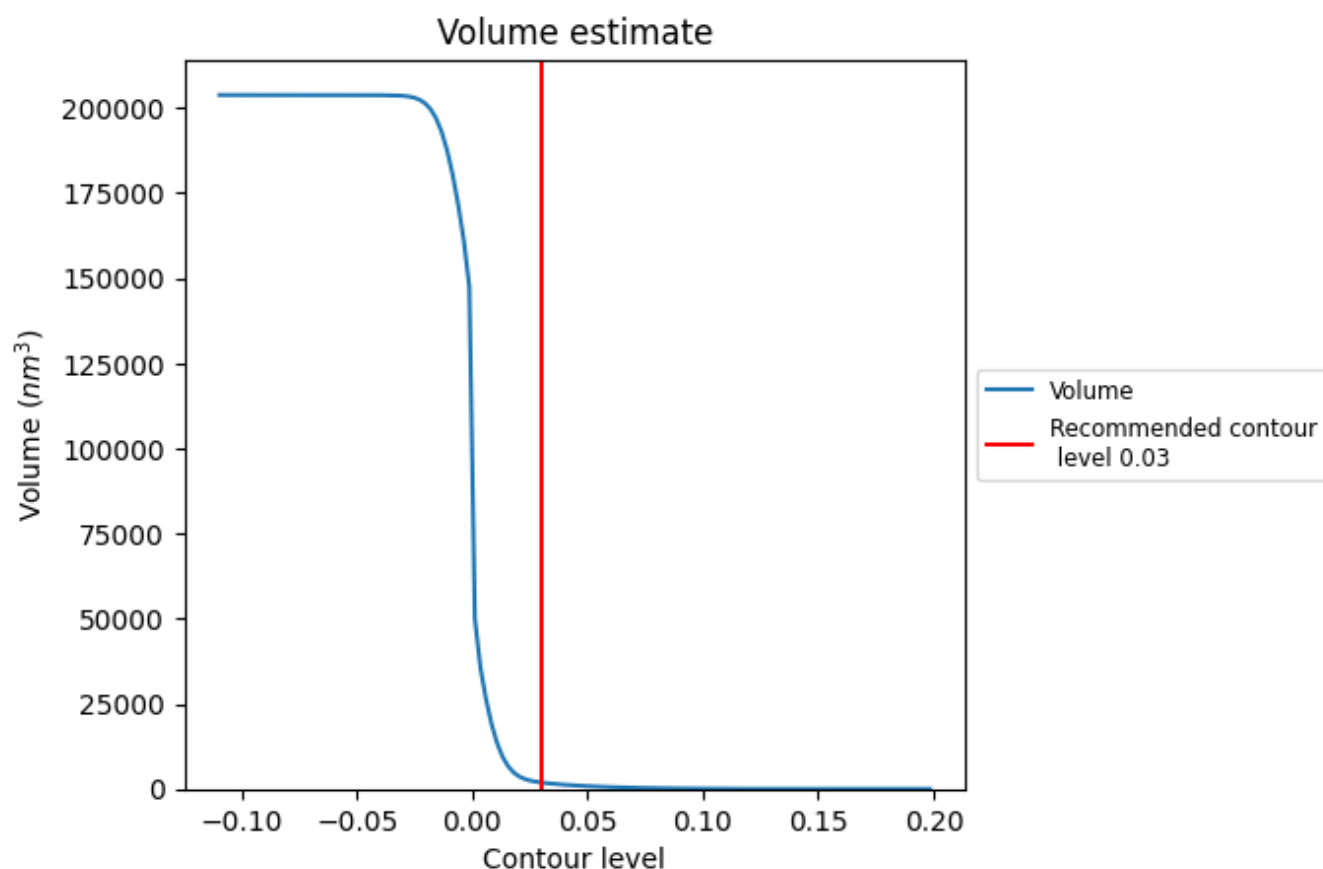
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

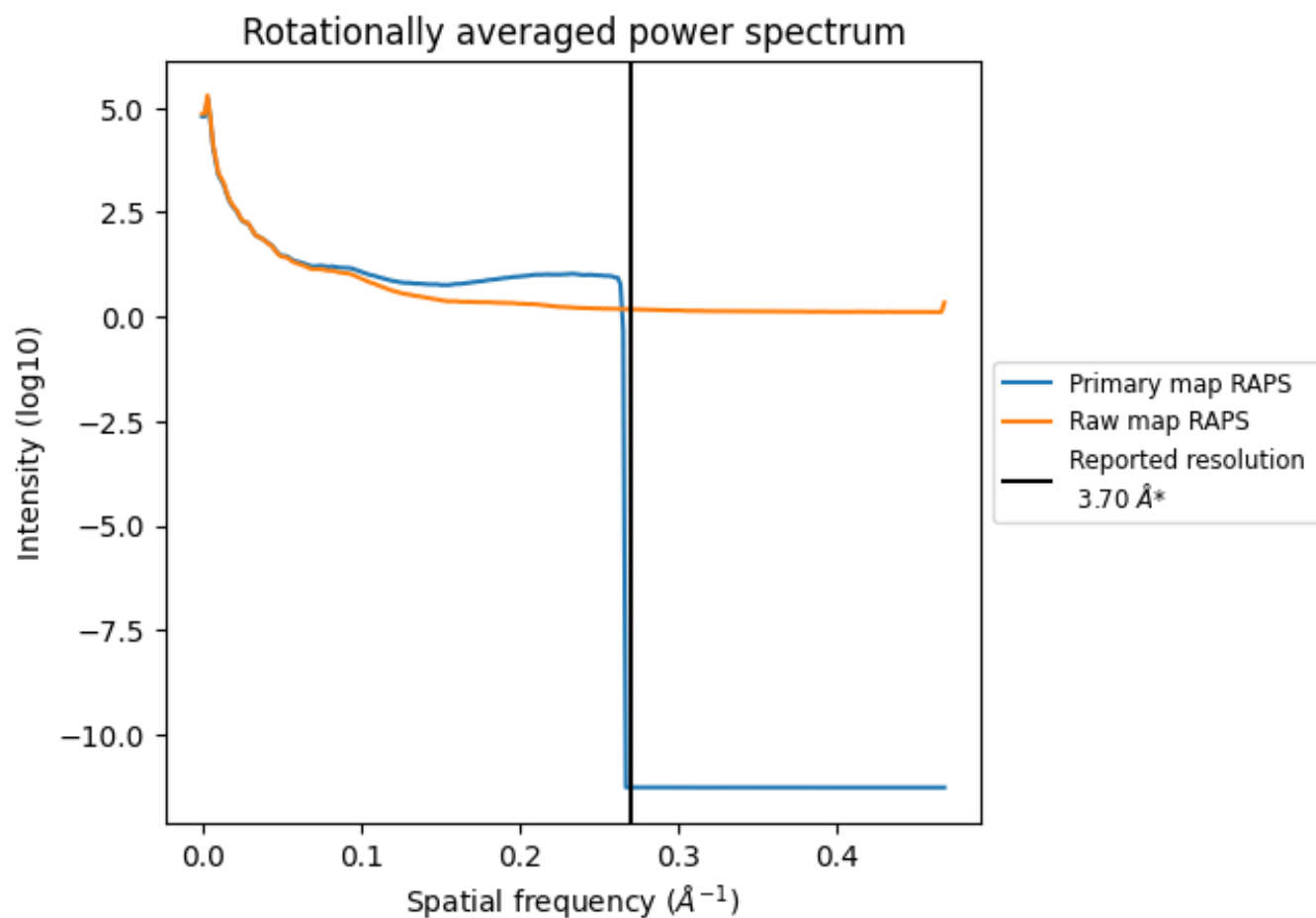
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1885 nm³; this corresponds to an approximate mass of 1703 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

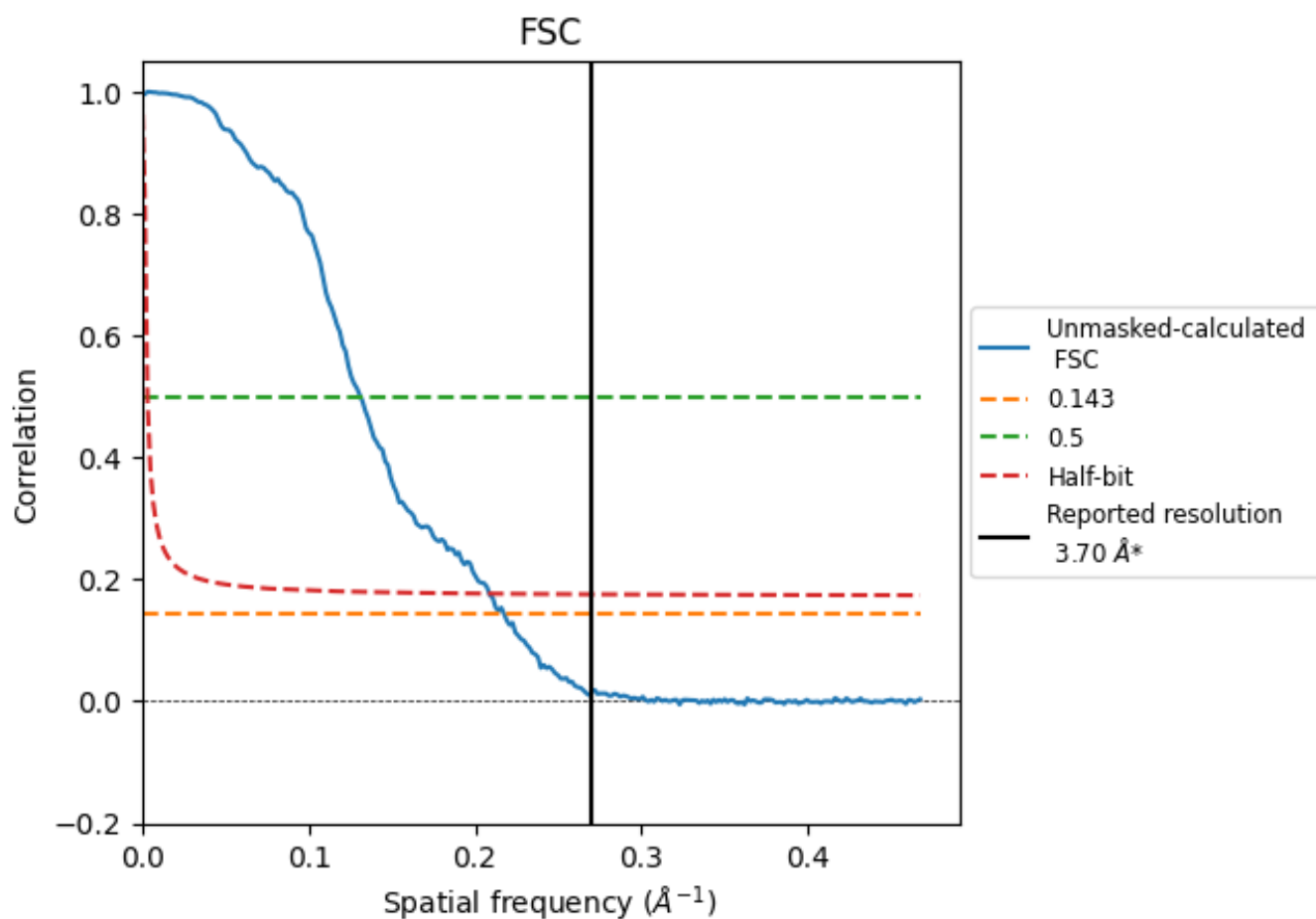


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.60	7.62	4.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.60 differs from the reported value 3.7 by more than 10 %

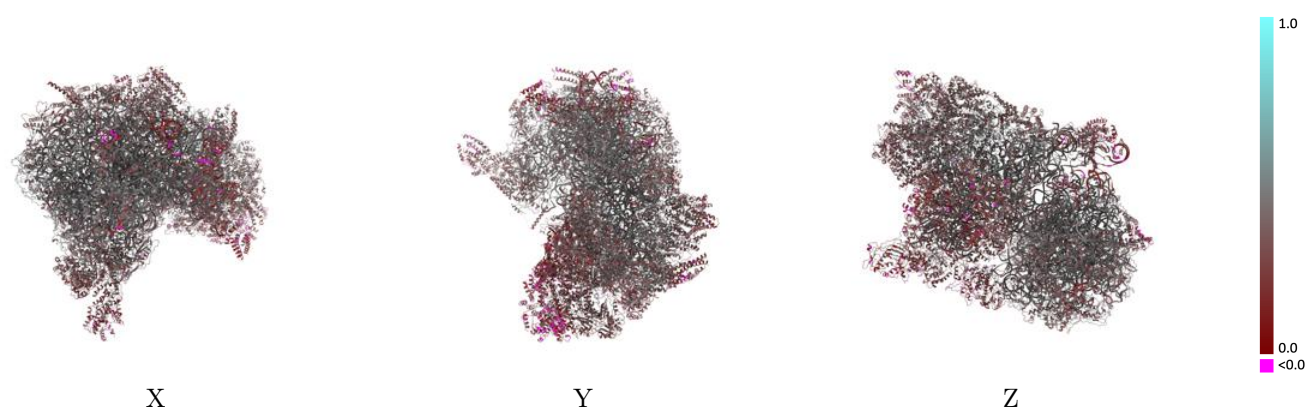
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-11032 and PDB model 6Z1P. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)

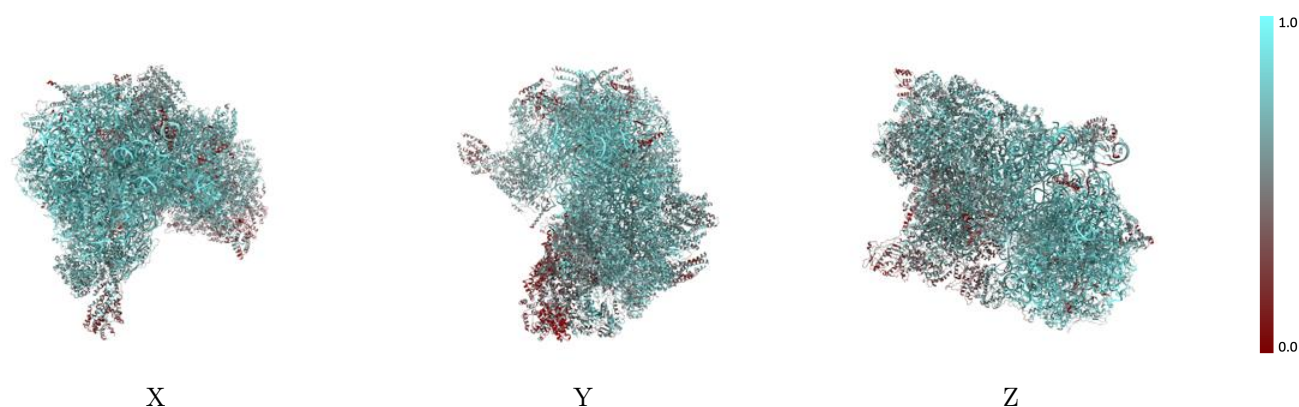
This section was not generated.

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



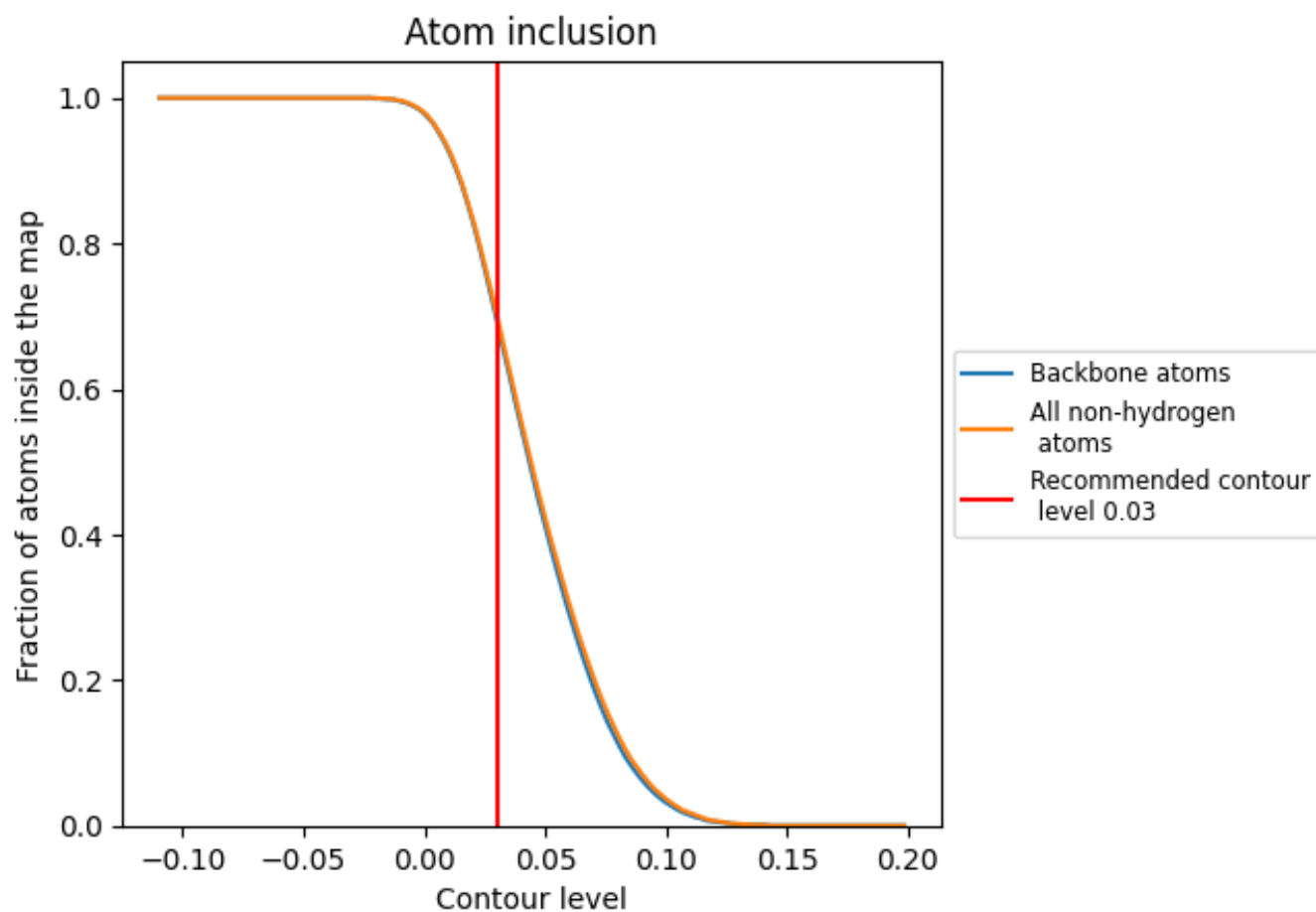
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 70% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7010	 0.3830
AA	 0.7610	 0.4440
AB	 0.7120	 0.4090
AC	 0.6710	 0.3650
AD	 0.9000	 0.5190
AE	 0.6910	 0.4150
AF	 0.7750	 0.4570
AG	 0.7700	 0.4630
AH	 0.5040	 0.2540
AI	 0.6990	 0.3960
AJ	 0.7350	 0.4430
AK	 0.3640	 0.1780
AL	 0.7860	 0.4570
AM	 0.6830	 0.3790
AN	 0.6470	 0.3750
AO	 0.7150	 0.3930
AP	 0.7070	 0.3860
AQ	 0.7820	 0.4570
AR	 0.5120	 0.2630
AS	 0.5920	 0.3190
AT	 0.5240	 0.2980
AU	 0.6740	 0.3660
AV	 0.7620	 0.4500
Aa	 0.8760	 0.4320
Ab	 0.8930	 0.4460
Ac	 0.7560	 0.4580
Ad	 0.7240	 0.4340
Ae	 0.7370	 0.4290
Af	 0.5020	 0.2960
Ag	 0.7410	 0.4160
Ah	 0.3770	 0.2760
Ai	 0.5970	 0.2870
Aj	 0.3770	 0.2440
Ak	 0.4290	 0.2720
Al	 0.7000	 0.3830



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Chain	Atom inclusion	Q-score
Am	 0.5010	 0.3110
An	 0.6150	 0.3510
Ao	 0.7230	 0.4260
Ap	 0.7460	 0.4650
Aq	 0.7380	 0.4290
Ar	 0.7470	 0.4510
As	 0.6910	 0.3850
At	 0.7580	 0.4460
Au	 0.7380	 0.4330
Av	 0.7540	 0.4390
Aw	 0.7330	 0.4300
Ax	 0.6960	 0.4060
Ay	 0.7380	 0.4240
Az	 0.6720	 0.3820
BA	 0.5620	 0.3540
BB	 0.6230	 0.3650
BC	 0.8860	 0.4930
BD	 0.6720	 0.3790
BE	 0.6720	 0.4120
BF	 0.7830	 0.4430
BG	 0.5390	 0.3170
BH	 0.7140	 0.3560
BI	 0.6640	 0.3950
BJ	 0.6600	 0.3690
BK	 0.7420	 0.4310
BL	 0.6970	 0.4100
BM	 0.3520	 0.2350
BN	 0.7120	 0.3860
BO	 0.3010	 0.2350
BP	 0.5720	 0.2930
BQ	 0.5210	 0.2920
BR	 0.5920	 0.3300
BS	 0.3970	 0.2270
BT	 0.6090	 0.3160
BU	 0.4710	 0.2790
BV	 0.5000	 0.2710
BW	 0.2190	 0.2080
BX	 0.5670	 0.3580
BY	 0.5390	 0.2720
Ba	 0.8740	 0.4210
Bb	 0.8430	 0.4080
Bc	 0.6980	 0.4420

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Chain	Atom inclusion	Q-score
Bd	 0.5330	 0.3400
Be	 0.6930	 0.4220
Bf	 0.7070	 0.4390
Bg	 0.6850	 0.4030
Bh	 0.4650	 0.3010
Bi	 0.6010	 0.3720
Bj	 0.6400	 0.3880
Bk	 0.5930	 0.3520
Bl	 0.7120	 0.4240
Bm	 0.3900	 0.2720
Bn	 0.6310	 0.3780
Bo	 0.7270	 0.4180
Bp	 0.6990	 0.4030
Bq	 0.5590	 0.3700
Br	 0.6390	 0.3620
Bs	 0.5130	 0.3060
Bt	 0.6910	 0.4000
Bu	 0.6140	 0.3590
Bv	 0.5990	 0.3290
Bw	 0.5100	 0.3060
Bx	 0.4970	 0.3070
By	 0.5480	 0.3250
Bz	 0.6660	 0.3690