wwPDB EM Validation Summary Report ⓘ

Jul 4, 2024 – 12:12 am BST

PDB ID	:	6ZSE
EMDB ID	:	EMD-11395
Title	:	Human mitochondrial ribosome in complex with mRNA, A/P-tRNA and P/E-tRNA
Authors	:	Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.
Deposited on	:	2020-07-15
Resolution	:	5.00 Å(reported)

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

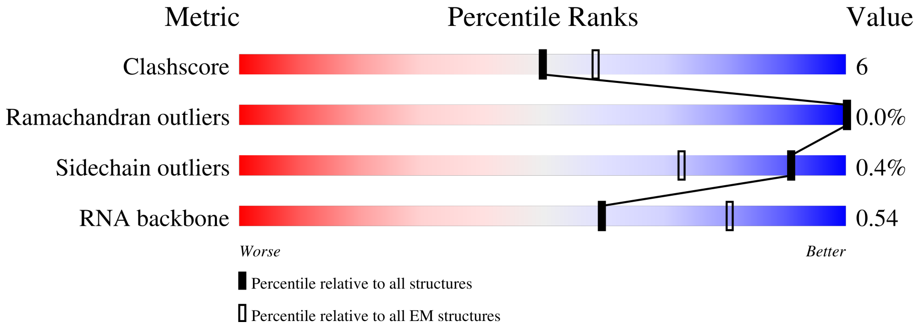
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

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

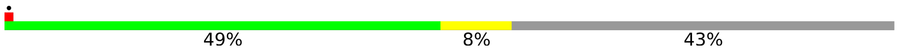
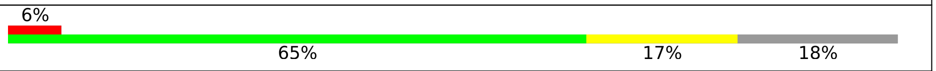
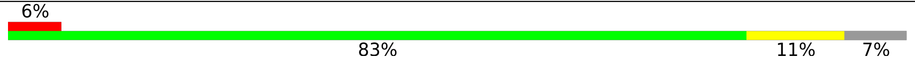
The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	0	188	
2	1	65	
3	2	92	
4	3	188	
5	4	103	
6	5	423	
7	6	380	

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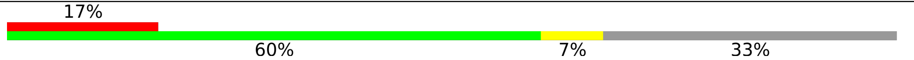
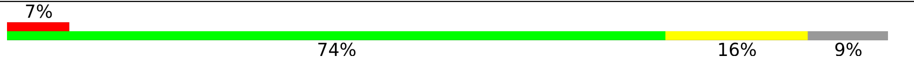
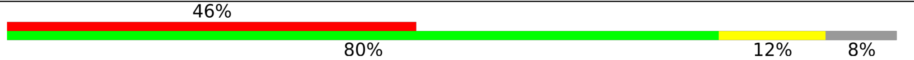
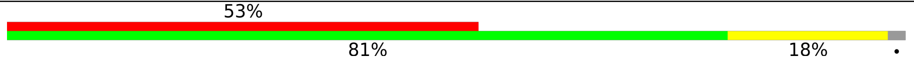
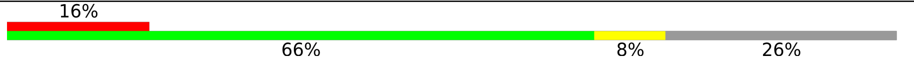
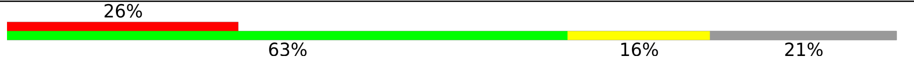
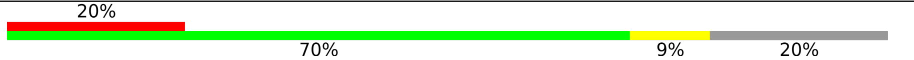
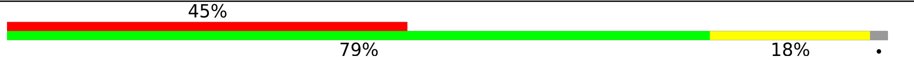
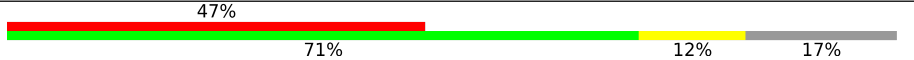
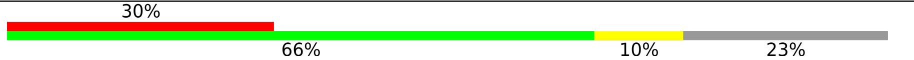
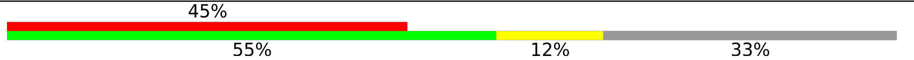
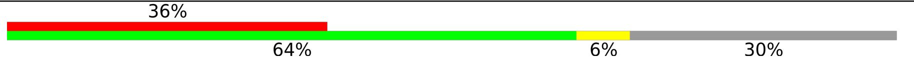
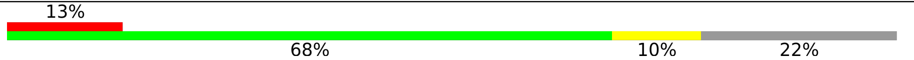
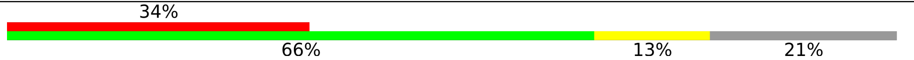
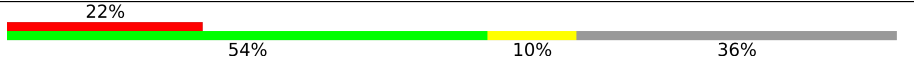
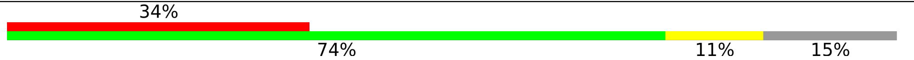
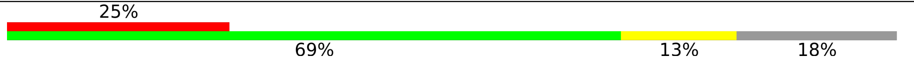
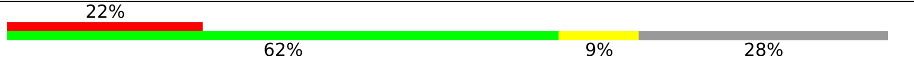
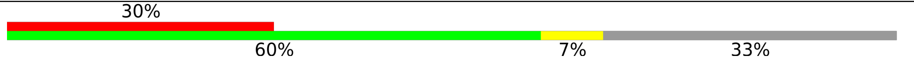
Mol	Chain	Length	Quality of chain
8	7	338	
9	8	206	
10	9	137	
11	XA	1561	
12	A0	218	
13	A1	323	
14	A2	118	
15	A3	199	
16	A4	689	
17	AA	924	
18	AB	296	
19	AC	167	
20	AD	430	
21	AE	125	
22	AF	242	
23	AG	396	
24	AH	201	
25	AI	194	
26	AJ	138	
27	AK	128	
28	AL	257	
29	AM	137	
30	AN	130	
31	AO	258	
32	AP	142	

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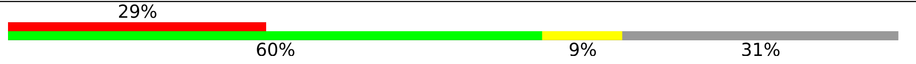
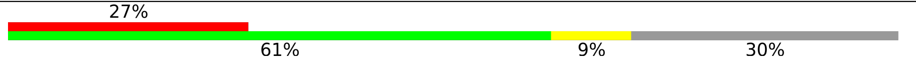
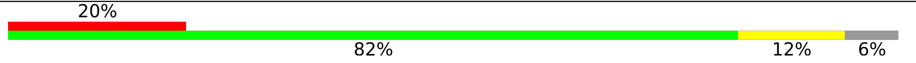
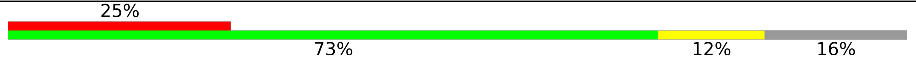
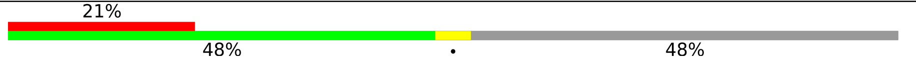
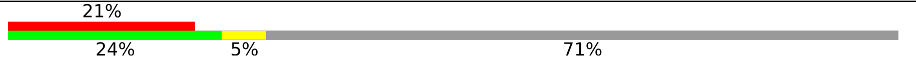
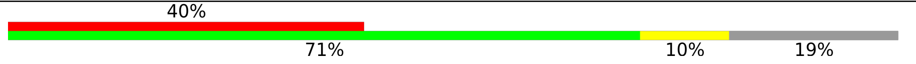
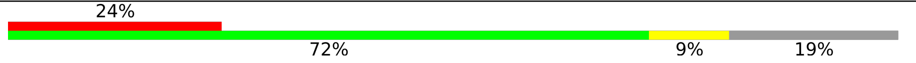
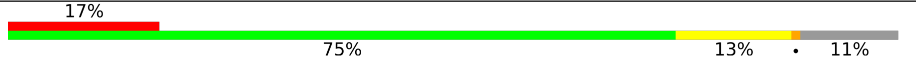
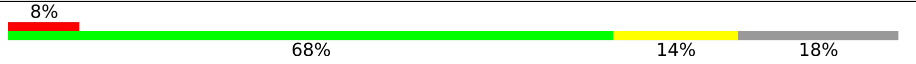
Mol	Chain	Length	Quality of chain
33	AQ	87	
34	AR	360	
35	AS	190	
36	AT	173	
37	AU	205	
38	AV	414	
39	AW	187	
40	AX	398	
41	AY	395	
42	AZ	106	
43	XB	72	
44	XD	305	
45	XE	348	
46	XF	311	
47	XH	267	
48	XI	261	
49	XJ	192	
50	XK	178	
51	XL	145	
52	XM	296	
53	XN	251	
54	XO	175	
55	XP	180	
56	XQ	292	
57	XR	149	

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Mol	Chain	Length	Quality of chain
58	XS	205	• 70% 8% 22%
59	XT	206	70% 10% 19%
60	XU	153	• 82% 10% 8%
61	XV	216	6% 79% 15% 6%
62	XW	148	• 61% 14% • 25%
63	XX	256	• 82% 12% 5%
64	XY	250	56% 15% 29%
65	XZ	161	• 68% 6% 25%
66	a	142	6% 68% 32%
67	b	215	69% 31%
68	c	332	• 83% 17%
69	d	306	8% 70% 29%
70	e	279	20% 75% • 24%
71	f	212	14% 67% 33%
72	g	166	• 79% • 20%
73	h	158	• 68% 32%
74	i	128	• 75% • 24%
75	j	123	• 70% 30%
76	k	112	6% 85% 15%
77	l	138	9% 58% 42%
78	m	128	8% 47% 53%
79	o	102	• 91% • 8%
80	p	206	• 62% 38%
81	q	222	16% 74% 26%
82	r	196	• 78% 22%

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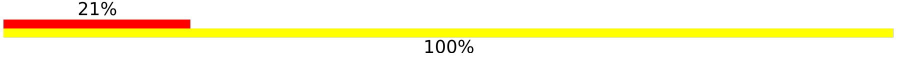
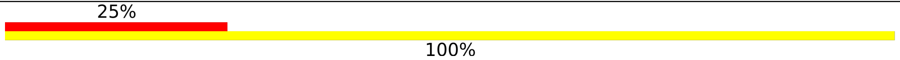
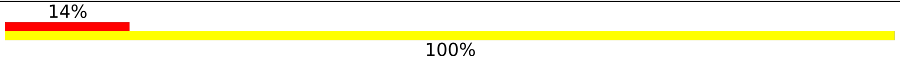
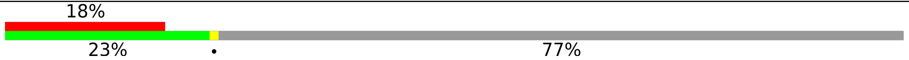
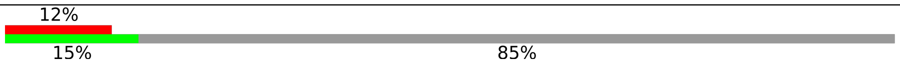
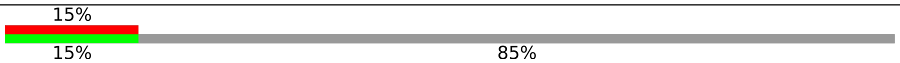
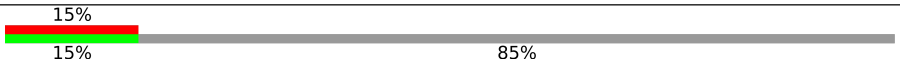
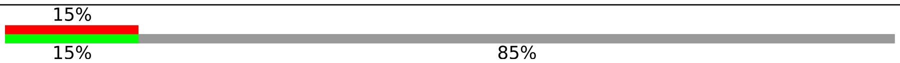
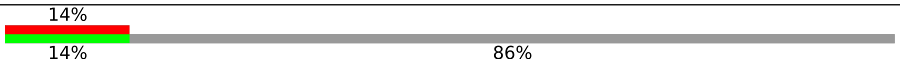
Mol	Chain	Length	Quality of chain
83	r1	14	
84	r2	76	
85	r3	73	
86	s	439	
87	t1	198	
87	t2	198	
87	t3	198	
87	t4	198	
87	t5	198	
87	t6	198	
88	A	8	

2 Entry composition (i)

There are 92 unique types of molecules in this entry. The entry contains 313629 atoms, of which 143000 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	0	108	1783	545	903	172	157	6	0	0

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	1	53	919	281	480	84	72	2	0	0

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2	46	782	233	406	83	59	1	0	0

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	3	95	1714	539	883	162	127	3	0	0

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	4	38	703	217	362	72	48	4	0	0

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	5	393	6405	2070	3201	559	564	11	0	0

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	354	Total 5787	C 1881	H 2840	N 525	O 532	S 9	0	0

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	291	Total 4737	C 1514	H 2372	N 401	O 432	S 18	0	0

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	139	Total 2377	C 747	H 1202	N 208	O 218	S 2	0	0

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	9	124	Total 1983	C 644	H 987	N 170	O 180	S 2	0	0

- Molecule 11 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	XA	1499	Total 47992	C 14284	H 16159	N 5756	O 10294	P 1499	0	0

- Molecule 12 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	A0	201	Total 3369	C 1065	H 1685	N 322	O 292	S 5	0	0

- Molecule 13 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	A1	275	Total 4491	C 1414	H 2261	N 380	O 425	S 11	0	0

- Molecule 14 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	A2	116	1889	574	964	181	162	8	0	0

- Molecule 15 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	A3	69	1292	393	682	130	86	1	0	0

- Molecule 16 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	A4	552	8955	2866	4485	756	820	28	0	0

- Molecule 17 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
17	AA	924	29592	8800	9964	3540	6364	924	0	0

- Molecule 18 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	AB	218	3545	1135	1769	322	309	10	0	0

- Molecule 19 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	AC	132	2170	699	1088	195	184	4	0	0

- Molecule 20 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	AD	343	5499	1706	2783	515	482	13	0	0

- Molecule 21 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	AE	122	1973	614	1001	177	177	4	0	0

- Molecule 22 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	AF	201	3384	1069	1716	305	283	11	0	0

- Molecule 23 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	AG	304	4995	1593	2490	444	454	14	0	0

- Molecule 24 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	AH	135	2241	712	1136	187	203	3	0	0

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	AI	136	2063	637	1052	192	178	4	0	0

- Molecule 26 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	AJ	108	1725	521	887	169	142	6	0	0

- Molecule 27 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	AK	101	1746	537	885	179	140	5	0	0

- Molecule 28 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	AL	164	2855	883	1473	257	235	7	0	0

- Molecule 29 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	AM	116	1871	582	951	182	150	6	0	0

- Molecule 30 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	AN	107	1754	549	908	153	141	3	0	0

- Molecule 31 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	AO	185	3018	970	1490	285	267	6	0	0

- Molecule 32 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	AP	95	1561	493	796	132	132	8	0	0

- Molecule 33 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	AQ	85	1483	455	749	149	123	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	variant	UNP P82921

- Molecule 34 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	AR	250	4134	1314	2074	353	385	8	0	0

- Molecule 35 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	AS	133	2203	709	1103	196	194	1	0	0

- Molecule 36 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	AT	162	2672	850	1342	231	238	11	0	0

- Molecule 37 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	AU	173	2932	900	1471	294	263	4	0	0

- Molecule 38 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	AV	349	5729	1841	2862	478	536	12	0	0

- Molecule 39 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	AW	97	1551	486	785	137	139	4	0	0

- Molecule 40 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	AX	348	5617	1802	2803	491	510	11	0	0

- Molecule 41 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	AY	113	1868	621	912	157	176	2	0	0

- Molecule 42 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	AZ	86	1465	467	734	131	129	4	0	0

- Molecule 43 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
43	XB	59	1890	563	635	227	406	59	0	0

- Molecule 44 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	XD	236	3738	1145	1896	373	315	9	0	0

- Molecule 45 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	XE	304	4798	1539	2402	416	430	11	0	0

- Molecule 46 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	XF	250	4057	1294	2044	365	348	6	0	0

- Molecule 47 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
47	XH	95	1616	498	832	152	134	0	0

- Molecule 48 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	XI	211	3474	1086	1783	303	291	11	0	0

- Molecule 49 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	XJ	170	2658	825	1367	230	234	2	0	0

- Molecule 50 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	XK	177	2899	934	1448	259	251	7	0	0

- Molecule 51 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	XL	115	1830	559	941	171	154	5	0	0

- Molecule 52 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	XM	287	4681	1472	2376	425	402	6	0	0

- Molecule 53 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	XN	221	3586	1138	1808	325	305	10	0	0

- Molecule 54 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	XO	152	2528	784	1283	239	215	7	0	0

- Molecule 55 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	XP	143	2326	729	1162	223	207	5	0	0

- Molecule 56 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	XQ	238	4000	1268	2022	352	349	9	0	0

- Molecule 57 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	XR	140	2367	732	1214	231	186	4	0	0

- Molecule 58 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	XS	160	2638	829	1354	226	225	4	0	0

- Molecule 59 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	XT	166	2778	875	1410	254	232	7	0	0

- Molecule 60 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	XU	141	2335	743	1164	222	203	3	0	0

- Molecule 61 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
61	XV	202	3304	1051	1656	294	295	8	0	0

- Molecule 62 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	XW	111	Total	C	H	N	O	S	0	0
			1769	558	898	164	146	3		

- Molecule 63 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	XX	243	Total	C	H	N	O	S	0	0
			4089	1317	2054	351	362	5		

- Molecule 64 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	XY	178	Total	C	H	N	O	S	0	0
			3109	981	1575	295	254	4		

- Molecule 65 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	XZ	120	Total	C	H	N	O	S	0	0
			2008	626	1030	183	166	3		

- Molecule 66 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	a	97	Total	C	H	N	O	S	0	0
			1590	512	777	145	151	5		

- Molecule 67 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	b	148	Total	C	H	N	O	S	0	0
			2358	733	1180	229	213	3		

- Molecule 68 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	c	275	Total	C	H	N	O	S	0	0
			4437	1415	2220	383	410	9		

- Molecule 69 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
69	d	216	3501	1125	1743	305	315	13	0	0

- Molecule 70 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
70	e	213	3463	1105	1732	304	317	5	0	0

- Molecule 71 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
71	f	143	2313	737	1164	187	221	4	0	0

- Molecule 72 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
72	g	132	2183	710	1086	191	194	2	0	0

- Molecule 73 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
73	h	108	1748	560	866	154	165	3	0	0

- Molecule 74 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
74	i	97	1684	532	857	165	126	4	0	0

- Molecule 75 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
75	j	86	1367	426	678	134	127	2	0	0

- Molecule 76 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	k	95	Total 1477	C 456	H 745	N 139	O 132	S 5	0	0

- Molecule 77 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	l	80	Total 1327	C 427	H 654	N 118	O 125	S 3	0	0

- Molecule 78 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	m	60	Total 1025	C 309	H 525	N 104	O 85	S 2	0	0

- Molecule 79 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	o	94	Total 1601	C 501	H 804	N 165	O 128	S 3	0	0

- Molecule 80 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	p	127	Total 2141	C 661	H 1083	N 201	O 192	S 4	0	0

- Molecule 81 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	q	164	Total 2738	C 858	H 1359	N 267	O 249	S 5	0	0

- Molecule 82 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	r	152	Total 2514	C 792	H 1267	N 239	O 208	S 8	0	0

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
83	r1	14	252	126	28	84	14	0	0

- Molecule 84 is a RNA chain called A/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
84	r2	76	1485	723	230	456	76	0	0

- Molecule 85 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
85	r3	73	1420	692	216	439	73	0	0

- Molecule 86 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
86	s	370	6058	1946	3022	542	534	14	0	0

- Molecule 87 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
87	t1	46	733	228	379	56	70	2	0
87	t2	30	506	154	268	38	46	0	0
87	t3	30	506	154	268	38	46	0	0
87	t4	29	484	148	255	36	45	0	0
87	t5	29	484	148	255	36	45	0	0
87	t6	27	450	137	236	34	43	0	0

- Molecule 88 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
88	A	8	140	53	67	9	10	1	0	0

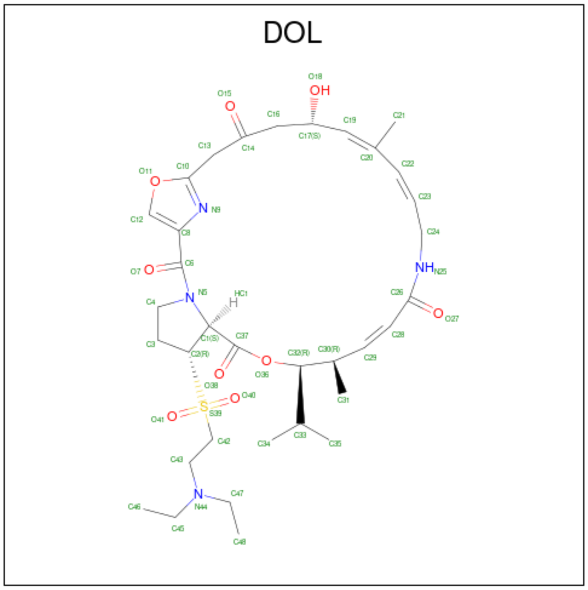
- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
89	0	1	Total Zn 1 1	0
89	4	1	Total Zn 1 1	0
89	AB	1	Total Zn 1 1	0
89	AO	1	Total Zn 1 1	0
89	AP	1	Total Zn 1 1	0
89	AT	1	Total Zn 1 1	0
89	r	1	Total Zn 1 1	0

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

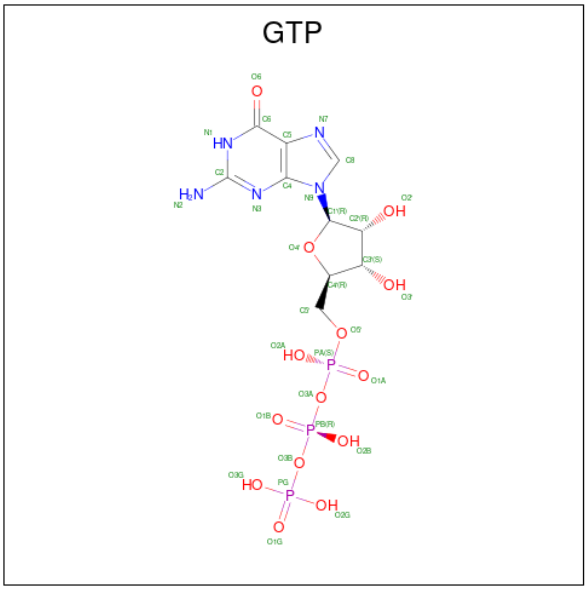
Mol	Chain	Residues	Atoms	AltConf
90	XA	141	Total Mg 141 141	0
90	AA	46	Total Mg 46 46	0
90	XD	1	Total Mg 1 1	0
90	XE	1	Total Mg 1 1	0
90	XI	1	Total Mg 1 1	0
90	XM	2	Total Mg 2 2	0
90	XW	1	Total Mg 1 1	0
90	g	1	Total Mg 1 1	0
90	o	1	Total Mg 1 1	0

- Molecule 91 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: $C_{34}H_{50}N_4O_9S$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
91	XA	1	98	34	50	4	9	1	0

- Molecule 92 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



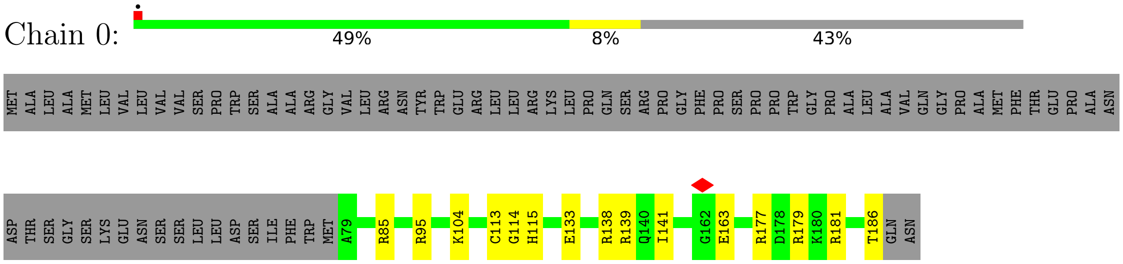
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
92	AX	1	42	10	10	5	14	3	0

3 Residue-property plots

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

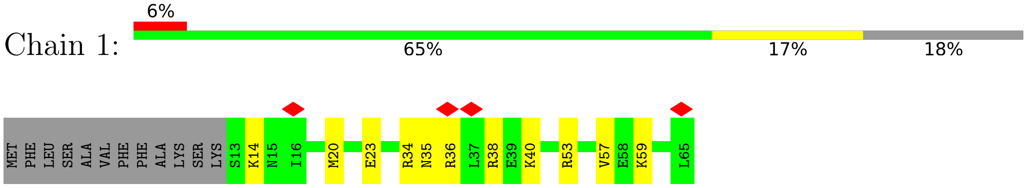
- Molecule 1: 39S ribosomal protein L32, mitochondrial

Chain 0:



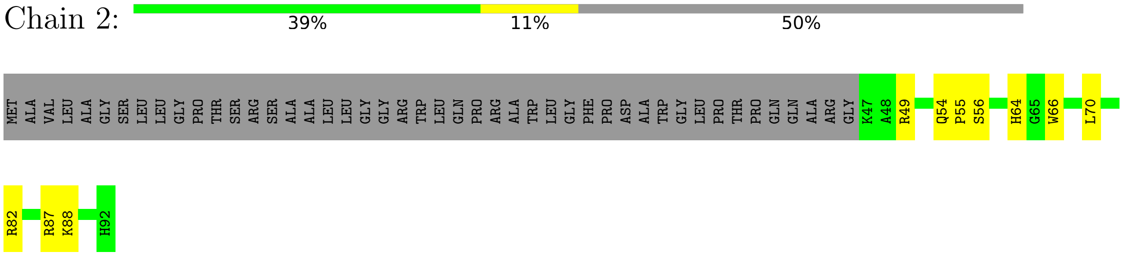
- Molecule 2: 39S ribosomal protein L33, mitochondrial

Chain 1:



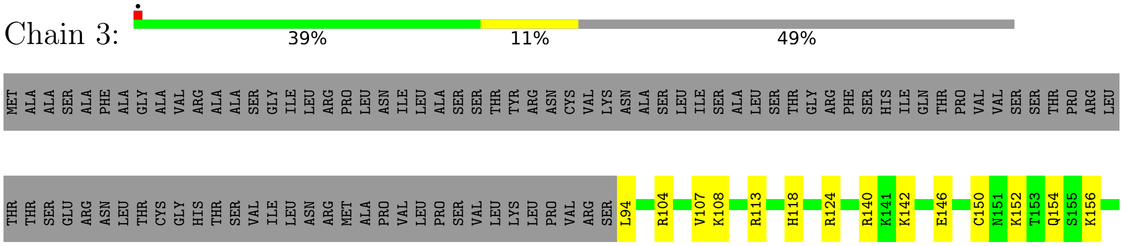
- Molecule 3: 39S ribosomal protein L34, mitochondrial

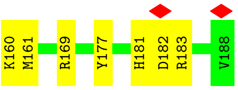
Chain 2:



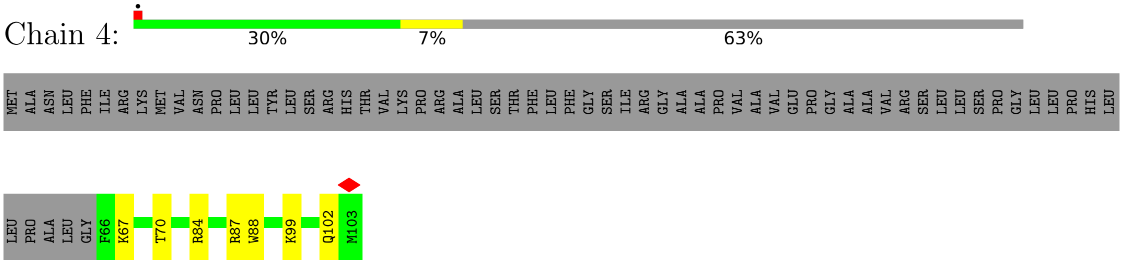
- Molecule 4: 39S ribosomal protein L35, mitochondrial

Chain 3:

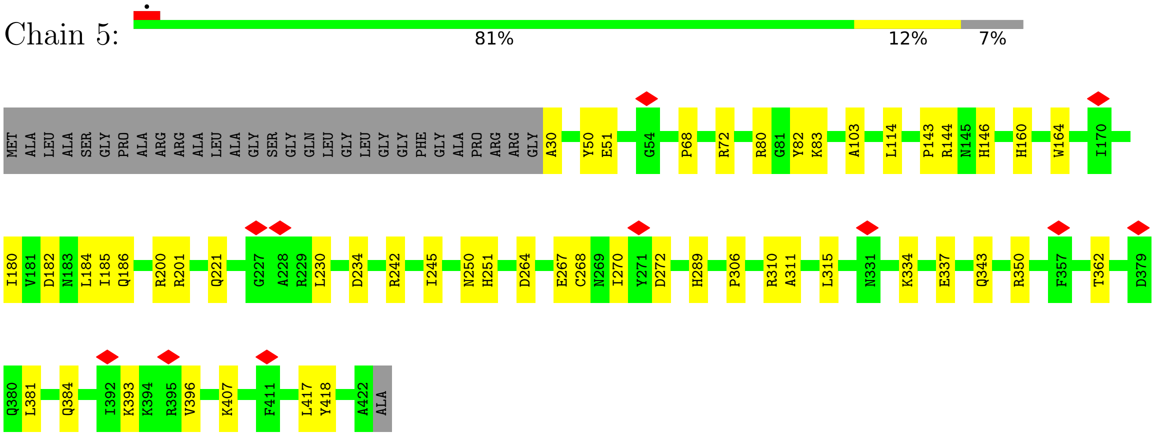




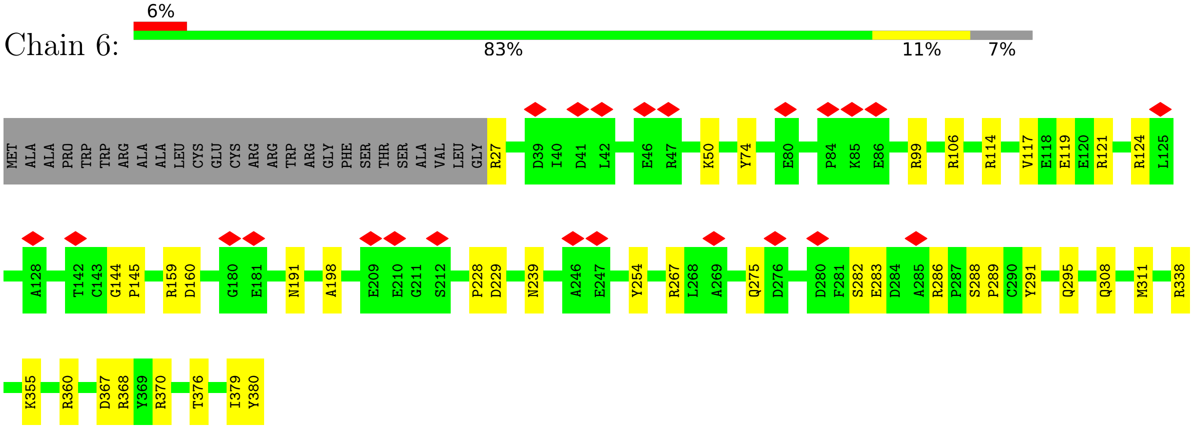
- Molecule 5: 39S ribosomal protein L36, mitochondrial



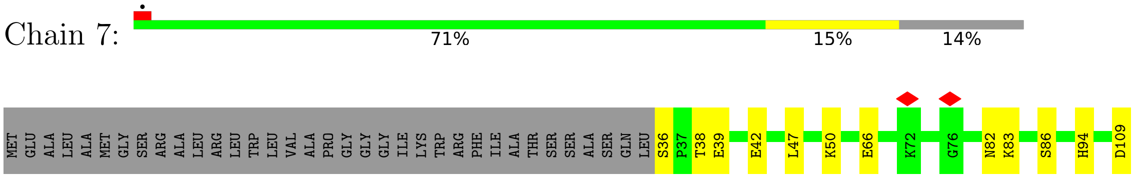
- Molecule 6: 39S ribosomal protein L37, mitochondrial

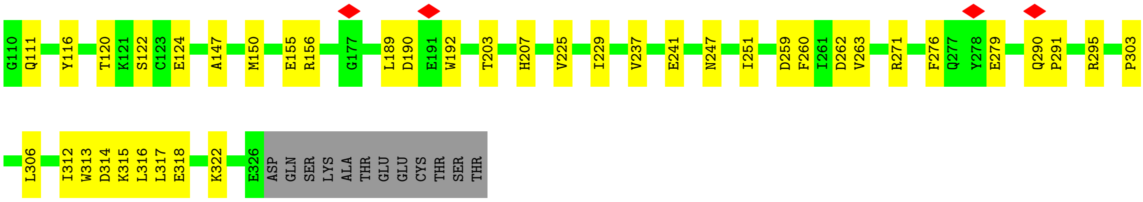


- Molecule 7: 39S ribosomal protein L38, mitochondrial



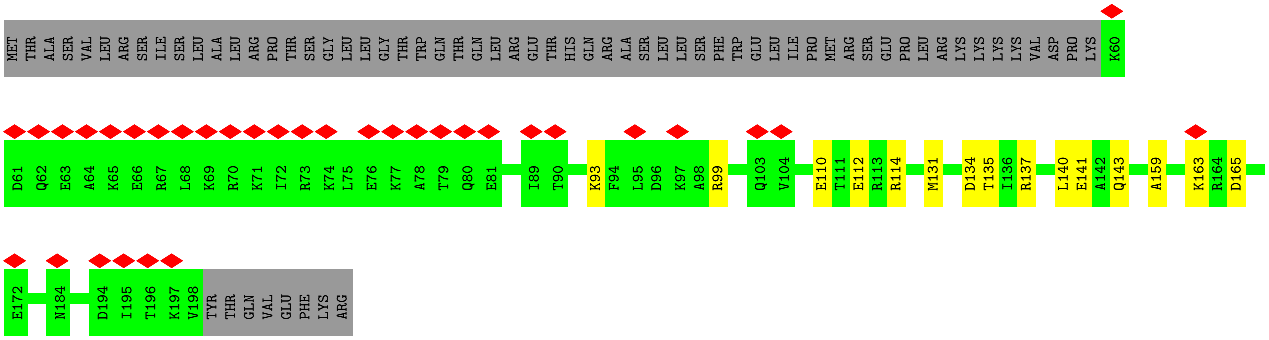
- Molecule 8: 39S ribosomal protein L39, mitochondrial





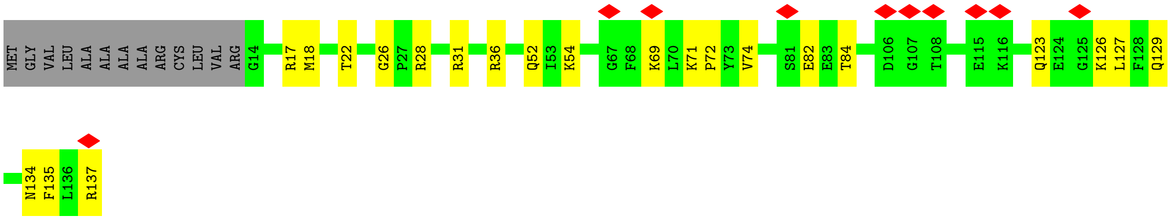
- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:



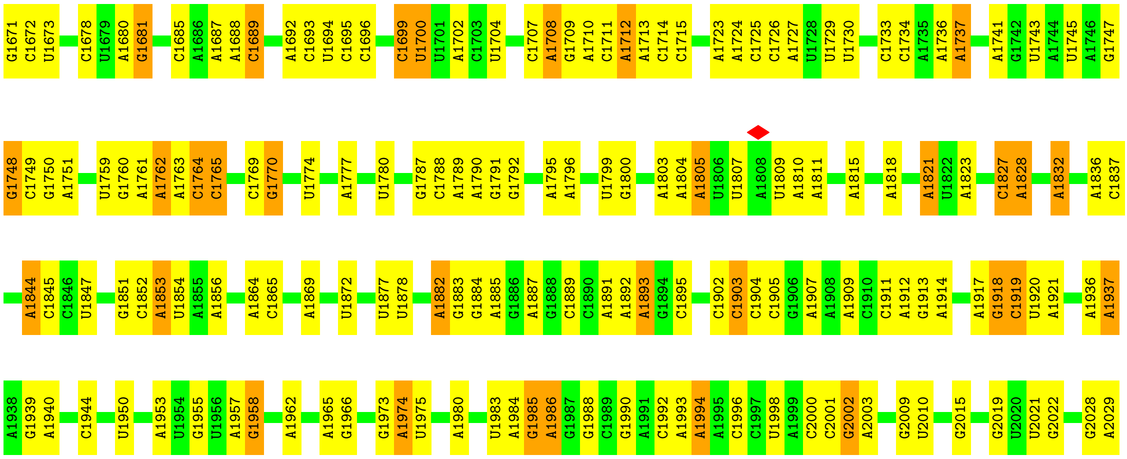
- Molecule 10: 39S ribosomal protein L41, mitochondrial

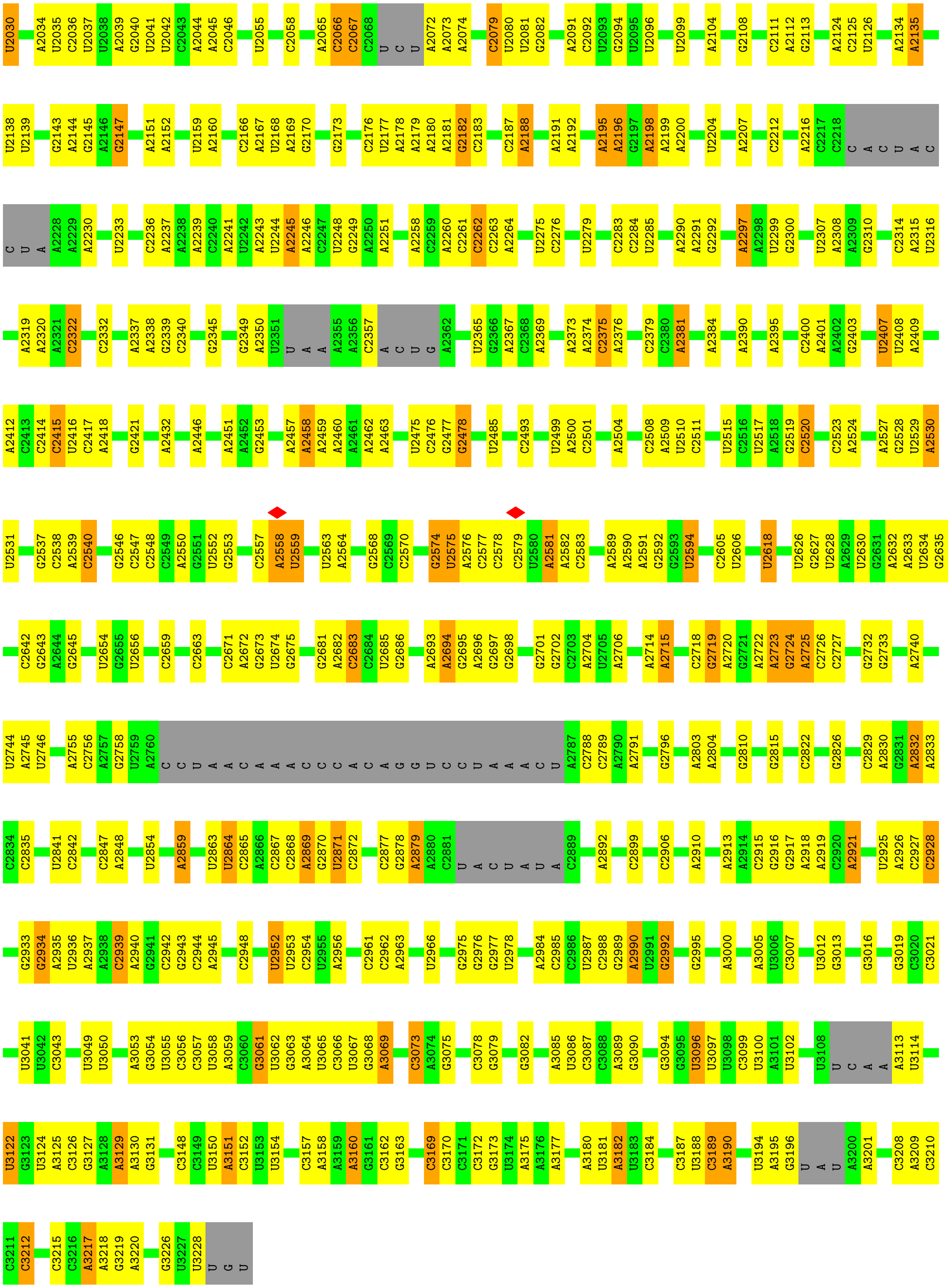
Chain 9:



- Molecule 11: 16S mitochondrial rRNA

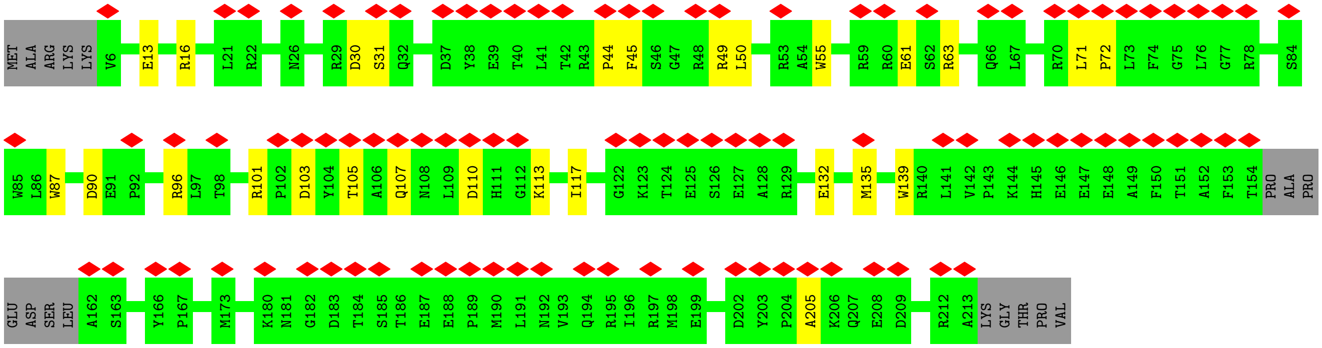
Chain XA:





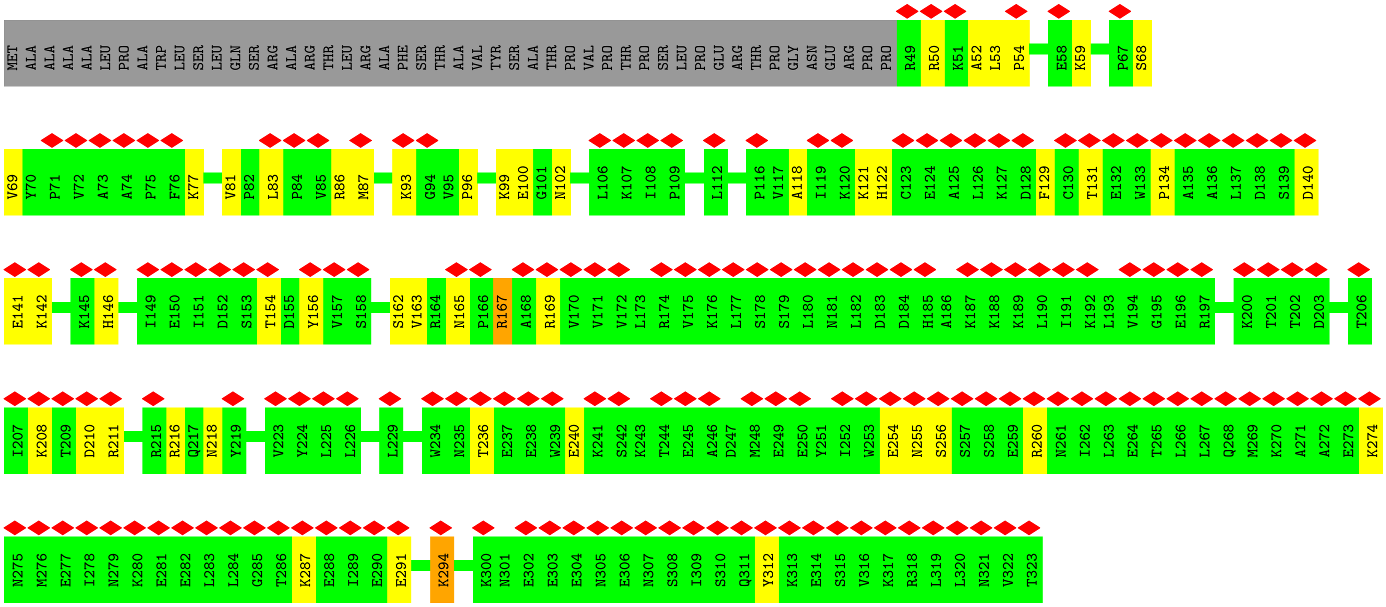
- Molecule 12: 28S ribosomal protein S34, mitochondrial

Chain A0:

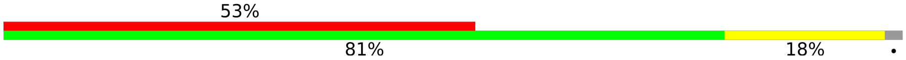


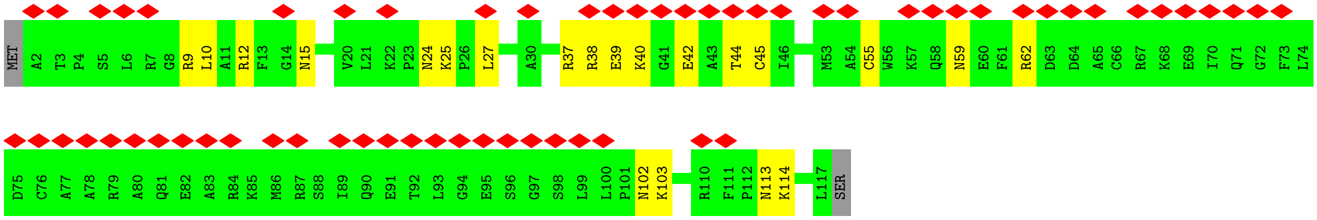
- Molecule 13: 28S ribosomal protein S35, mitochondrial

Chain A1:

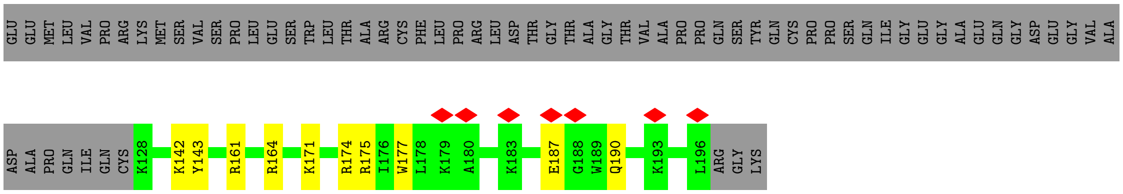
- Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2:




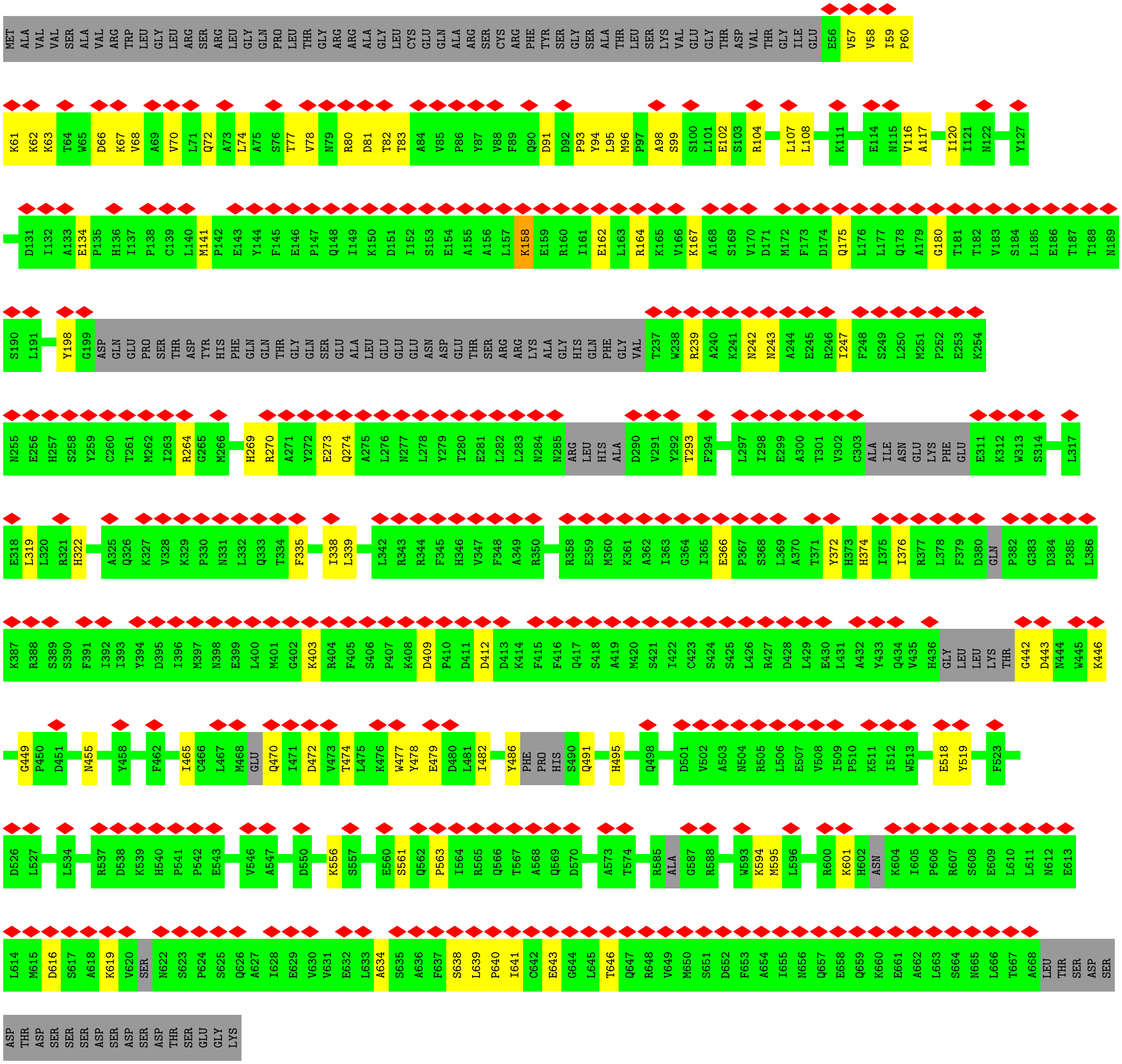
- Molecule 15: Aurora kinase A-interacting protein

Chain A3:

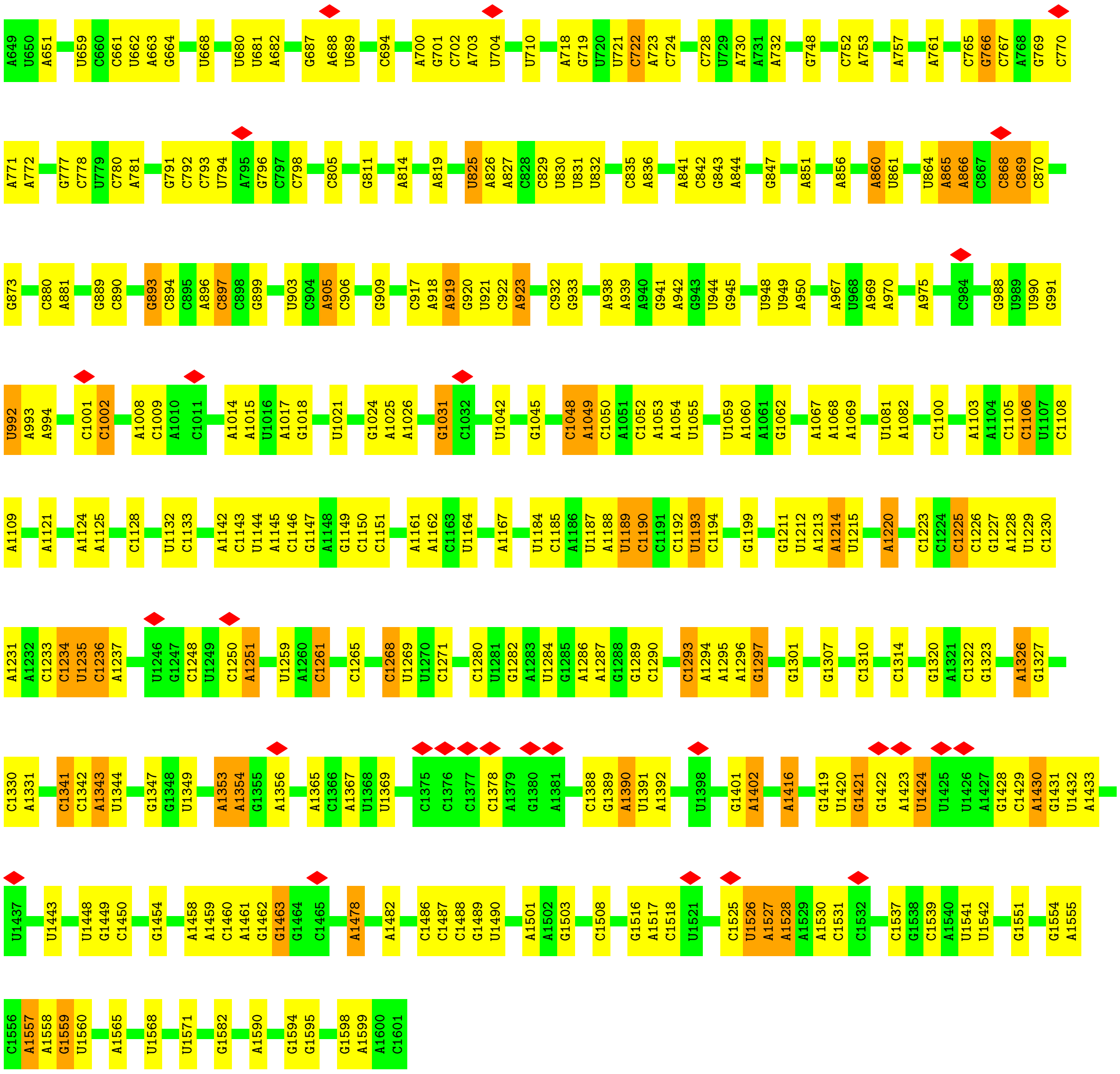
- Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4:



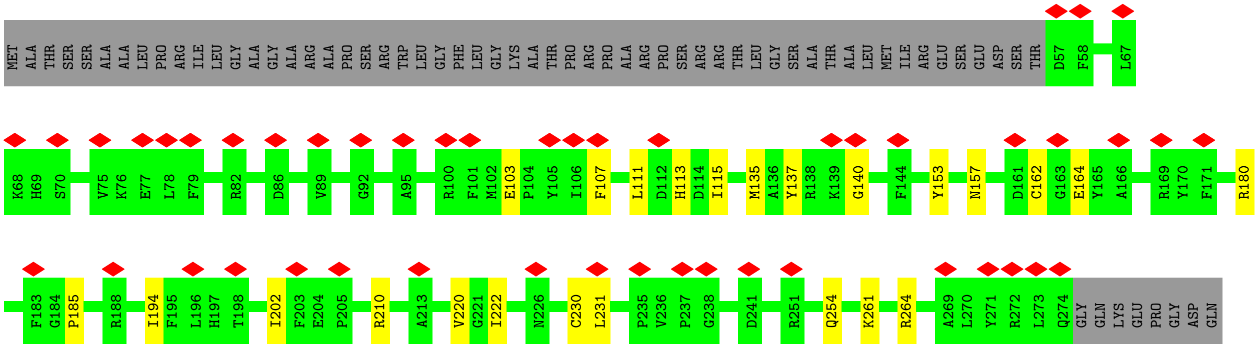
- Molecule 17: 12S mitochondrial rRNA

Chain AA:

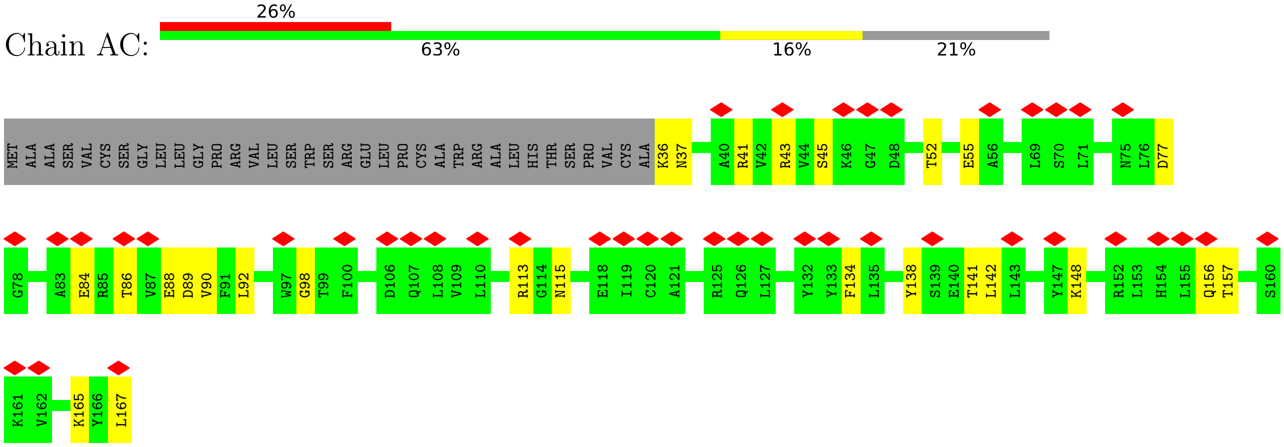


- Molecule 18: 28S ribosomal protein S2, mitochondrial

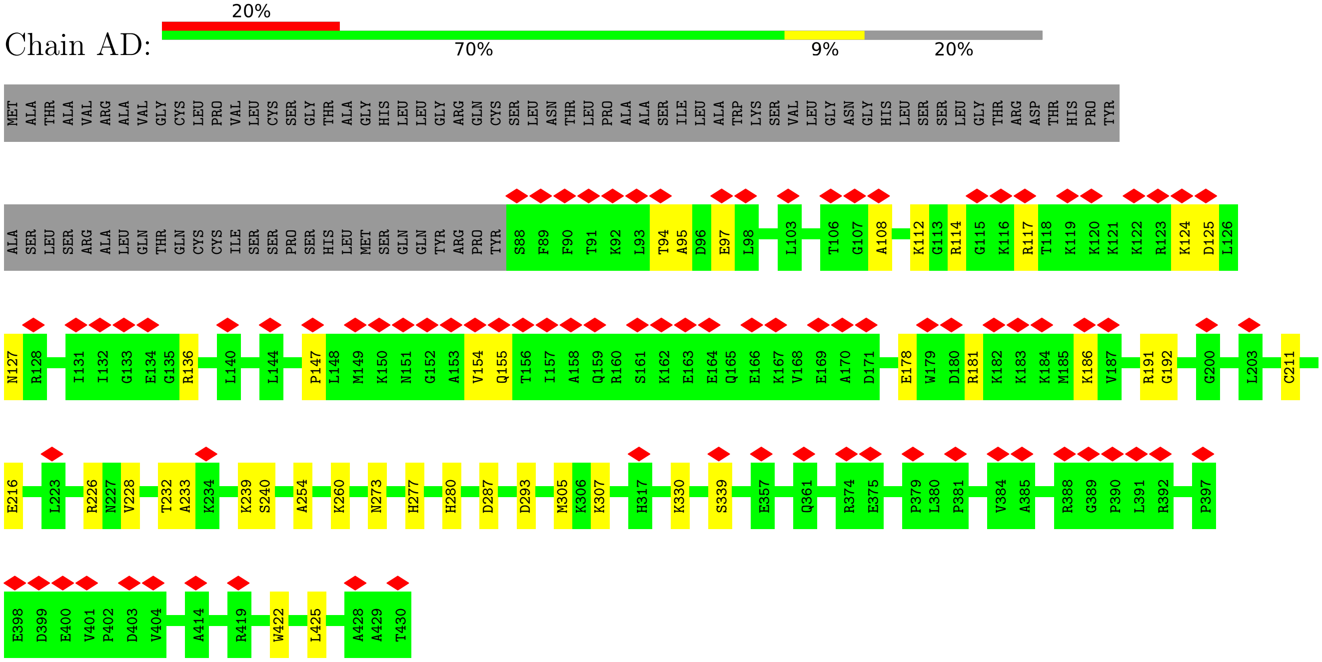
Chain AB:



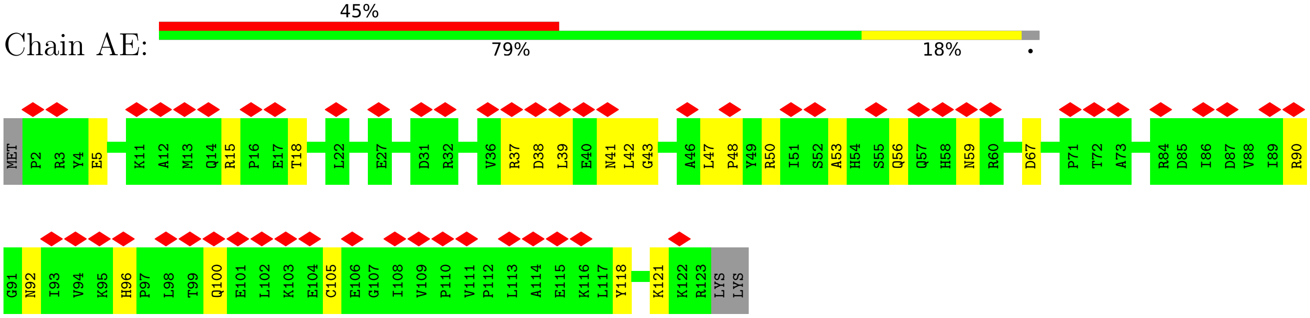
- Molecule 19: 28S ribosomal protein S24, mitochondrial



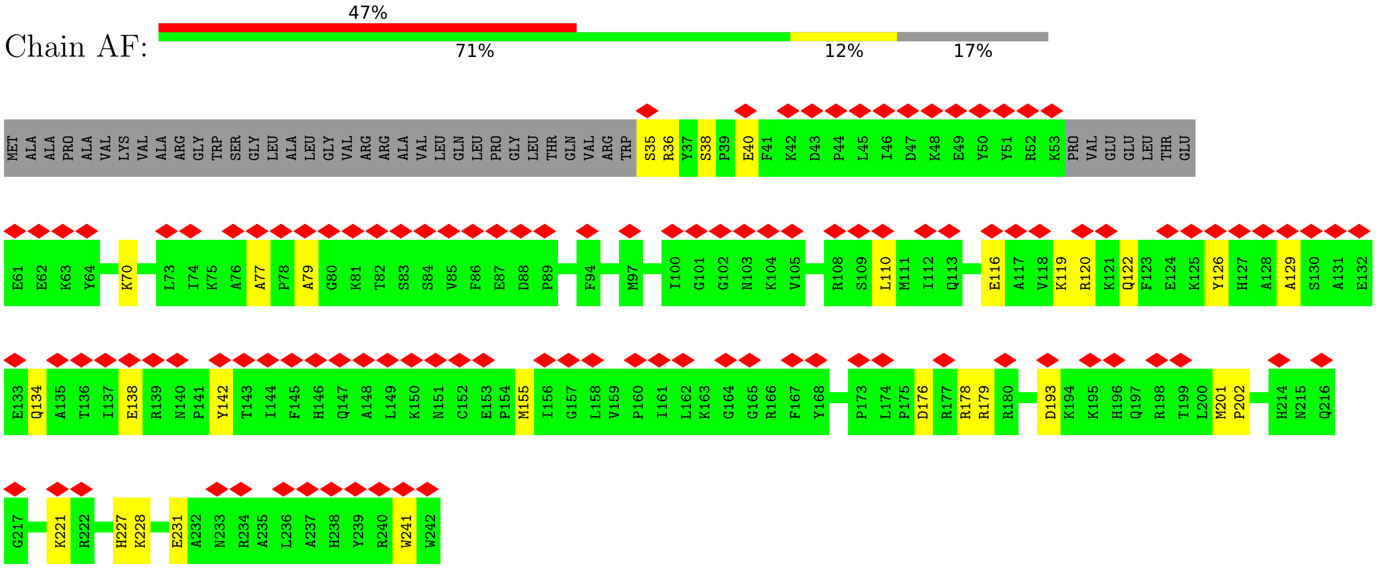
- Molecule 20: 28S ribosomal protein S5, mitochondrial



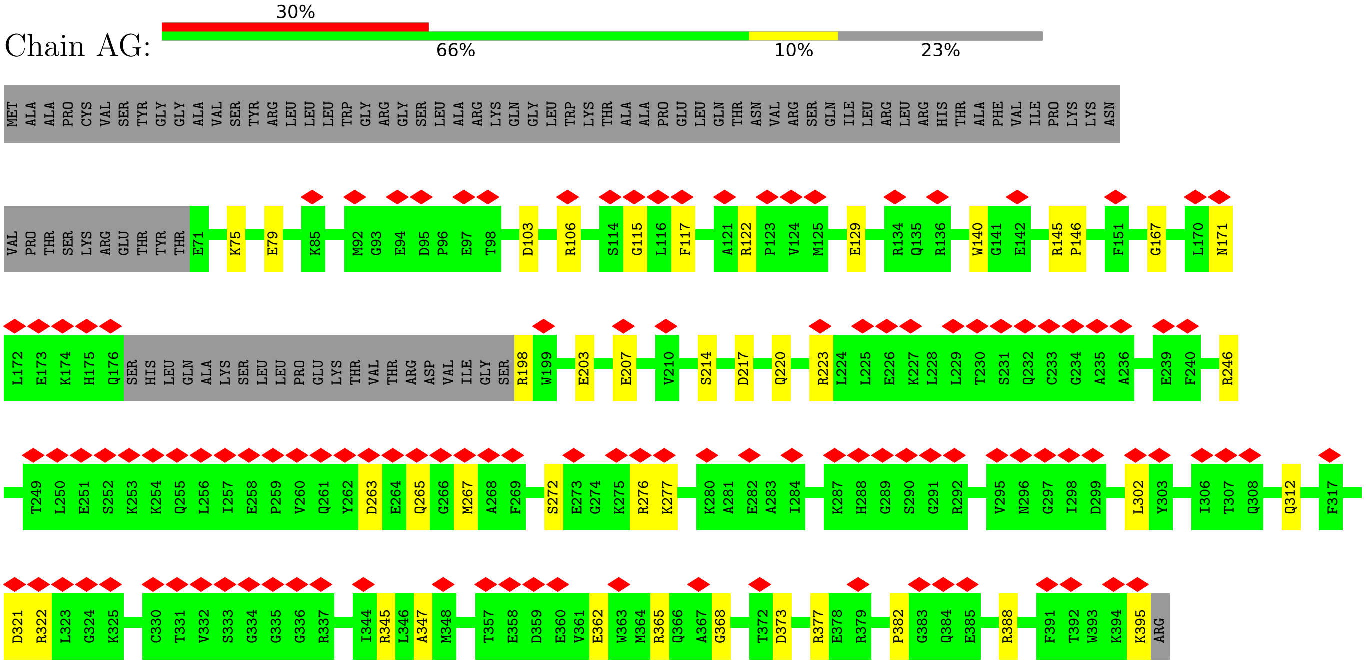
- Molecule 21: 28S ribosomal protein S6, mitochondrial



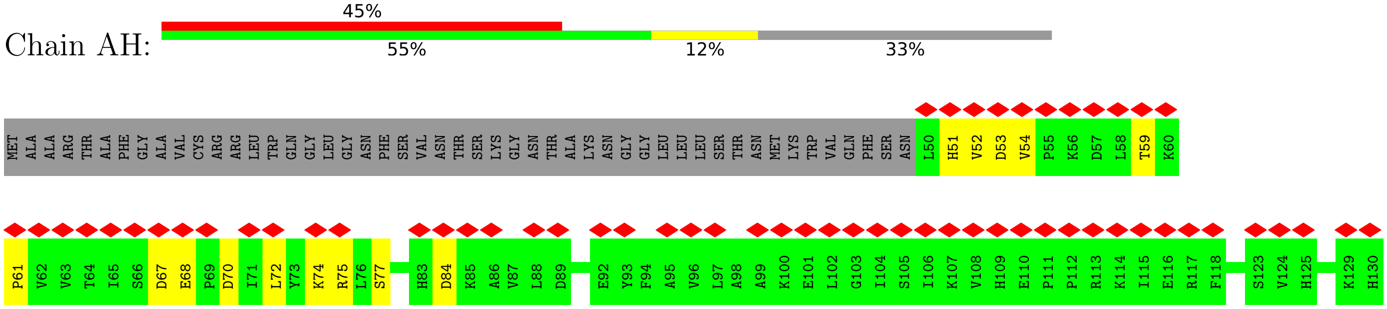
- Molecule 22: 28S ribosomal protein S7, mitochondrial

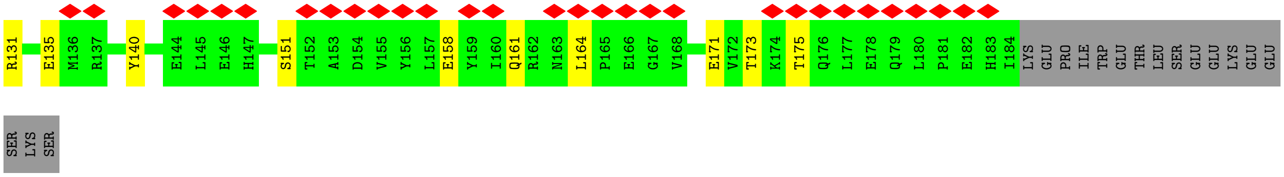


- Molecule 23: 28S ribosomal protein S9, mitochondrial



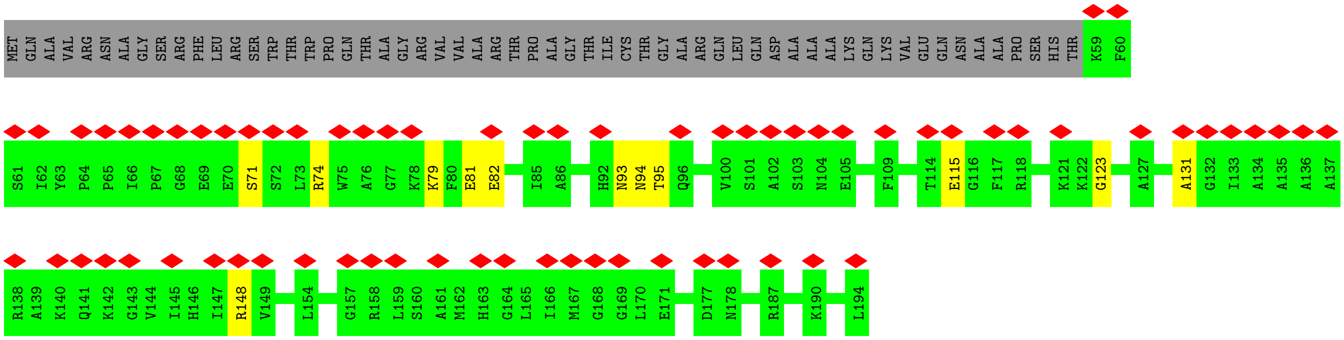
- Molecule 24: 28S ribosomal protein S10, mitochondrial





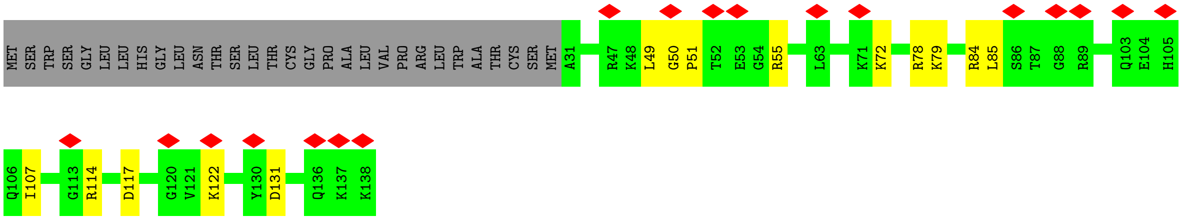
- Molecule 25: 28S ribosomal protein S11, mitochondrial

Chain AI:



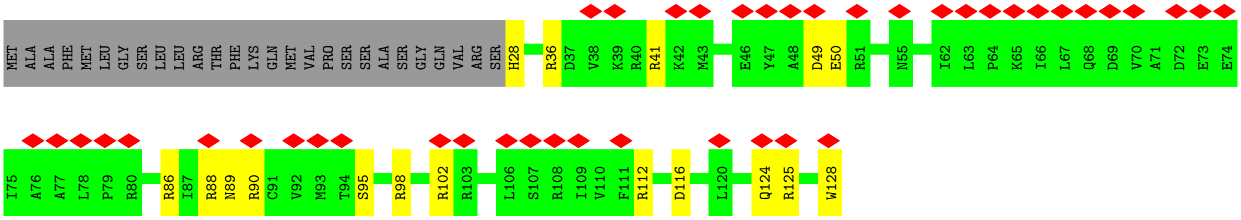
- Molecule 26: 28S ribosomal protein S12, mitochondrial

Chain AJ:



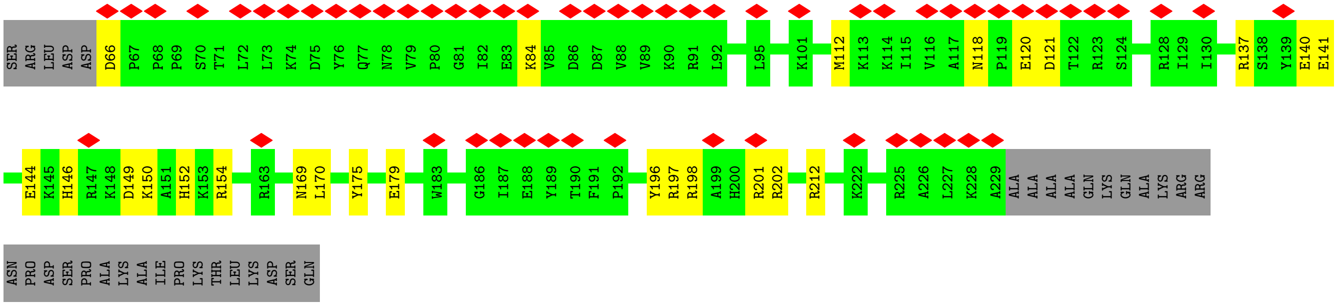
- Molecule 27: 28S ribosomal protein S14, mitochondrial

Chain AK:



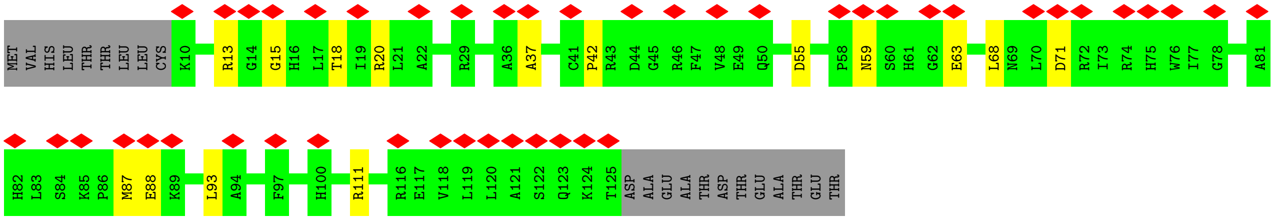
- Molecule 28: 28S ribosomal protein S15, mitochondrial

Chain AL:



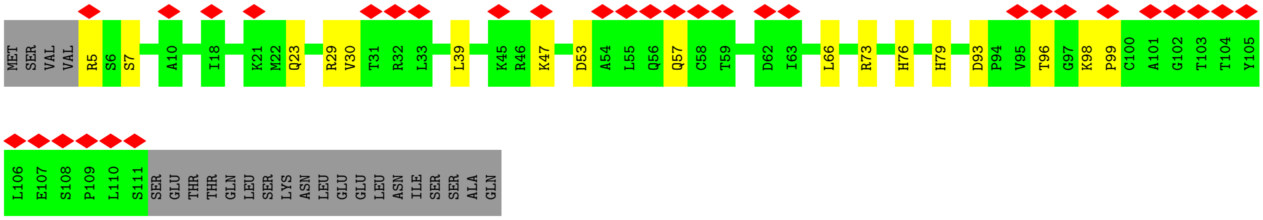
- Molecule 29: 28S ribosomal protein S16, mitochondrial

Chain AM:



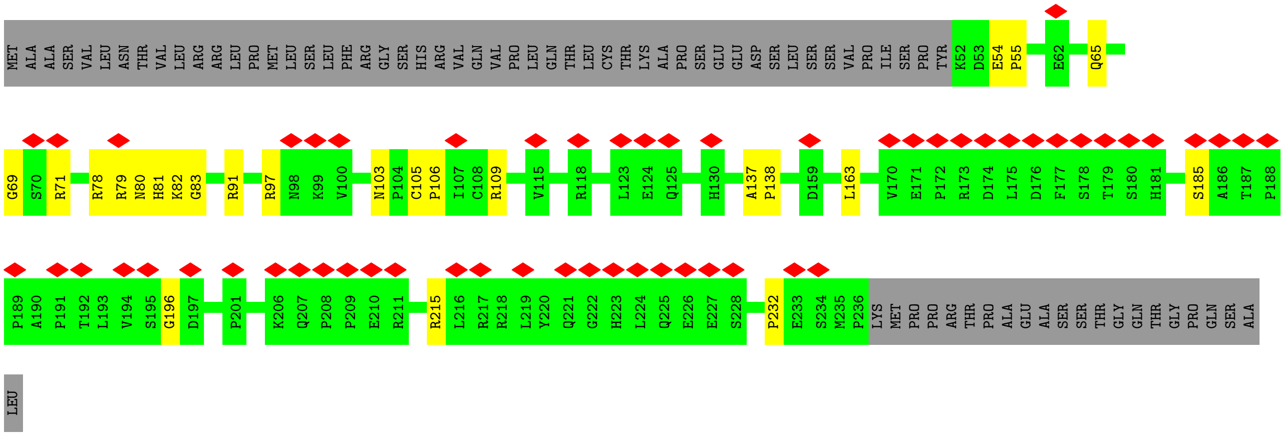
- Molecule 30: 28S ribosomal protein S17, mitochondrial

Chain AN:



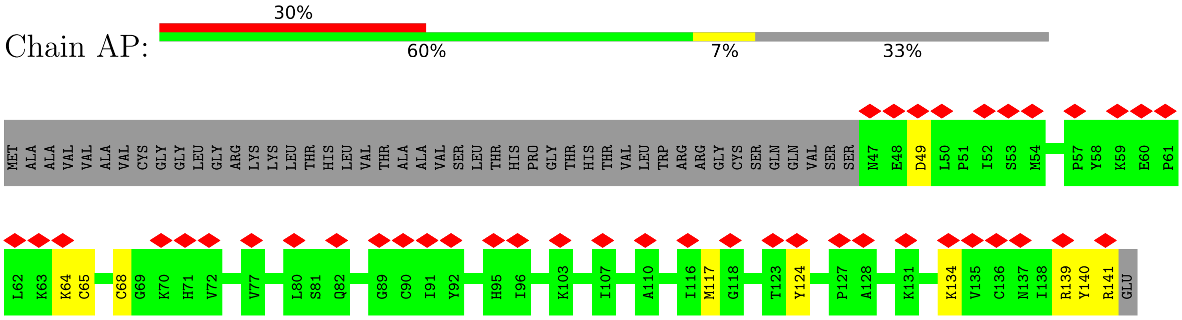
- Molecule 31: 28S ribosomal protein S18b, mitochondrial

Chain AO:



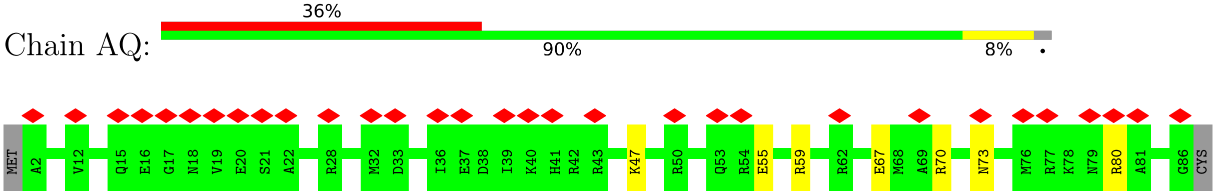
- Molecule 32: 28S ribosomal protein S18c, mitochondrial

Chain AP:



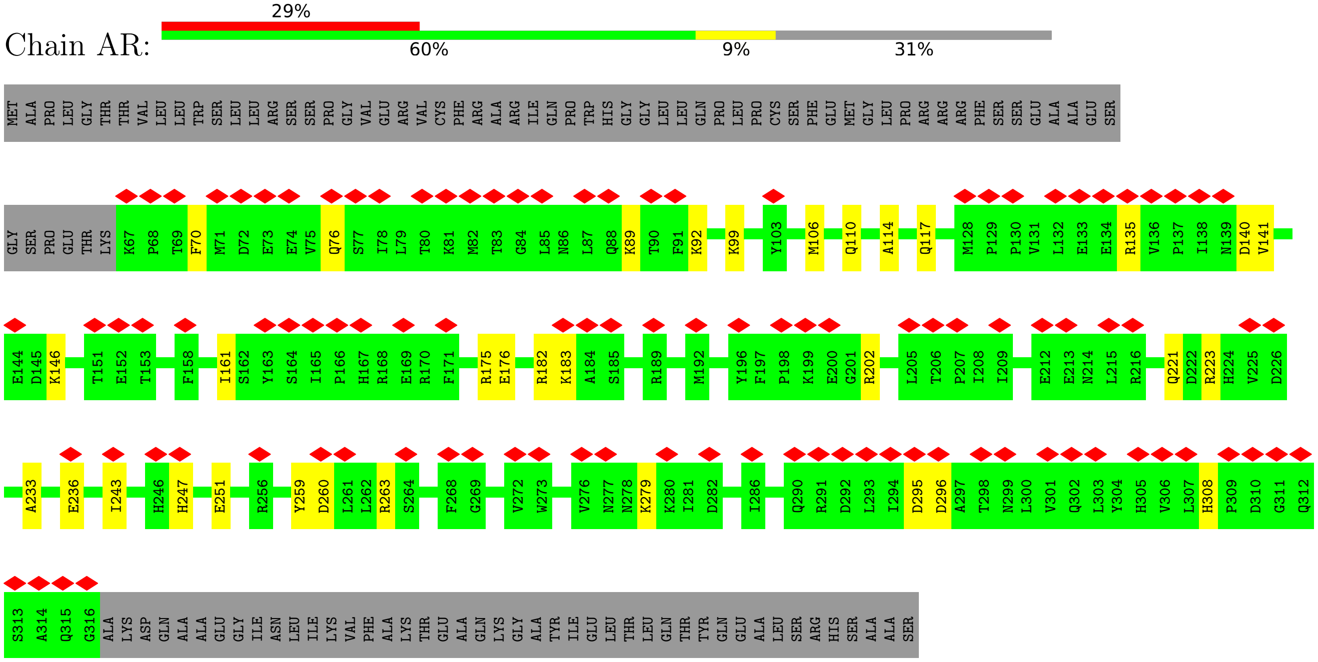
- Molecule 33: 28S ribosomal protein S21, mitochondrial

Chain AQ:



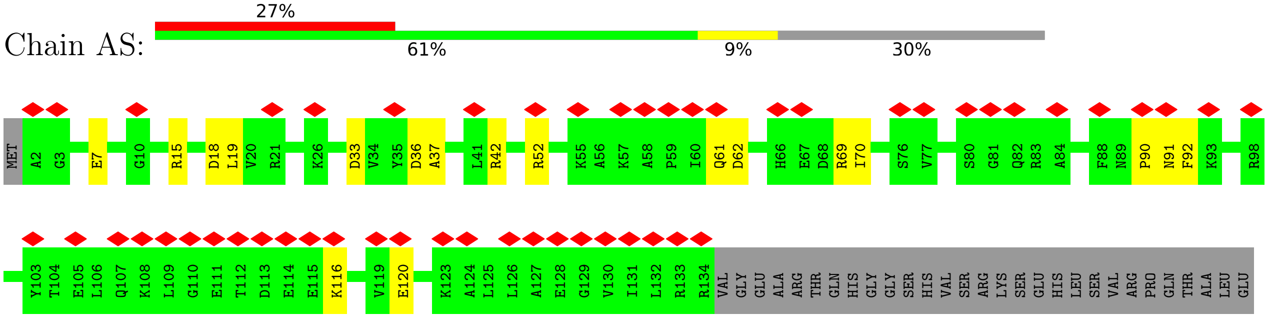
- Molecule 34: 28S ribosomal protein S22, mitochondrial

Chain AR:

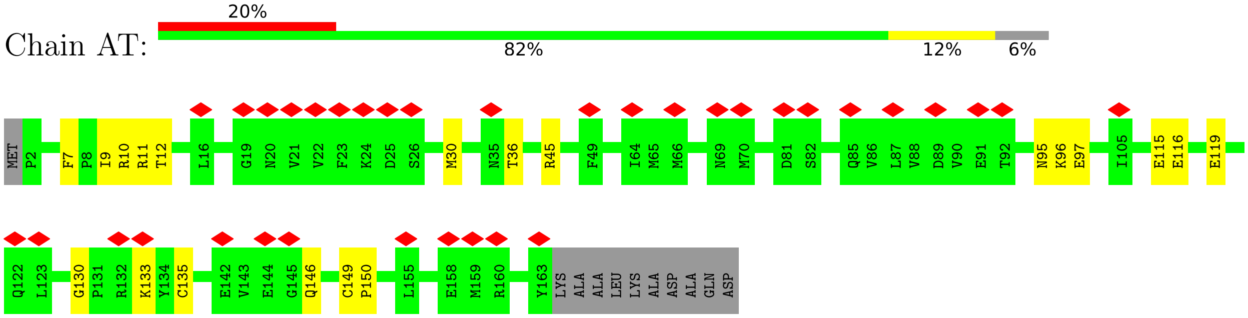


- Molecule 35: 28S ribosomal protein S23, mitochondrial

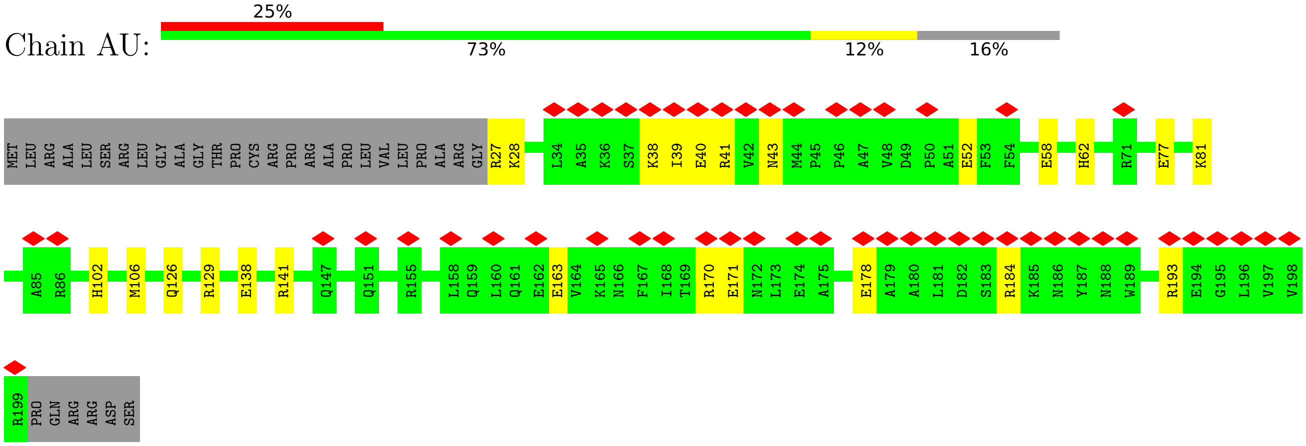
Chain AS:



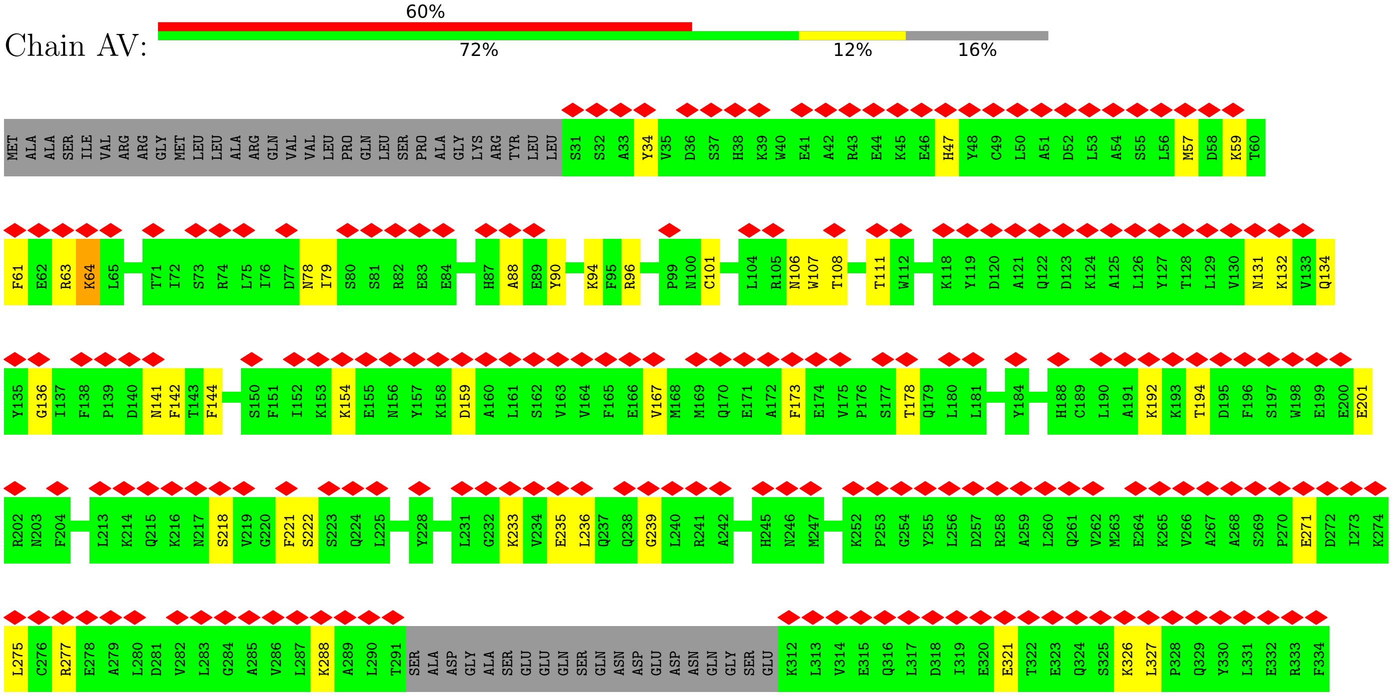
- Molecule 36: 28S ribosomal protein S25, mitochondrial

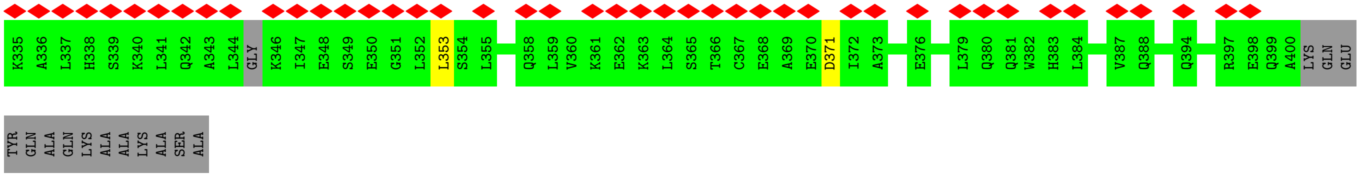


- Molecule 37: 28S ribosomal protein S26, mitochondrial



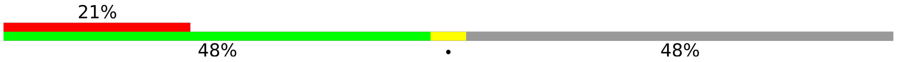
- Molecule 38: 28S ribosomal protein S27, mitochondrial

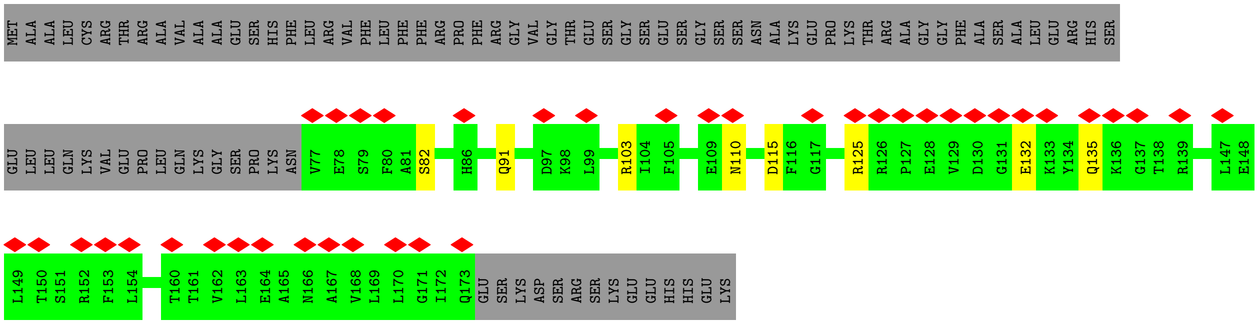




- Molecule 39: 28S ribosomal protein S28, mitochondrial

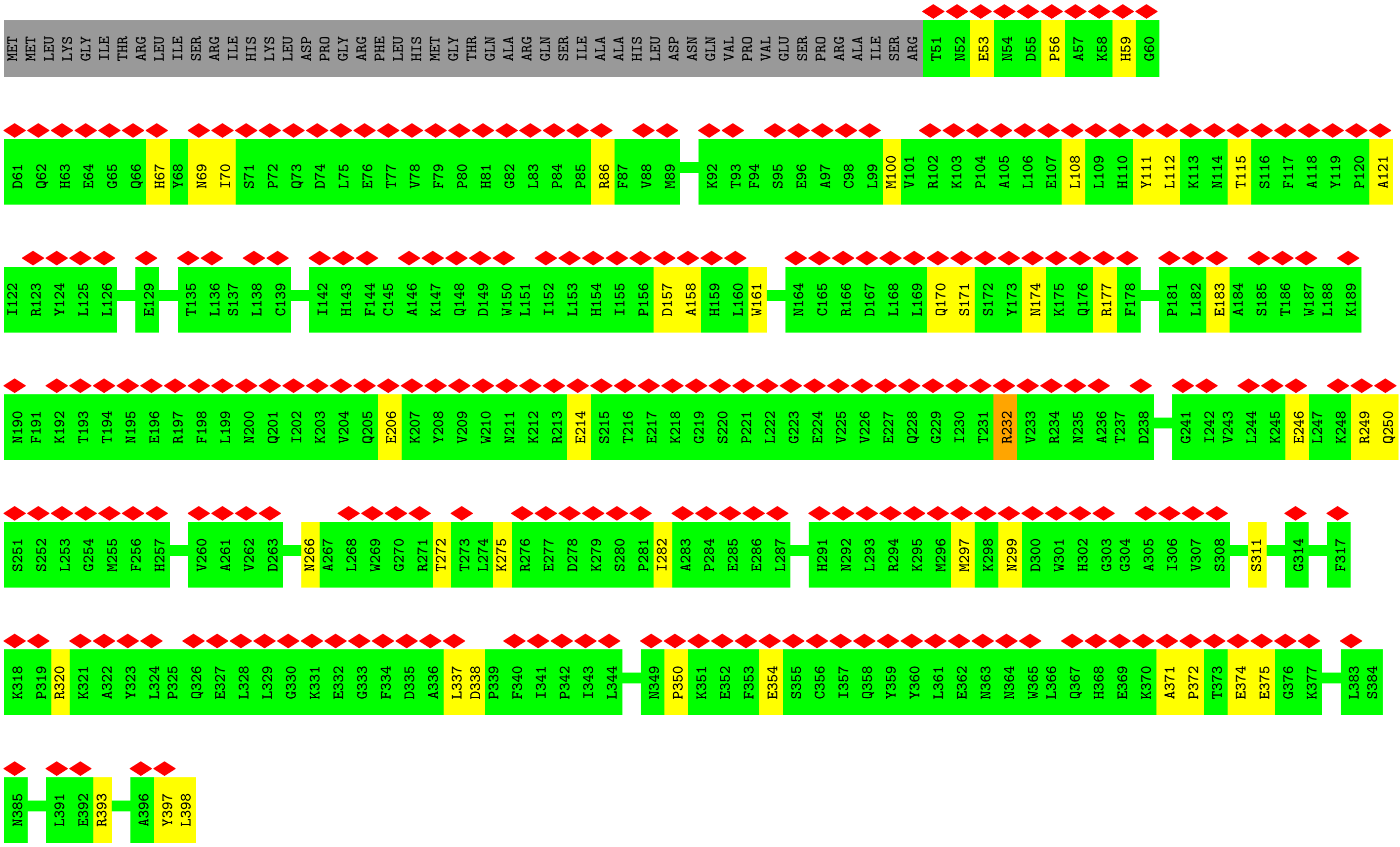
Chain AW:





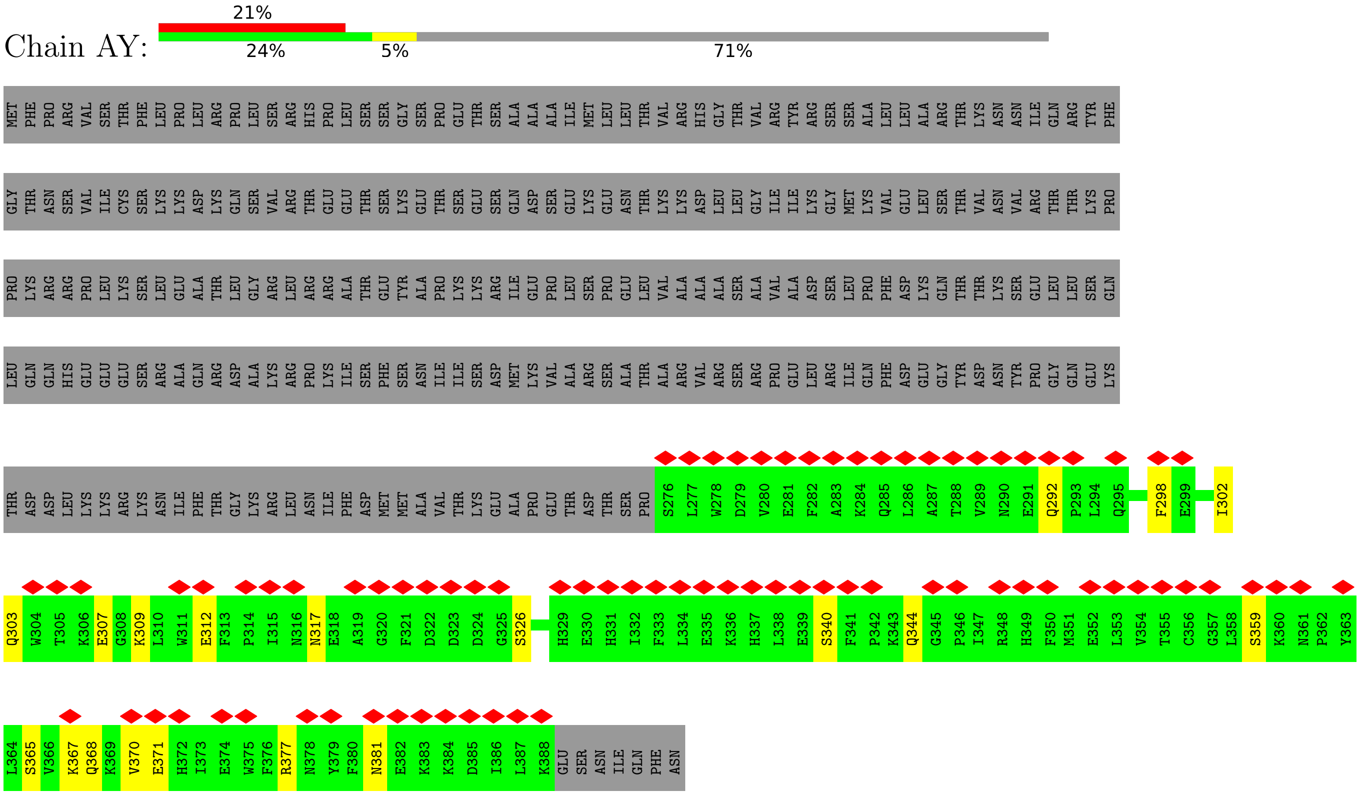
- Molecule 40: 28S ribosomal protein S29, mitochondrial

Chain AX:



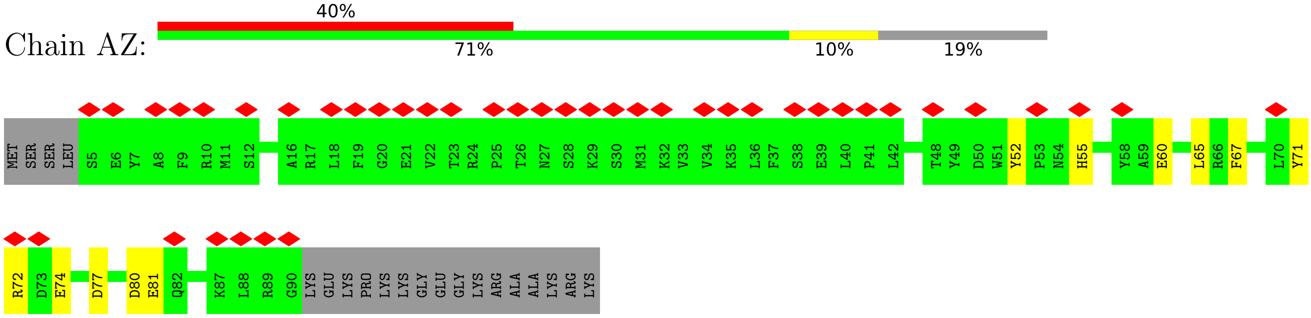
- Molecule 41: 28S ribosomal protein S31, mitochondrial

Chain AY:



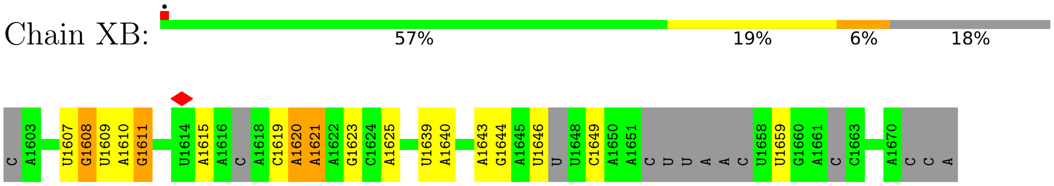
- Molecule 42: 28S ribosomal protein S33, mitochondrial

Chain AZ:



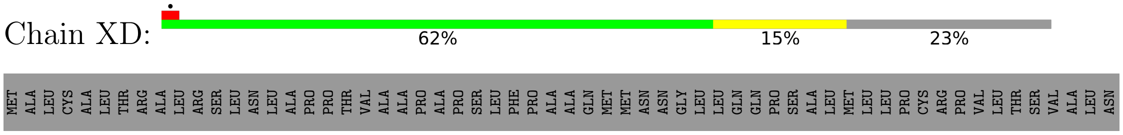
- Molecule 43: mitochondrial tRNAVal

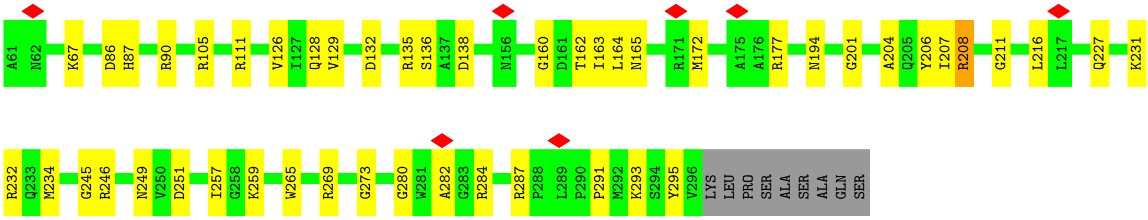
Chain XB:



- Molecule 44: 39S ribosomal protein L2, mitochondrial

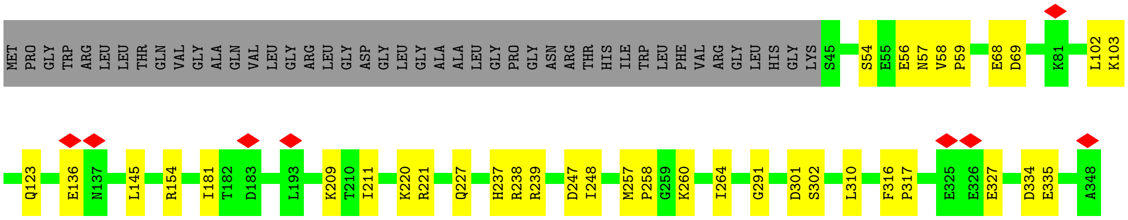
Chain XD:





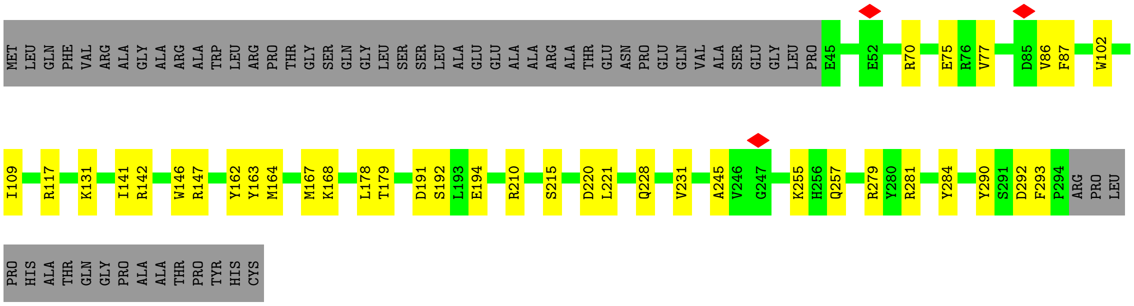
- Molecule 45: 39S ribosomal protein L3, mitochondrial

Chain XE:



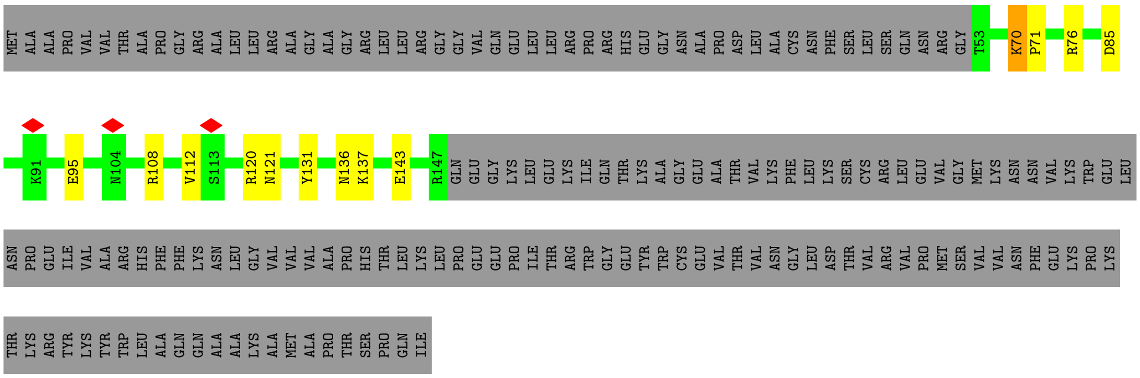
- Molecule 46: 39S ribosomal protein L4, mitochondrial

Chain XF:

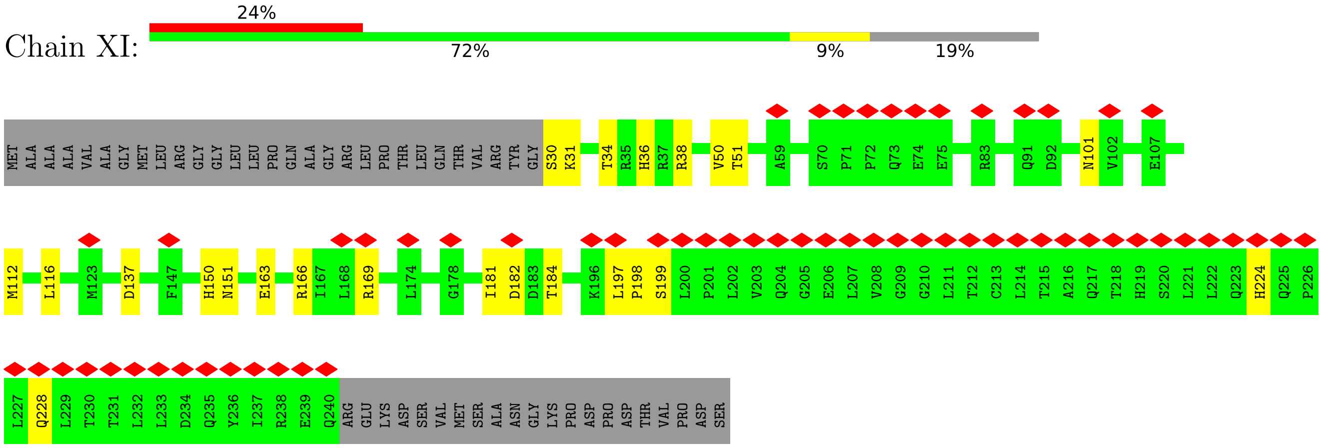


- Molecule 47: 39S ribosomal protein L9, mitochondrial

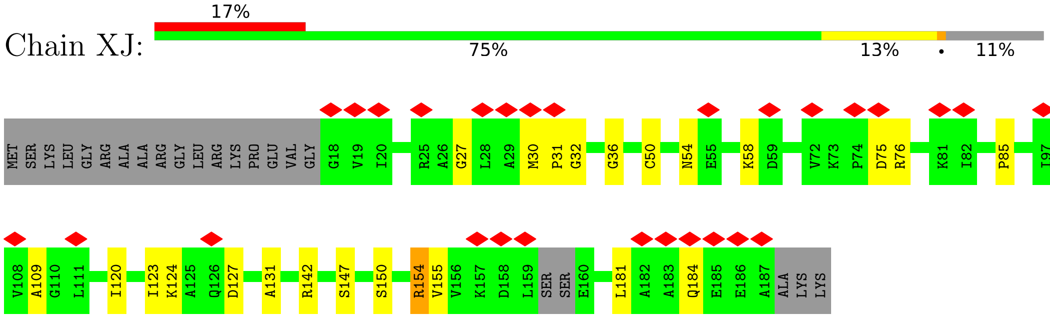
Chain XH:



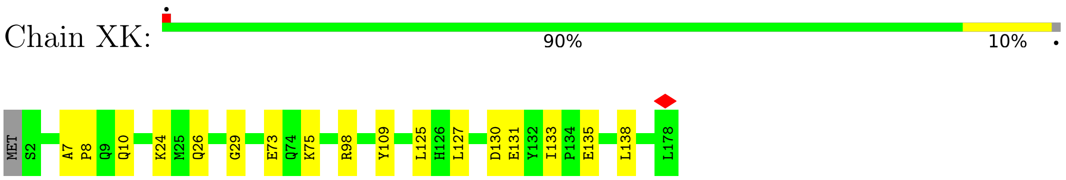
- Molecule 48: 39S ribosomal protein L10, mitochondrial



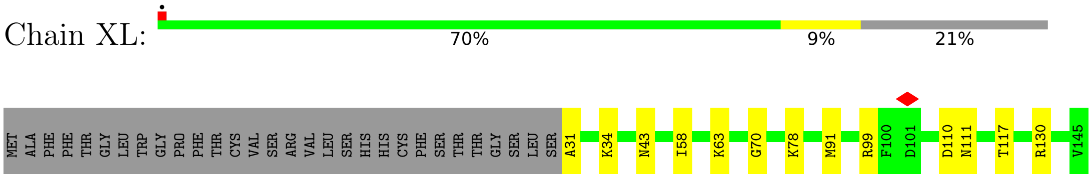
- Molecule 49: 39S ribosomal protein L11, mitochondrial



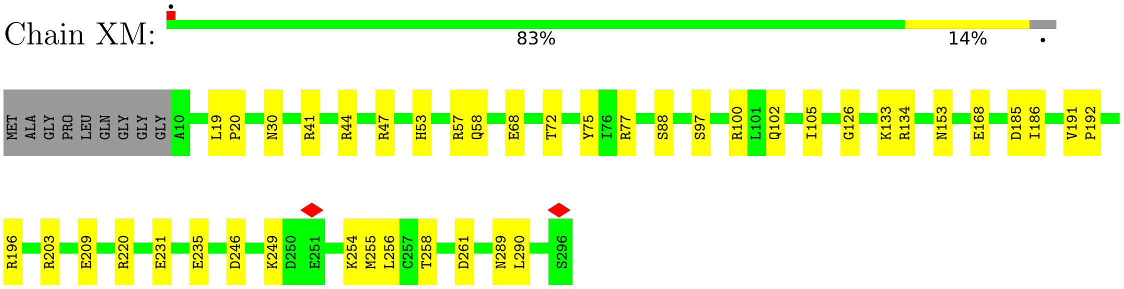
- Molecule 50: 39S ribosomal protein L13, mitochondrial



- Molecule 51: 39S ribosomal protein L14, mitochondrial

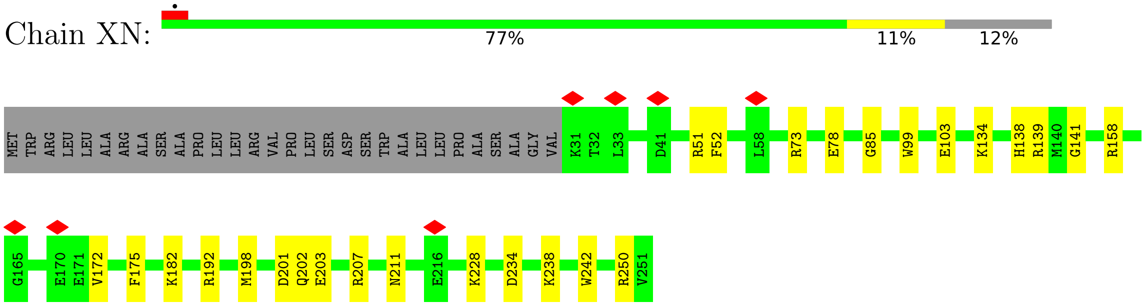


- Molecule 52: 39S ribosomal protein L15, mitochondrial



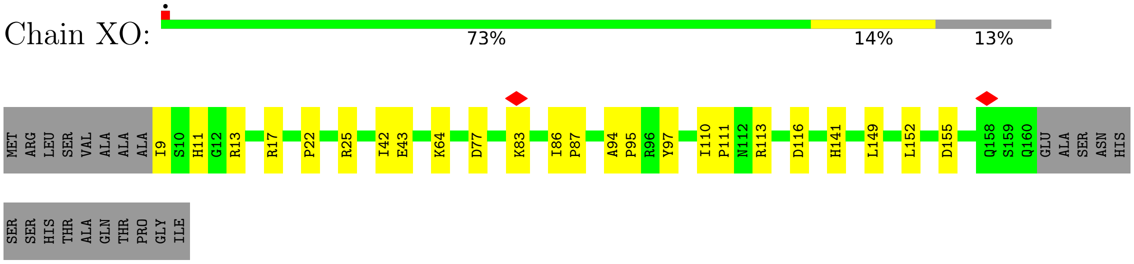
- Molecule 53: 39S ribosomal protein L16, mitochondrial

Chain XN:



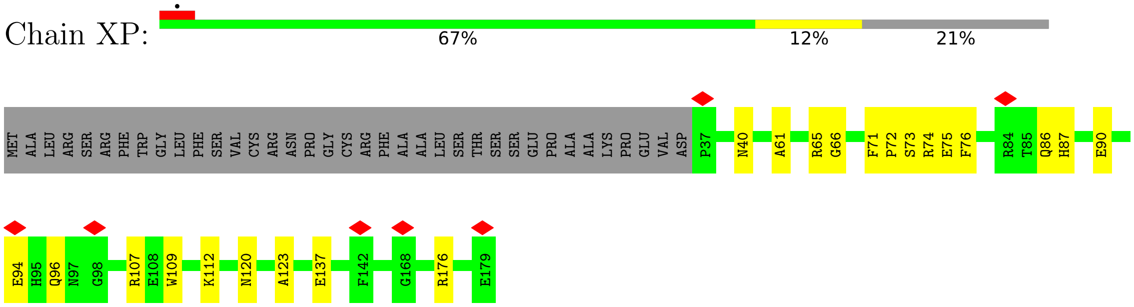
- Molecule 54: 39S ribosomal protein L17, mitochondrial

Chain XO:



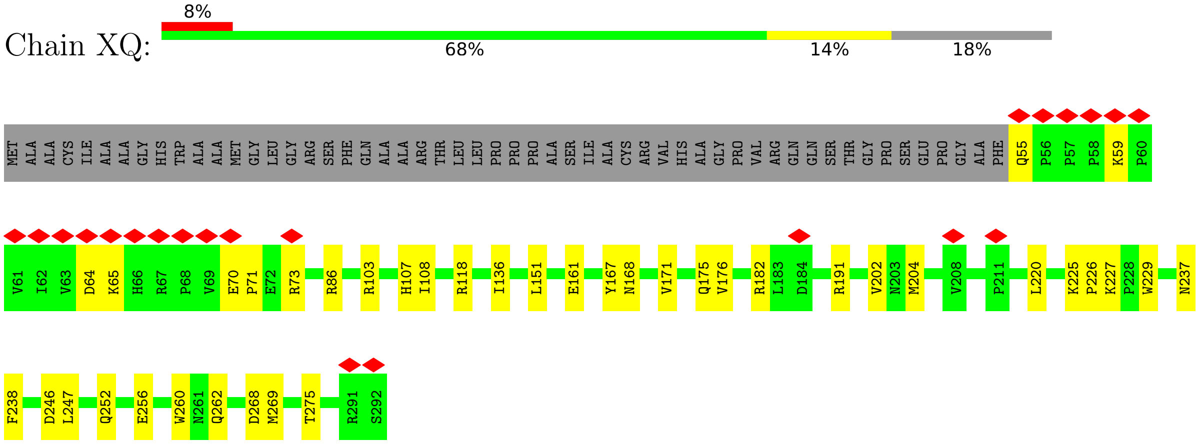
- Molecule 55: 39S ribosomal protein L18, mitochondrial

Chain XP:



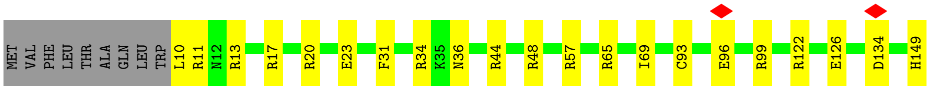
- Molecule 56: 39S ribosomal protein L19, mitochondrial

Chain XQ:



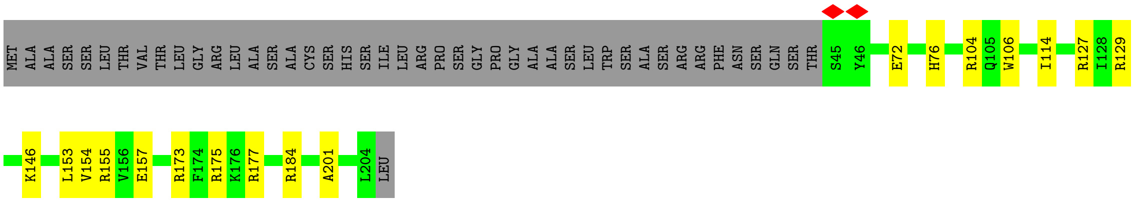
- Molecule 57: 39S ribosomal protein L20, mitochondrial

Chain XR:



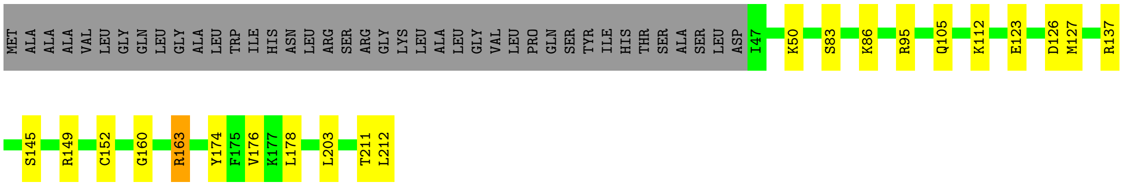
- Molecule 58: 39S ribosomal protein L21, mitochondrial

Chain XS:



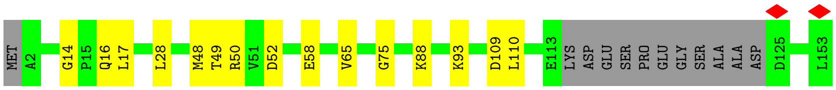
- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT:



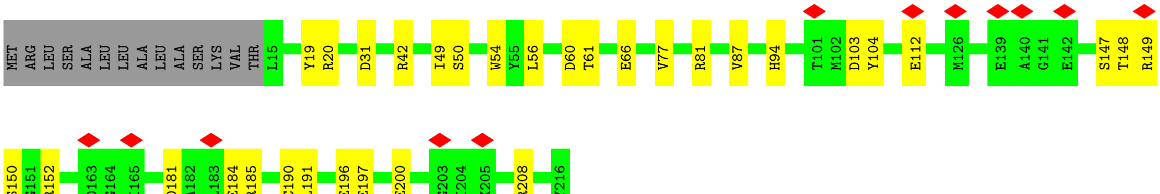
- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU:



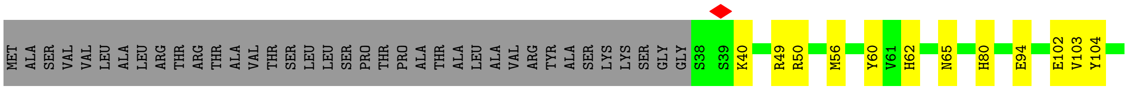
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV:

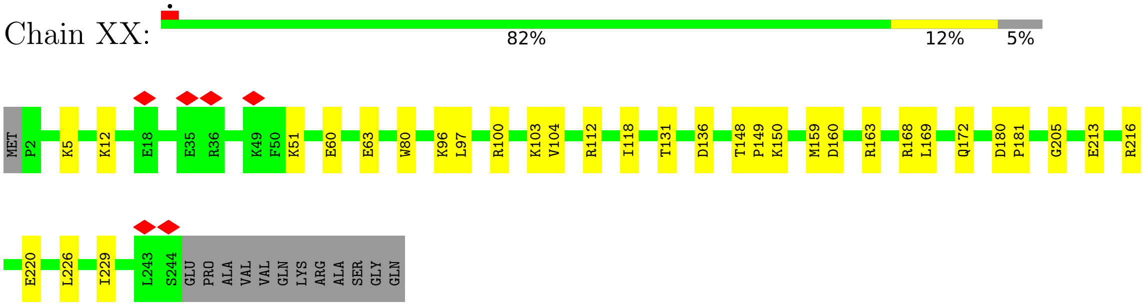


- Molecule 62: 39S ribosomal protein L27, mitochondrial

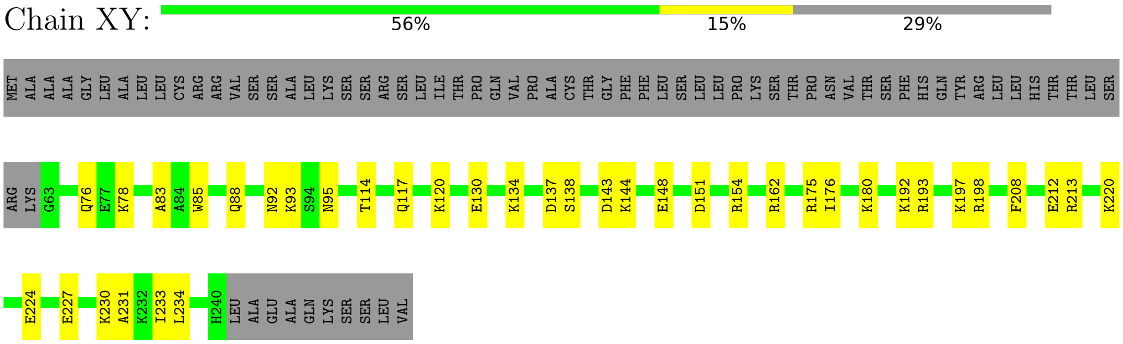
Chain XW:



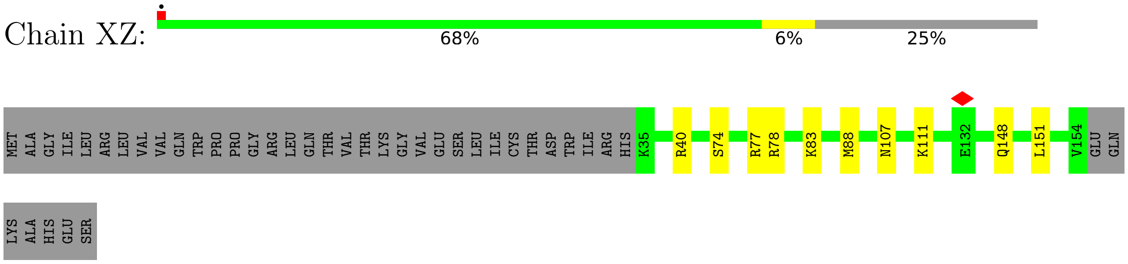
- Molecule 63: 39S ribosomal protein L28, mitochondrial



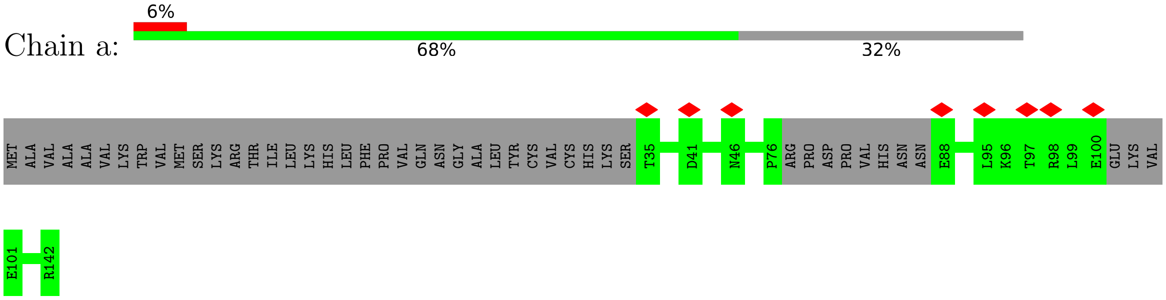
- Molecule 64: 39S ribosomal protein L47, mitochondrial



- Molecule 65: 39S ribosomal protein L30, mitochondrial

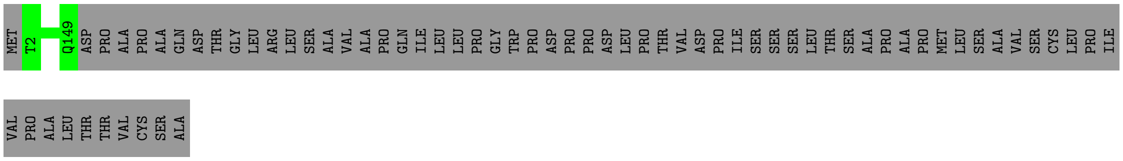


- Molecule 66: 39S ribosomal protein L42, mitochondrial



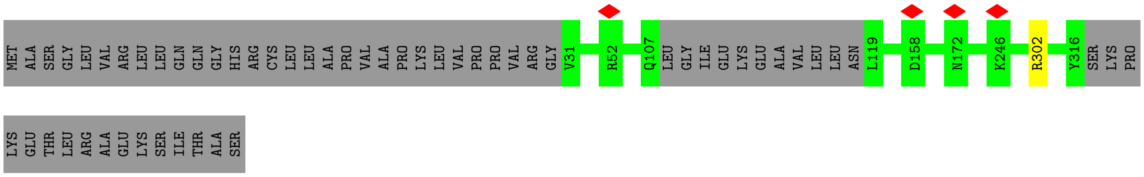
- Molecule 67: 39S ribosomal protein L43, mitochondrial

Chain b:



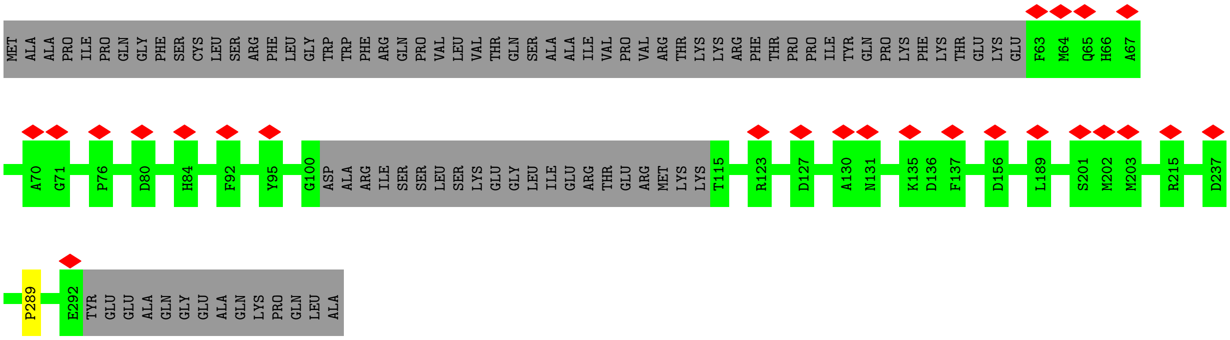
- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c:



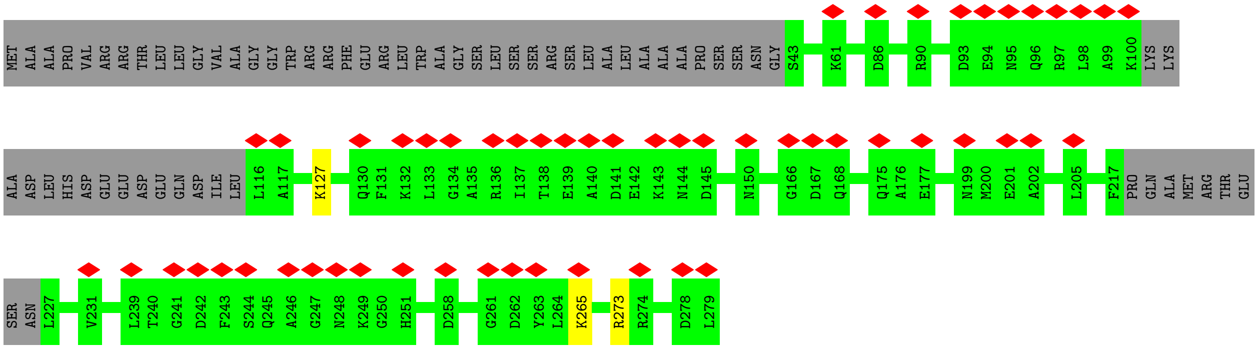
- Molecule 69: 39S ribosomal protein L45, mitochondrial

Chain d:



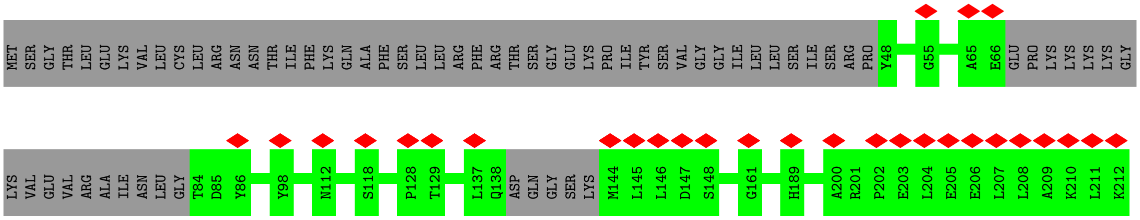
- Molecule 70: 39S ribosomal protein L46, mitochondrial

Chain e:

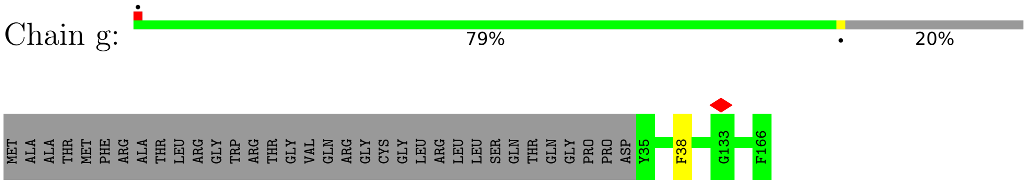


- Molecule 71: 39S ribosomal protein L48, mitochondrial

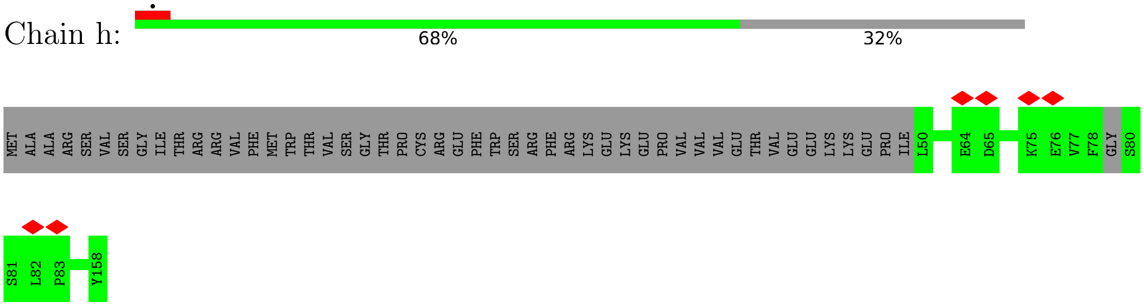
Chain f:



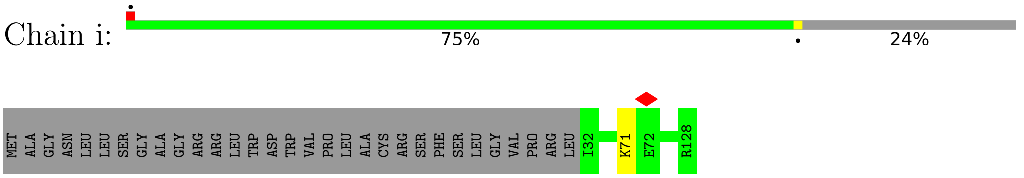
- Molecule 72: 39S ribosomal protein L49, mitochondrial



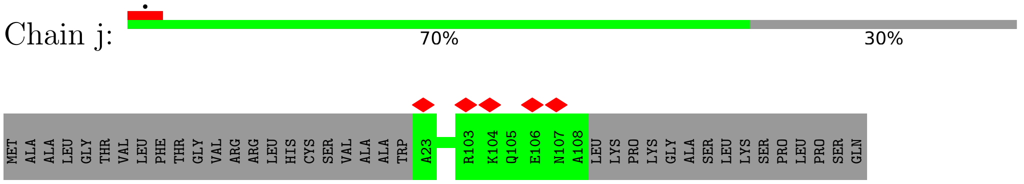
- Molecule 73: 39S ribosomal protein L50, mitochondrial



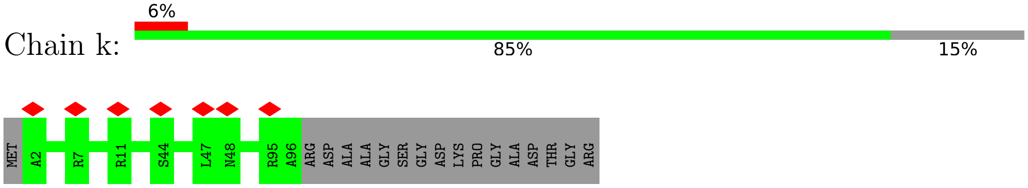
- Molecule 74: 39S ribosomal protein L51, mitochondrial



- Molecule 75: 39S ribosomal protein L52, mitochondrial

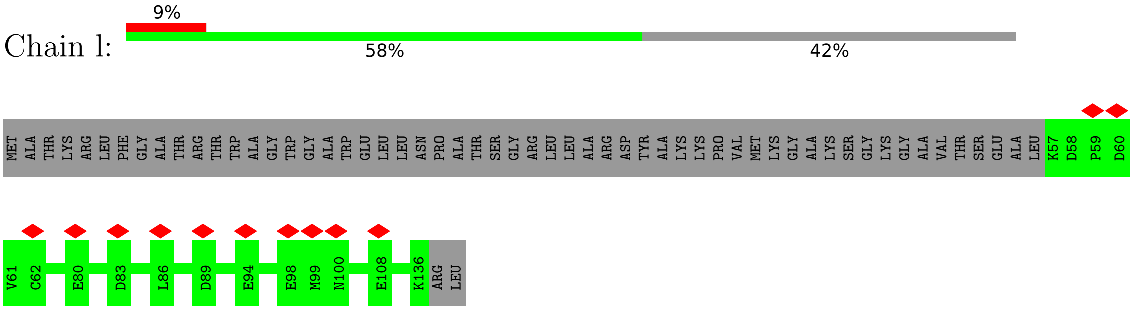


- Molecule 76: 39S ribosomal protein L53, mitochondrial



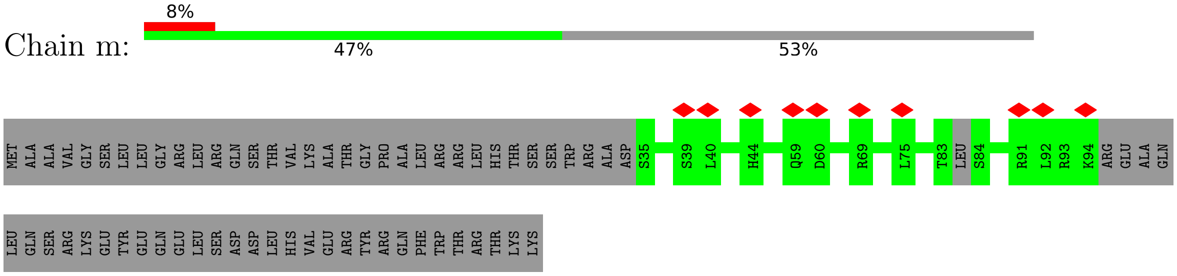
- Molecule 77: 39S ribosomal protein L54, mitochondrial

Chain l:



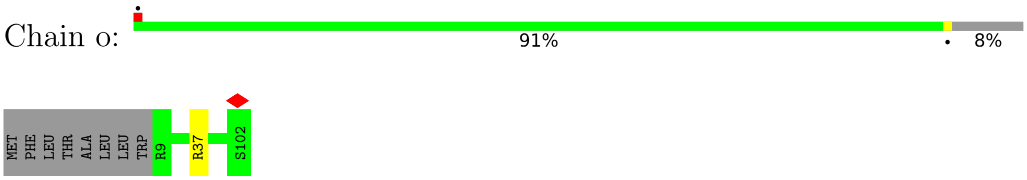
- Molecule 78: 39S ribosomal protein L55, mitochondrial

Chain m:



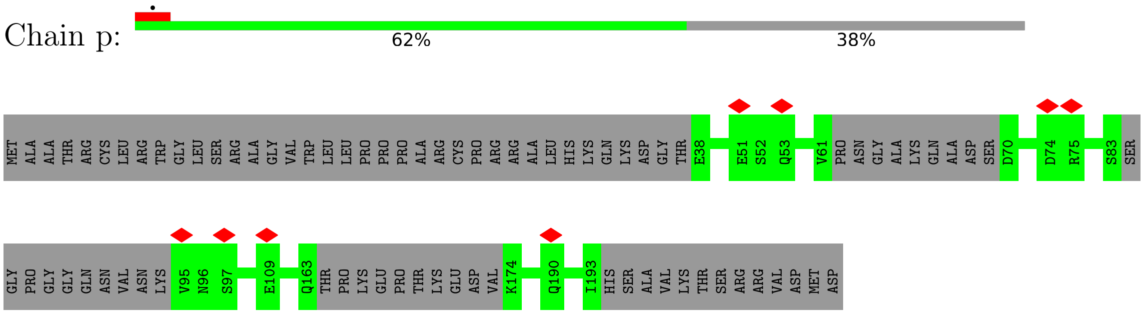
- Molecule 79: Ribosomal protein 63, mitochondrial

Chain o:



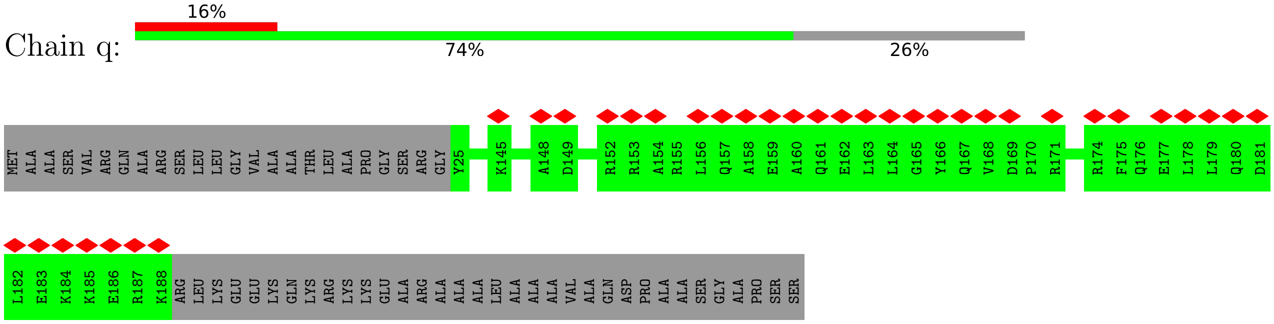
- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



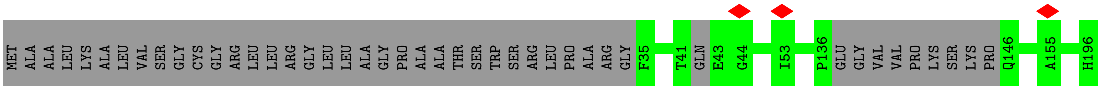
- Molecule 81: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



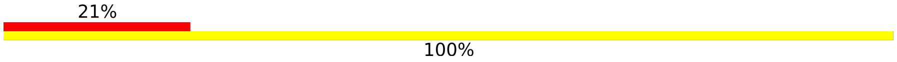
- Molecule 82: 39S ribosomal protein S18a, mitochondrial

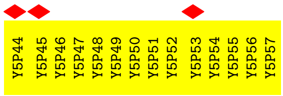
Chain r:



- Molecule 83: mRNA

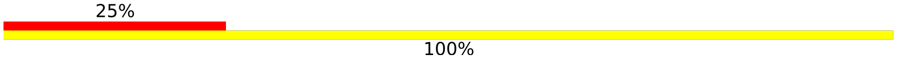
Chain r1:

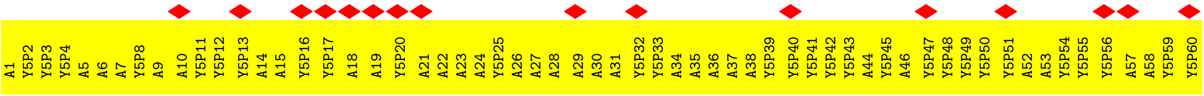


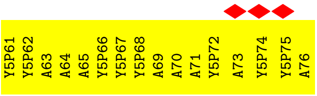


- Molecule 84: A/P-tRNA

Chain r2:

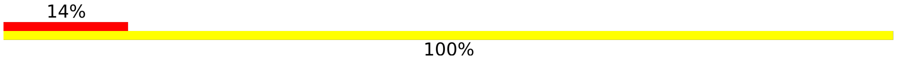


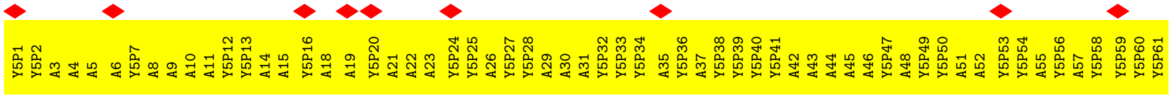


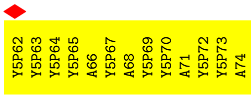


- Molecule 85: P/E-tRNA

Chain r3:

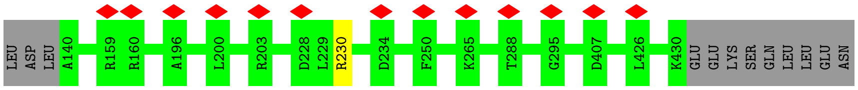




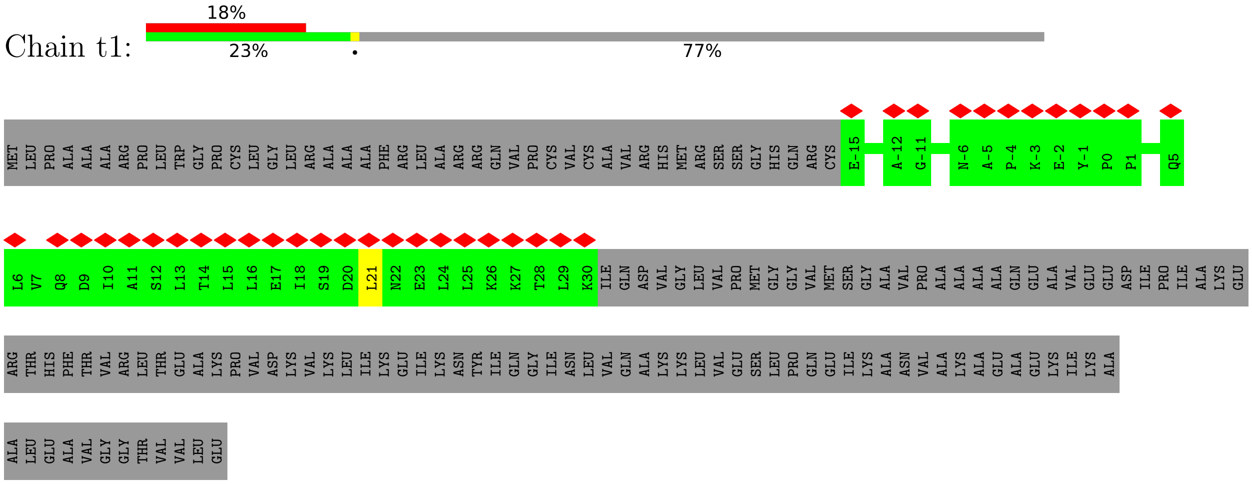


- Molecule 86: 39S ribosomal protein S30, mitochondrial

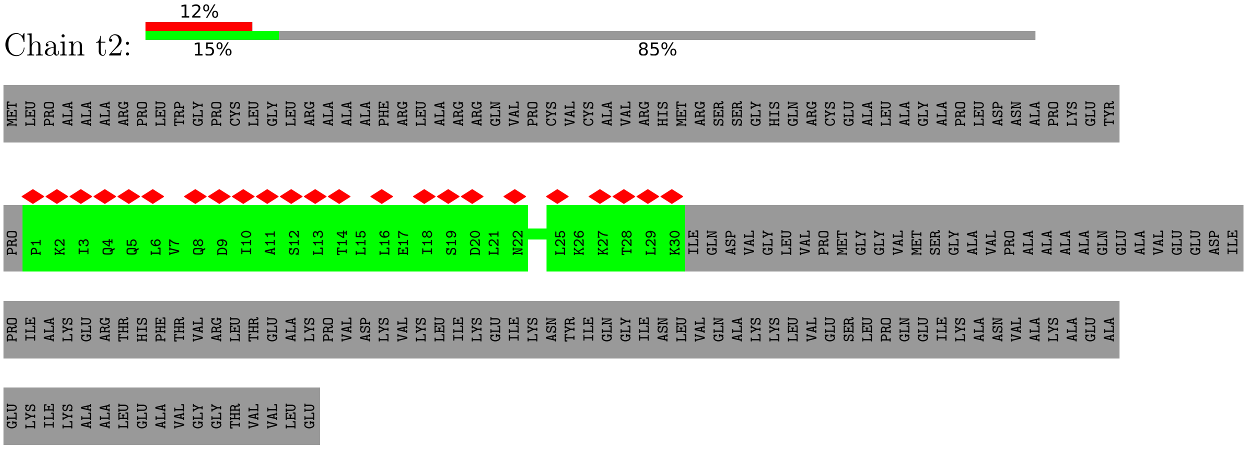
Chain s:



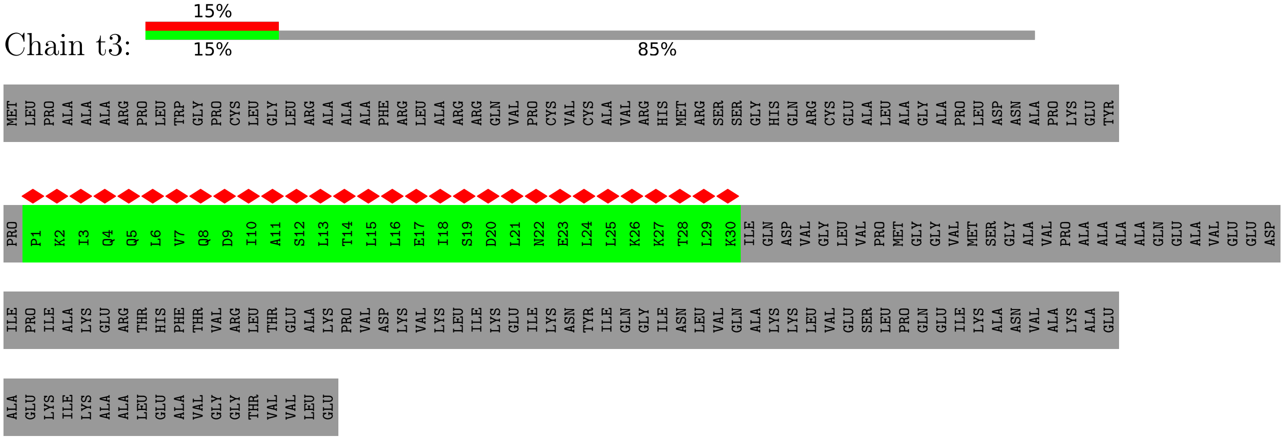
- Molecule 87: 39S ribosomal protein L12, mitochondrial



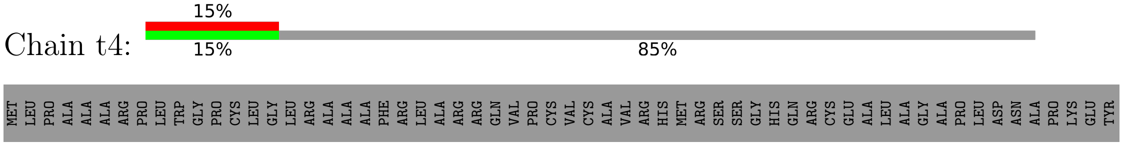
- Molecule 87: 39S ribosomal protein L12, mitochondrial

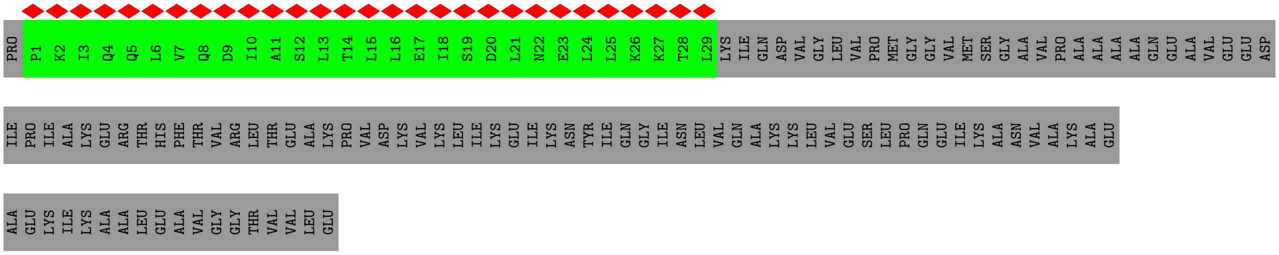


- Molecule 87: 39S ribosomal protein L12, mitochondrial

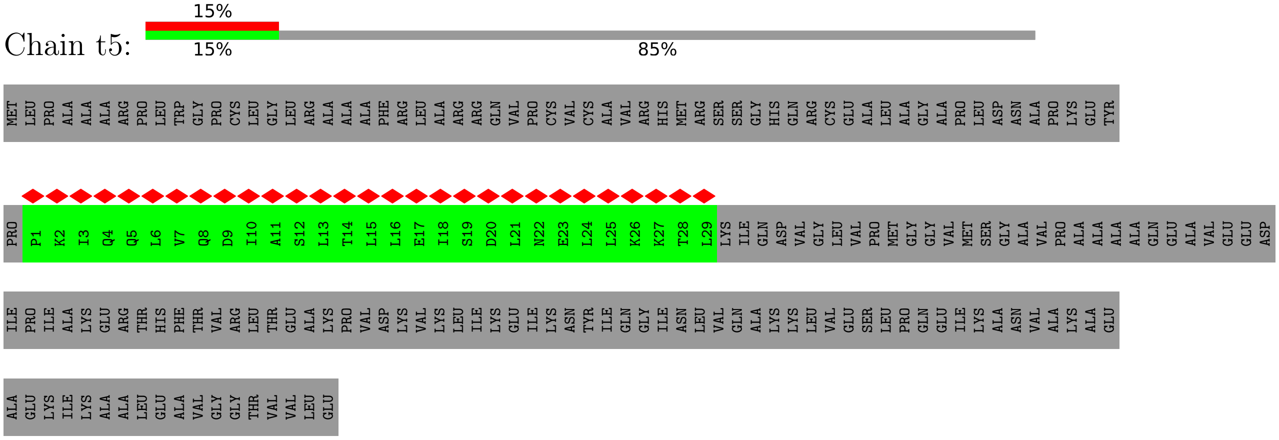


- Molecule 87: 39S ribosomal protein L12, mitochondrial

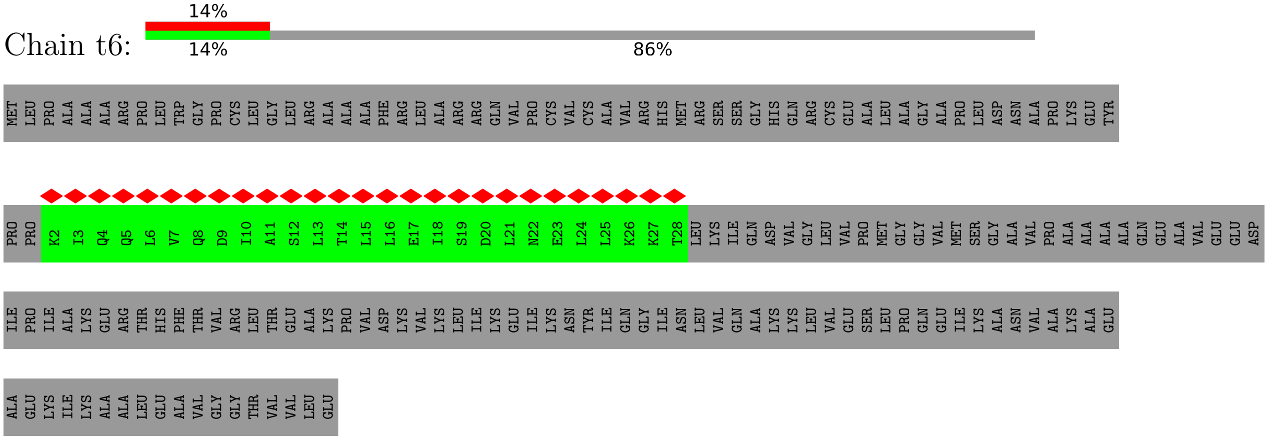




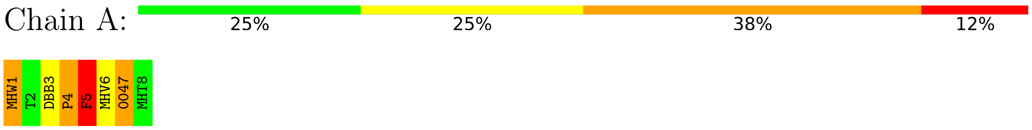
- Molecule 87: 39S ribosomal protein L12, mitochondrial



- Molecule 87: 39S ribosomal protein L12, mitochondrial



- Molecule 88: Quinupristin



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4966	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 ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.112	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: P5P, DOL, MHU, MHT, MHV, DBB, MHW, MG, Y5P, 004, GTP, 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	0	0.27	0/895	0.43	0/1201
2	1	0.26	0/444	0.46	0/591
3	2	0.30	0/382	0.43	0/507
4	3	0.31	0/852	0.43	0/1136
5	4	0.26	0/349	0.44	0/461
6	5	0.26	0/3299	0.42	0/4495
7	6	0.27	0/3041	0.41	0/4137
8	7	0.25	0/2419	0.42	0/3267
9	8	0.25	0/1199	0.38	0/1612
10	9	0.28	0/1024	0.41	0/1379
11	XA	0.32	0/35615	0.79	0/55429
12	A0	0.23	0/1727	0.42	0/2338
13	A1	0.24	0/2276	0.40	0/3079
14	A2	0.24	0/939	0.41	0/1256
15	A3	0.25	0/621	0.42	0/820
16	A4	0.25	0/4559	0.41	0/6149
17	AA	0.20	0/21952	0.75	0/34164
18	AB	0.24	0/1819	0.40	0/2462
19	AC	0.24	0/1112	0.42	0/1505
20	AD	0.24	0/2768	0.42	0/3707
21	AE	0.23	0/989	0.43	0/1335
22	AF	0.24	0/1708	0.39	0/2291
23	AG	0.25	0/2559	0.41	0/3429
24	AH	0.24	0/1128	0.43	0/1529
25	AI	0.25	0/1031	0.42	0/1390
26	AJ	0.25	0/854	0.46	0/1148
27	AK	0.22	0/879	0.39	0/1182
28	AL	0.24	0/1406	0.39	0/1878
29	AM	0.24	0/941	0.41	0/1265
30	AN	0.24	0/864	0.43	0/1169
31	AO	0.24	0/1580	0.38	0/2150
32	AP	0.24	0/782	0.38	0/1050

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
33	AQ	0.23	0/746	0.41	0/993
34	AR	0.27	0/2103	0.43	0/2842
35	AS	0.25	0/1127	0.40	0/1518
36	AT	0.25	0/1361	0.41	0/1829
37	AU	0.24	0/1482	0.39	0/1987
38	AV	0.24	0/2925	0.40	0/3948
39	AW	0.24	0/778	0.44	0/1048
40	AX	0.24	0/2884	0.43	0/3903
41	AY	0.25	0/985	0.38	0/1329
42	AZ	0.24	0/748	0.38	0/1000
43	XB	0.20	0/1400	0.73	0/2168
44	XD	0.26	0/1879	0.45	0/2527
45	XE	0.28	0/2465	0.44	0/3344
46	XF	0.30	0/2071	0.45	0/2817
47	XH	0.25	0/798	0.44	0/1073
48	XI	0.25	0/1727	0.43	0/2340
49	XJ	0.24	0/1309	0.40	0/1764
50	XK	0.30	0/1495	0.41	0/2029
51	XL	0.26	0/904	0.43	0/1218
52	XM	0.29	0/2359	0.43	0/3185
53	XN	0.28	0/1825	0.44	0/2458
54	XO	0.26	0/1269	0.43	0/1708
55	XP	0.25	0/1190	0.41	0/1611
56	XQ	0.26	0/2026	0.44	0/2734
57	XR	0.31	0/1174	0.45	0/1572
58	XS	0.28	0/1311	0.46	0/1778
59	XT	0.30	0/1402	0.44	0/1886
60	XU	0.27	0/1200	0.41	0/1623
61	XV	0.26	0/1693	0.44	0/2297
62	XW	0.28	0/893	0.46	0/1204
63	XX	0.32	1/2090 (0.0%)	0.41	0/2825
64	XY	0.26	0/1571	0.42	0/2106
65	XZ	0.29	0/1003	0.45	0/1354
66	a	0.26	0/838	0.43	0/1138
67	b	0.28	0/1202	0.46	0/1626
68	c	0.26	0/2264	0.41	0/3059
69	d	0.25	0/1807	0.42	0/2450
70	e	0.24	0/1766	0.42	0/2382
71	f	0.25	0/1168	0.42	0/1573
72	g	0.30	0/1134	0.48	0/1547
73	h	0.25	0/905	0.41	0/1233
74	i	0.30	0/849	0.45	0/1135
75	j	0.27	0/703	0.41	0/947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	k	0.24	0/743	0.44	0/1003
77	l	0.24	0/692	0.37	0/939
78	m	0.23	0/508	0.49	0/682
79	o	0.29	0/818	0.45	0/1097
80	p	0.23	0/1071	0.41	0/1433
81	q	0.25	0/1413	0.40	0/1906
82	r	0.27	0/1282	0.42	0/1734
86	s	0.26	0/3114	0.42	0/4225
87	t1	0.25	0/366	0.37	0/497
87	t2	0.21	0/238	0.37	0/319
87	t3	0.21	0/238	0.35	0/319
87	t4	0.22	0/229	0.37	0/308
87	t5	0.21	0/229	0.35	0/308
87	t6	0.23	0/213	0.39	0/286
88	A	0.55	0/13	0.66	0/15
All	All	0.27	1/176009 (0.0%)	0.57	0/249690

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
48	XI	0	1
70	e	0	1
88	A	2	3
All	All	2	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	XX	149	PRO	N-CD	7.70	1.58	1.47

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
88	A	2	THR	CB
88	A	4	PRO	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
88	A	3	DBB	Peptide
88	A	4	PRO	Peptide
88	A	5	MHU	Peptide
48	XI	197	LEU	Peptide
70	e	265	LYS	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	0	880	903	903	12	0
2	1	439	480	480	9	0
3	2	376	406	406	14	0
4	3	831	883	883	17	0
5	4	341	362	362	7	0
6	5	3204	3201	3201	31	0
7	6	2947	2840	2840	31	0
8	7	2365	2372	2371	31	0
9	8	1175	1202	1202	9	0
10	9	996	987	987	17	0
11	XA	31833	16159	16168	352	0
12	A0	1684	1685	1685	16	0
13	A1	2230	2261	2261	68	0
14	A2	925	964	964	13	0
15	A3	610	682	682	11	0
16	A4	4470	4485	4486	127	0
17	AA	19628	9964	9971	159	0
18	AB	1776	1769	1769	17	0
19	AC	1082	1088	1088	25	0
20	AD	2716	2783	2784	32	0
21	AE	972	1001	1001	18	0
22	AF	1668	1716	1716	23	0
23	AG	2505	2490	2490	31	0
24	AH	1105	1136	1136	38	0
25	AI	1011	1052	1052	6	0
26	AJ	838	887	887	13	0
27	AK	861	885	885	13	0
28	AL	1382	1473	1472	19	0
29	AM	920	951	951	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	AN	846	908	908	13	0
31	AO	1528	1490	1490	18	0
32	AP	765	796	796	8	0
33	AQ	734	749	749	6	0
34	AR	2060	2074	2074	24	0
35	AS	1100	1103	1103	12	0
36	AT	1330	1342	1342	11	0
37	AU	1461	1471	1471	17	0
38	AV	2867	2862	2862	26	0
39	AW	766	785	785	5	0
40	AX	2814	2803	2802	27	0
41	AY	956	912	911	21	0
42	AZ	731	734	734	9	0
43	XB	1255	635	640	9	0
44	XD	1842	1896	1896	40	0
45	XE	2396	2402	2402	27	0
46	XF	2013	2044	2044	25	0
47	XH	784	832	832	9	0
48	XI	1691	1783	1783	15	0
49	XJ	1291	1367	1364	16	0
50	XK	1451	1448	1448	12	0
51	XL	889	941	941	8	0
52	XM	2305	2376	2376	30	0
53	XN	1778	1808	1808	17	0
54	XO	1245	1283	1283	18	0
55	XP	1164	1162	1162	16	0
56	XQ	1978	2022	2022	30	0
57	XR	1153	1214	1214	18	0
58	XS	1284	1354	1354	12	0
59	XT	1368	1410	1410	16	0
60	XU	1171	1164	1164	9	0
61	XV	1648	1656	1654	24	0
62	XW	871	898	898	18	0
63	XX	2035	2054	2054	21	0
64	XY	1534	1575	1575	33	0
65	XZ	978	1030	1030	8	0
66	a	813	777	777	0	0
67	b	1178	1180	1180	0	0
68	c	2217	2220	2220	0	0
69	d	1758	1743	1742	0	0
70	e	1731	1732	1732	0	0
71	f	1149	1164	1164	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	g	1097	1086	1085	0	0
73	h	882	866	867	0	0
74	i	827	857	857	0	0
75	j	689	678	678	0	0
76	k	732	745	745	0	0
77	l	673	654	653	0	0
78	m	500	525	525	0	0
79	o	797	804	804	0	0
80	p	1058	1083	1083	0	0
81	q	1379	1359	1359	0	0
82	r	1247	1267	1267	0	0
83	r1	252	0	169	0	0
84	r2	1485	0	835	0	0
85	r3	1420	0	807	0	0
86	s	3036	3022	3022	0	0
87	t1	354	379	374	0	0
87	t2	238	268	270	0	0
87	t3	238	268	270	0	0
87	t4	229	255	257	0	0
87	t5	229	255	257	0	0
87	t6	214	236	236	0	0
88	A	73	67	64	7	0
89	0	1	0	0	0	0
89	4	1	0	0	0	0
89	AB	1	0	0	0	0
89	AO	1	0	0	0	0
89	AP	1	0	0	0	0
89	AT	1	0	0	0	0
89	r	1	0	0	0	0
90	AA	46	0	0	0	0
90	XA	141	0	0	0	0
90	XD	1	0	0	0	0
90	XE	1	0	0	0	0
90	XI	1	0	0	0	0
90	XM	2	0	0	0	0
90	XW	1	0	0	0	0
90	g	1	0	0	0	0
90	o	1	0	0	0	0
91	XA	48	50	50	1	0
92	AX	32	10	12	1	0
All	All	170629	143000	144825	1391	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 6.

The worst 5 of 1391 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)
16:A4:449:GLY:HA2	41:AY:292:GLN:NE2	1.33	1.40
13:A1:162:SER:OG	16:A4:134:GLU:CG	2.03	1.05
16:A4:449:GLY:CA	41:AY:292:GLN:NE2	2.22	1.03
13:A1:162:SER:OG	16:A4:134:GLU:HG3	1.60	1.00
17:AA:701:G:N2	17:AA:841:A:O2’	1.99	0.95

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	102 (96%)	4 (4%)	0	100	100
2	1	51/65 (78%)	47 (92%)	4 (8%)	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
5	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
6	5	391/423 (92%)	365 (93%)	26 (7%)	0	100	100
7	6	350/380 (92%)	325 (93%)	25 (7%)	0	100	100
8	7	283/338 (84%)	266 (94%)	17 (6%)	0	100	100
9	8	137/206 (66%)	129 (94%)	8 (6%)	0	100	100
10	9	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
12	A0	197/218 (90%)	187 (95%)	10 (5%)	0	100	100
13	A1	273/323 (84%)	258 (94%)	15 (6%)	0	100	100
14	A2	114/118 (97%)	111 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	A3	67/199 (34%)	67 (100%)	0	0	100	100
16	A4	526/689 (76%)	493 (94%)	33 (6%)	0	100	100
18	AB	216/296 (73%)	210 (97%)	6 (3%)	0	100	100
19	AC	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
20	AD	341/430 (79%)	327 (96%)	14 (4%)	0	100	100
21	AE	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
22	AF	197/242 (81%)	193 (98%)	4 (2%)	0	100	100
23	AG	300/396 (76%)	290 (97%)	10 (3%)	0	100	100
24	AH	133/201 (66%)	127 (96%)	6 (4%)	0	100	100
25	AI	134/194 (69%)	129 (96%)	5 (4%)	0	100	100
26	AJ	106/138 (77%)	97 (92%)	9 (8%)	0	100	100
27	AK	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
28	AL	162/257 (63%)	160 (99%)	2 (1%)	0	100	100
29	AM	114/137 (83%)	112 (98%)	2 (2%)	0	100	100
30	AN	105/130 (81%)	101 (96%)	4 (4%)	0	100	100
31	AO	183/258 (71%)	179 (98%)	4 (2%)	0	100	100
32	AP	93/142 (66%)	87 (94%)	6 (6%)	0	100	100
33	AQ	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
34	AR	248/360 (69%)	238 (96%)	10 (4%)	0	100	100
35	AS	131/190 (69%)	123 (94%)	8 (6%)	0	100	100
36	AT	160/173 (92%)	150 (94%)	10 (6%)	0	100	100
37	AU	171/205 (83%)	169 (99%)	2 (1%)	0	100	100
38	AV	341/414 (82%)	322 (94%)	19 (6%)	0	100	100
39	AW	95/187 (51%)	91 (96%)	4 (4%)	0	100	100
40	AX	342/398 (86%)	327 (96%)	15 (4%)	0	100	100
41	AY	111/395 (28%)	102 (92%)	9 (8%)	0	100	100
42	AZ	84/106 (79%)	82 (98%)	2 (2%)	0	100	100
44	XD	234/305 (77%)	214 (92%)	18 (8%)	2 (1%)	17	56
45	XE	302/348 (87%)	287 (95%)	15 (5%)	0	100	100
46	XF	248/311 (80%)	240 (97%)	8 (3%)	0	100	100
47	XH	93/267 (35%)	90 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	XI	209/261 (80%)	192 (92%)	17 (8%)	0	100	100
49	XJ	168/192 (88%)	157 (94%)	11 (6%)	0	100	100
50	XK	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
51	XL	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
52	XM	285/296 (96%)	272 (95%)	13 (5%)	0	100	100
53	XN	219/251 (87%)	210 (96%)	9 (4%)	0	100	100
54	XO	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
55	XP	141/180 (78%)	131 (93%)	10 (7%)	0	100	100
56	XQ	236/292 (81%)	223 (94%)	13 (6%)	0	100	100
57	XR	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
58	XS	158/205 (77%)	153 (97%)	5 (3%)	0	100	100
59	XT	164/206 (80%)	156 (95%)	8 (5%)	0	100	100
60	XU	137/153 (90%)	132 (96%)	5 (4%)	0	100	100
61	XV	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
62	XW	109/148 (74%)	105 (96%)	4 (4%)	0	100	100
63	XX	241/256 (94%)	231 (96%)	10 (4%)	0	100	100
64	XY	176/250 (70%)	171 (97%)	5 (3%)	0	100	100
65	XZ	118/161 (73%)	116 (98%)	2 (2%)	0	100	100
66	a	93/142 (66%)	86 (92%)	7 (8%)	0	100	100
67	b	146/215 (68%)	137 (94%)	9 (6%)	0	100	100
68	c	271/332 (82%)	259 (96%)	12 (4%)	0	100	100
69	d	212/306 (69%)	200 (94%)	11 (5%)	1 (0%)	29	68
70	e	207/279 (74%)	200 (97%)	7 (3%)	0	100	100
71	f	137/212 (65%)	131 (96%)	6 (4%)	0	100	100
72	g	130/166 (78%)	121 (93%)	8 (6%)	1 (1%)	19	60
73	h	106/158 (67%)	100 (94%)	6 (6%)	0	100	100
74	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
75	j	84/123 (68%)	84 (100%)	0	0	100	100
76	k	93/112 (83%)	86 (92%)	7 (8%)	0	100	100
77	l	78/138 (56%)	73 (94%)	5 (6%)	0	100	100
78	m	58/128 (45%)	54 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	o	92/102 (90%)	87 (95%)	5 (5%)	0	100	100
80	p	119/206 (58%)	113 (95%)	6 (5%)	0	100	100
81	q	162/222 (73%)	159 (98%)	3 (2%)	0	100	100
82	r	144/196 (74%)	136 (94%)	8 (6%)	0	100	100
86	s	366/439 (83%)	349 (95%)	17 (5%)	0	100	100
87	t1	45/198 (23%)	41 (91%)	4 (9%)	0	100	100
87	t2	28/198 (14%)	28 (100%)	0	0	100	100
87	t3	28/198 (14%)	28 (100%)	0	0	100	100
87	t4	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
87	t5	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
87	t6	25/198 (13%)	25 (100%)	0	0	100	100
88	A	2/8 (25%)	0	1 (50%)	1 (50%)	0	0
All	All	13778/19168 (72%)	13136 (95%)	637 (5%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
88	A	4	PRO
72	g	38	PHE
44	XD	207	ILE
44	XD	208	ARG
69	d	289	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	50/60 (83%)	50 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	352 (100%)	1 (0%)	92	95
7	6	313/332 (94%)	312 (100%)	1 (0%)	92	95
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	128/190 (67%)	128 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	176/190 (93%)	175 (99%)	1 (1%)	86	92
13	A1	253/291 (87%)	249 (98%)	4 (2%)	62	79
14	A2	99/101 (98%)	97 (98%)	2 (2%)	55	73
15	A3	63/166 (38%)	63 (100%)	0	100	100
16	A4	494/609 (81%)	490 (99%)	4 (1%)	81	89
18	AB	192/249 (77%)	192 (100%)	0	100	100
19	AC	115/143 (80%)	115 (100%)	0	100	100
20	AD	283/357 (79%)	281 (99%)	2 (1%)	84	90
21	AE	104/107 (97%)	104 (100%)	0	100	100
22	AF	178/209 (85%)	177 (99%)	1 (1%)	86	92
23	AG	264/342 (77%)	264 (100%)	0	100	100
24	AH	125/180 (69%)	125 (100%)	0	100	100
25	AI	104/147 (71%)	104 (100%)	0	100	100
26	AJ	93/118 (79%)	93 (100%)	0	100	100
27	AK	91/113 (80%)	91 (100%)	0	100	100
28	AL	152/226 (67%)	151 (99%)	1 (1%)	84	90
29	AM	95/113 (84%)	95 (100%)	0	100	100
30	AN	93/115 (81%)	93 (100%)	0	100	100
31	AO	166/230 (72%)	165 (99%)	1 (1%)	86	92
32	AP	86/123 (70%)	85 (99%)	1 (1%)	71	84
33	AQ	77/79 (98%)	77 (100%)	0	100	100
34	AR	229/318 (72%)	228 (100%)	1 (0%)	91	94
35	AS	115/164 (70%)	115 (100%)	0	100	100
36	AT	150/157 (96%)	148 (99%)	2 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	AU	149/174 (86%)	148 (99%)	1 (1%)	84	90
38	AV	315/364 (86%)	312 (99%)	3 (1%)	76	86
39	AW	84/158 (53%)	84 (100%)	0	100	100
40	AX	307/351 (88%)	305 (99%)	2 (1%)	84	90
41	AY	104/357 (29%)	104 (100%)	0	100	100
42	AZ	79/95 (83%)	79 (100%)	0	100	100
44	XD	190/245 (78%)	189 (100%)	1 (0%)	88	93
45	XE	259/290 (89%)	259 (100%)	0	100	100
46	XF	217/262 (83%)	217 (100%)	0	100	100
47	XH	86/228 (38%)	85 (99%)	1 (1%)	71	84
48	XI	194/232 (84%)	194 (100%)	0	100	100
49	XJ	133/150 (89%)	132 (99%)	1 (1%)	81	89
50	XK	155/156 (99%)	155 (100%)	0	100	100
51	XL	98/124 (79%)	98 (100%)	0	100	100
52	XM	245/249 (98%)	244 (100%)	1 (0%)	91	94
53	XN	188/211 (89%)	188 (100%)	0	100	100
54	XO	133/150 (89%)	133 (100%)	0	100	100
55	XP	125/155 (81%)	125 (100%)	0	100	100
56	XQ	220/256 (86%)	220 (100%)	0	100	100
57	XR	118/126 (94%)	117 (99%)	1 (1%)	81	89
58	XS	145/180 (81%)	145 (100%)	0	100	100
59	XT	146/176 (83%)	145 (99%)	1 (1%)	84	90
60	XU	126/135 (93%)	126 (100%)	0	100	100
61	XV	179/191 (94%)	179 (100%)	0	100	100
62	XW	91/119 (76%)	88 (97%)	3 (3%)	38	61
63	XX	219/229 (96%)	218 (100%)	1 (0%)	88	93
64	XY	161/223 (72%)	161 (100%)	0	100	100
65	XZ	111/147 (76%)	111 (100%)	0	100	100
66	a	93/133 (70%)	93 (100%)	0	100	100
67	b	130/186 (70%)	130 (100%)	0	100	100
68	c	241/288 (84%)	240 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	d	196/274 (72%)	196 (100%)	0	100	100
70	e	185/236 (78%)	183 (99%)	2 (1%)	73	85
71	f	128/188 (68%)	128 (100%)	0	100	100
72	g	122/148 (82%)	122 (100%)	0	100	100
73	h	103/148 (70%)	103 (100%)	0	100	100
74	i	86/110 (78%)	85 (99%)	1 (1%)	71	84
75	j	68/97 (70%)	68 (100%)	0	100	100
76	k	80/90 (89%)	80 (100%)	0	100	100
77	l	74/116 (64%)	74 (100%)	0	100	100
78	m	54/113 (48%)	54 (100%)	0	100	100
79	o	80/87 (92%)	79 (99%)	1 (1%)	69	82
80	p	117/181 (65%)	117 (100%)	0	100	100
81	q	141/178 (79%)	141 (100%)	0	100	100
82	r	138/169 (82%)	138 (100%)	0	100	100
86	s	326/381 (86%)	325 (100%)	1 (0%)	92	95
87	t1	41/158 (26%)	40 (98%)	1 (2%)	49	69
87	t2	29/158 (18%)	29 (100%)	0	100	100
87	t3	29/158 (18%)	29 (100%)	0	100	100
87	t4	28/158 (18%)	28 (100%)	0	100	100
87	t5	28/158 (18%)	28 (100%)	0	100	100
87	t6	26/158 (16%)	26 (100%)	0	100	100
88	A	2/2 (100%)	2 (100%)	0	100	100
All	All	12396/16509 (75%)	12351 (100%)	45 (0%)	91	94

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	XD	231	LYS
62	XW	56	MET
47	XH	70	LYS
57	XR	44	ARG
63	XX	12	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
31	AO	119	ASN
82	r	123	HIS
41	AY	292	GLN
72	g	139	GLN
38	AV	329	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	XA	1490/1561 (95%)	270 (18%)	7 (0%)
17	AA	916/924 (99%)	167 (18%)	6 (0%)
43	XB	54/72 (75%)	10 (18%)	0
83	r1	0/14	-	-
84	r2	0/76	-	-
85	r3	0/73	-	-
All	All	2460/2720 (90%)	447 (18%)	13 (0%)

5 of 447 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	XA	1681	G
11	XA	1685	C
11	XA	1689	C
11	XA	1692	A
11	XA	1693	C

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	AA	687	G
17	AA	770	C
17	AA	1420	U
17	AA	1234	C
17	AA	1419	G

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	Y5P	r2	12	84	14,19,20	3.14	3 (21%)	18,26,29	0.60	0
84	Y5P	r2	66	84	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
85	Y5P	r3	69	85	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
84	P5P	r2	70	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	Y5P	r3	7	85	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
84	Y5P	r2	3	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
88	004	A	7	88	9,10,11	1.08	1 (11%)	9,12,14	1.80	3 (33%)
84	P5P	r2	6	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	45	85	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
84	Y5P	r2	55	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
85	Y5P	r3	67	85	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
84	P5P	r2	46	84	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r2	76	84	16,23,24	0.97	1 (6%)	14,33,36	1.96	3 (21%)
85	Y5P	r3	39	85	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	61	85	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
83	Y5P	r1	44	83	14,19,20	3.15	3 (21%)	18,26,29	0.58	0
84	P5P	r2	71	84	16,23,24	0.94	1 (6%)	14,33,36	1.96	3 (21%)
85	P5P	r3	11	85	16,23,24	0.97	1 (6%)	14,33,36	1.96	3 (21%)
84	Y5P	r2	41	84	14,19,20	3.15	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	56	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
84	P5P	r2	24	84	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r3	42	85	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	1	84	16,23,24	0.94	1 (6%)	14,33,36	1.96	3 (21%)
85	Y5P	r3	27	85	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
84	Y5P	r2	16	84	14,19,20	3.16	3 (21%)	18,26,29	0.53	0
85	P5P	r3	8	85	16,23,24	0.97	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r2	45	84	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
85	P5P	r3	19	85	16,23,24	0.97	1 (6%)	14,33,36	2.00	3 (21%)
84	Y5P	r2	11	84	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
88	MHV	A	6	88	7,9,10	0.35	0	7,11,13	1.73	2 (28%)
84	Y5P	r2	54	84	14,19,20	3.13	3 (21%)	18,26,29	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	P5P	r3	3	85	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
84	P5P	r2	28	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	22	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	53	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
84	P5P	r2	57	84	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
84	P5P	r2	9	84	16,23,24	0.95	1 (6%)	14,33,36	2.03	3 (21%)
84	P5P	r2	36	83,84	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
84	P5P	r2	38	84	16,23,24	0.96	1 (6%)	14,33,36	1.96	3 (21%)
83	Y5P	r1	53	83	14,19,20	3.14	3 (21%)	18,26,29	0.61	0
84	Y5P	r2	61	84	14,19,20	3.12	3 (21%)	18,26,29	0.56	0
85	P5P	r3	44	85	16,23,24	0.95	1 (6%)	14,33,36	2.02	3 (21%)
85	P5P	r3	51	85	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	59	85	14,19,20	3.15	3 (21%)	18,26,29	0.54	0
85	Y5P	r3	38	85	14,19,20	3.15	3 (21%)	18,26,29	0.64	0
84	Y5P	r2	13	84	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
88	MHU	A	5	88	14,15,16	0.44	0	18,19,21	1.23	3 (16%)
84	P5P	r2	64	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	29	85	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r3	14	85	16,23,24	0.94	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r2	67	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	P5P	r2	65	84	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
84	P5P	r2	30	84	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
85	P5P	r3	46	85	16,23,24	0.97	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r2	17	84	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	60	85	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	34	85	14,19,20	3.14	4 (28%)	18,26,29	0.57	0
84	Y5P	r2	33	84	14,19,20	3.12	3 (21%)	18,26,29	0.63	0
85	P5P	r3	43	85	16,23,24	0.97	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	47	85	14,19,20	3.15	3 (21%)	18,26,29	0.63	0
84	P5P	r2	35	84	16,23,24	0.98	1 (6%)	14,33,36	1.95	3 (21%)
83	Y5P	r1	45	83	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	8	84	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
85	P5P	r3	4	85	16,23,24	0.98	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r2	73	84	16,23,24	0.96	1 (6%)	14,33,36	1.96	3 (21%)
88	DBB	A	3	88	4,5,6	0.56	0	1,5,7	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
83	Y5P	r1	48	83	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	70	85	14,19,20	3.12	4 (28%)	18,26,29	0.63	0
85	P5P	r3	52	85	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
85	P5P	r3	74	85	16,23,24	0.97	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	25	85	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
85	P5P	r3	35	85	16,23,24	0.99	1 (6%)	14,33,36	1.96	3 (21%)
85	P5P	r3	6	85	16,23,24	0.94	1 (6%)	14,33,36	1.99	3 (21%)
85	Y5P	r3	54	85	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
84	P5P	r2	37	84	16,23,24	0.96	1 (6%)	14,33,36	1.96	3 (21%)
85	P5P	r3	5	85	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	64	85	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
84	Y5P	r2	75	84	14,19,20	3.14	3 (21%)	18,26,29	0.65	0
84	Y5P	r2	49	84	14,19,20	3.13	3 (21%)	18,26,29	0.62	0
85	P5P	r3	31	85	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	50	85	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
85	P5P	r3	21	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	48	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r1	47	83	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
83	Y5P	r1	54	83	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
84	P5P	r2	10	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
84	P5P	r2	27	84	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
84	Y5P	r2	74	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	63	85	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
84	P5P	r2	23	84	16,23,24	0.97	1 (6%)	14,33,36	1.97	3 (21%)
84	Y5P	r2	59	84	14,19,20	3.16	3 (21%)	18,26,29	0.56	0
84	P5P	r2	21	84	16,23,24	0.94	1 (6%)	14,33,36	2.02	3 (21%)
84	P5P	r2	63	84	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
84	P5P	r2	19	84	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r2	40	84	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	32	84	14,19,20	3.15	3 (21%)	18,26,29	0.54	0
85	P5P	r3	9	85	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r2	50	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	51	84	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	49	83,84	14,19,20	3.14	3 (21%)	18,26,29	0.61	0
83	Y5P	r1	55	83	14,19,20	3.11	3 (21%)	18,26,29	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
84	Y5P	r2	2	84	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r1	56	20,83	14,19,20	3.13	3 (21%)	18,26,29	0.61	0
85	Y5P	r3	12	85	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	25	84	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	52	83	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	43	84	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
84	Y5P	r2	62	84	14,19,20	3.14	3 (21%)	18,26,29	0.60	0
84	Y5P	r2	20	84	14,19,20	3.14	4 (28%)	18,26,29	0.59	0
85	Y5P	r3	16	85	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
84	P5P	r2	44	84	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	30	85	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r2	42	84	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	72	85	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
85	Y5P	r3	20	85	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
85	Y5P	r3	2	85	14,19,20	3.13	3 (21%)	18,26,29	0.62	0
84	Y5P	r2	72	84	14,19,20	3.13	3 (21%)	18,26,29	0.58	0
85	Y5P	r3	49	85	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	P5P	r2	34	84	16,23,24	0.94	1 (6%)	14,33,36	2.00	3 (21%)
85	Y5P	r3	41	85	14,19,20	3.12	4 (28%)	18,26,29	0.64	0
85	Y5P	r3	56	85	14,19,20	3.12	3 (21%)	18,26,29	0.62	0
83	Y5P	r1	50	83	14,19,20	3.13	3 (21%)	18,26,29	0.61	0
83	Y5P	r1	51	83	14,19,20	3.12	3 (21%)	18,26,29	0.59	0
85	Y5P	r3	1	85	18,20,20	2.76	3 (16%)	25,29,29	0.69	0
84	Y5P	r2	39	84	14,19,20	3.13	3 (21%)	18,26,29	0.55	0
83	Y5P	r1	57	83	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	P5P	r2	69	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	P5P	r3	57	85	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
85	P5P	r3	10	85	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
88	MHW	A	1	88	9,9,10	0.82	0	10,11,13	3.06	3 (30%)
84	P5P	r2	7	84	16,23,24	0.96	1 (6%)	14,33,36	2.01	3 (21%)
85	Y5P	r3	28	85	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
84	P5P	r2	31	84	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	40	85	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
85	P5P	r3	23	85	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	53	85	14,19,20	3.15	3 (21%)	18,26,29	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
85	Y5P	r3	36	85	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
85	P5P	r3	15	85	16,23,24	0.99	1 (6%)	14,33,36	1.96	3 (21%)
85	P5P	r3	68	85	16,23,24	0.97	1 (6%)	14,33,36	1.96	3 (21%)
83	Y5P	r1	46	83	14,19,20	3.11	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	48	84	14,19,20	3.14	3 (21%)	18,26,29	0.65	0
85	P5P	r3	22	85	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	33	85	14,19,20	3.14	3 (21%)	18,26,29	0.53	0
84	Y5P	r2	4	84	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	32	85	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
84	P5P	r2	52	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	66	85	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
85	Y5P	r3	13	85	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
84	P5P	r2	29	84	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
84	Y5P	r2	47	84	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
84	P5P	r2	58	84	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
85	Y5P	r3	65	85	14,19,20	3.11	3 (21%)	18,26,29	0.66	0
85	Y5P	r3	62	85	14,19,20	3.13	3 (21%)	18,26,29	0.63	0
85	Y5P	r3	73	85	14,19,20	3.11	3 (21%)	18,26,29	0.57	0
84	P5P	r2	5	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	18	85	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
84	Y5P	r2	60	84	14,19,20	3.13	3 (21%)	18,26,29	0.60	0
84	Y5P	r2	68	84	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
84	P5P	r2	18	84	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	71	85	16,23,24	0.96	1 (6%)	14,33,36	1.96	3 (21%)
85	P5P	r3	26	85	16,23,24	0.96	1 (6%)	14,33,36	1.95	3 (21%)
85	P5P	r3	55	85	16,23,24	0.96	1 (6%)	14,33,36	1.97	3 (21%)
84	P5P	r2	15	84	16,23,24	0.96	1 (6%)	14,33,36	2.00	3 (21%)
84	P5P	r2	26	84	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
85	P5P	r3	37	85	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
85	Y5P	r3	58	85	14,19,20	3.13	3 (21%)	18,26,29	0.67	0
84	P5P	r2	14	84	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
85	Y5P	r3	24	85	14,19,20	3.13	3 (21%)	18,26,29	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	Y5P	r2	12	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	66	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	69	85	-	3/7/33/34	0/2/2/2
84	P5P	r2	70	84	-	0/3/25/26	0/3/3/3
85	Y5P	r3	7	85	-	3/7/33/34	0/2/2/2
84	Y5P	r2	3	84	-	2/7/33/34	0/2/2/2
88	004	A	7	88	-	1/4/6/8	0/1/1/1
84	P5P	r2	6	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	45	85	-	3/3/25/26	0/3/3/3
84	Y5P	r2	55	84	-	2/7/33/34	0/2/2/2
85	Y5P	r3	67	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	46	84	-	3/3/25/26	0/3/3/3
84	P5P	r2	76	84	-	1/3/25/26	0/3/3/3
85	Y5P	r3	39	85	-	3/7/33/34	0/2/2/2
85	Y5P	r3	61	85	-	2/7/33/34	0/2/2/2
83	Y5P	r1	44	83	-	2/7/33/34	0/2/2/2
84	P5P	r2	71	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	11	85	-	0/3/25/26	0/3/3/3
84	Y5P	r2	41	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	56	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	24	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	42	85	-	2/3/25/26	0/3/3/3
84	P5P	r2	1	84	-	3/3/25/26	0/3/3/3
85	Y5P	r3	27	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	16	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	8	85	-	0/3/25/26	0/3/3/3
84	Y5P	r2	45	84	-	3/7/33/34	0/2/2/2
85	P5P	r3	19	85	-	2/3/25/26	0/3/3/3
84	Y5P	r2	11	84	-	1/7/33/34	0/2/2/2
88	MHV	A	6	88	-	0/1/12/14	0/1/1/1
84	Y5P	r2	54	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	3	85	-	3/3/25/26	0/3/3/3
84	P5P	r2	28	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	22	84	-	1/3/25/26	0/3/3/3
84	P5P	r2	53	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	57	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	9	84	-	3/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	P5P	r2	36	83,84	-	0/3/25/26	0/3/3/3
84	P5P	r2	38	84	-	0/3/25/26	0/3/3/3
83	Y5P	r1	53	83	-	4/7/33/34	0/2/2/2
84	Y5P	r2	61	84	-	2/7/33/34	0/2/2/2
85	P5P	r3	44	85	-	0/3/25/26	0/3/3/3
85	P5P	r3	51	85	-	0/3/25/26	0/3/3/3
85	Y5P	r3	59	85	-	2/7/33/34	0/2/2/2
85	Y5P	r3	38	85	-	4/7/33/34	0/2/2/2
84	Y5P	r2	13	84	-	3/7/33/34	0/2/2/2
88	MHU	A	5	88	-	5/9/12/14	0/1/1/1
84	P5P	r2	64	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	29	85	-	3/3/25/26	0/3/3/3
85	P5P	r3	14	85	-	1/3/25/26	0/3/3/3
84	Y5P	r2	67	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	65	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	30	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	46	85	-	1/3/25/26	0/3/3/3
84	Y5P	r2	17	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	60	85	-	2/7/33/34	0/2/2/2
85	Y5P	r3	34	85	-	5/7/33/34	0/2/2/2
84	Y5P	r2	33	84	-	6/7/33/34	0/2/2/2
85	P5P	r3	43	85	-	1/3/25/26	0/3/3/3
85	Y5P	r3	47	85	-	4/7/33/34	0/2/2/2
84	P5P	r2	35	84	-	2/3/25/26	0/3/3/3
83	Y5P	r1	45	83	-	1/7/33/34	0/2/2/2
84	Y5P	r2	8	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	4	85	-	3/3/25/26	0/3/3/3
84	P5P	r2	73	84	-	2/3/25/26	0/3/3/3
88	DBB	A	3	88	-	0/3/4/6	-
83	Y5P	r1	48	83	-	1/7/33/34	0/2/2/2
85	Y5P	r3	70	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	52	85	-	0/3/25/26	0/3/3/3
85	P5P	r3	74	85	-	2/3/25/26	0/3/3/3
85	Y5P	r3	25	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	35	85	-	3/3/25/26	0/3/3/3
85	P5P	r3	6	85	-	0/3/25/26	0/3/3/3
85	Y5P	r3	54	85	-	3/7/33/34	0/2/2/2
84	P5P	r2	37	84	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	P5P	r3	5	85	-	1/3/25/26	0/3/3/3
85	Y5P	r3	64	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	75	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	49	84	-	3/7/33/34	0/2/2/2
85	P5P	r3	31	85	-	0/3/25/26	0/3/3/3
85	Y5P	r3	50	85	-	3/7/33/34	0/2/2/2
85	P5P	r3	21	85	-	3/3/25/26	0/3/3/3
85	P5P	r3	48	85	-	2/3/25/26	0/3/3/3
83	Y5P	r1	47	83	-	3/7/33/34	0/2/2/2
83	Y5P	r1	54	83	-	3/7/33/34	0/2/2/2
84	P5P	r2	10	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	27	84	-	0/3/25/26	0/3/3/3
84	Y5P	r2	74	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	63	85	-	3/7/33/34	0/2/2/2
84	P5P	r2	23	84	-	1/3/25/26	0/3/3/3
84	Y5P	r2	59	84	-	2/7/33/34	0/2/2/2
84	P5P	r2	21	84	-	2/3/25/26	0/3/3/3
84	P5P	r2	63	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	19	84	-	0/3/25/26	0/3/3/3
84	Y5P	r2	40	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	32	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	9	85	-	1/3/25/26	0/3/3/3
84	Y5P	r2	50	84	-	3/7/33/34	0/2/2/2
84	Y5P	r2	51	84	-	1/7/33/34	0/2/2/2
83	Y5P	r1	49	83,84	-	3/7/33/34	0/2/2/2
83	Y5P	r1	55	83	-	3/7/33/34	0/2/2/2
84	Y5P	r2	2	84	-	1/7/33/34	0/2/2/2
83	Y5P	r1	56	20,83	-	2/7/33/34	0/2/2/2
85	Y5P	r3	12	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	25	84	-	1/7/33/34	0/2/2/2
83	Y5P	r1	52	83	-	1/7/33/34	0/2/2/2
84	Y5P	r2	43	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	62	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	20	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	16	85	-	4/7/33/34	0/2/2/2
84	P5P	r2	44	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	30	85	-	2/3/25/26	0/3/3/3
84	Y5P	r2	42	84	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	Y5P	r3	72	85	-	2/7/33/34	0/2/2/2
85	Y5P	r3	20	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	2	85	-	4/7/33/34	0/2/2/2
84	Y5P	r2	72	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	49	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	34	84	-	0/3/25/26	0/3/3/3
85	Y5P	r3	41	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	56	85	-	7/7/33/34	0/2/2/2
83	Y5P	r1	50	83	-	2/7/33/34	0/2/2/2
83	Y5P	r1	51	83	-	2/7/33/34	0/2/2/2
85	Y5P	r3	1	85	-	4/10/34/34	0/2/2/2
84	Y5P	r2	39	84	-	1/7/33/34	0/2/2/2
83	Y5P	r1	57	83	-	1/7/33/34	0/2/2/2
84	P5P	r2	69	84	-	3/3/25/26	0/3/3/3
85	P5P	r3	57	85	-	2/3/25/26	0/3/3/3
85	P5P	r3	10	85	-	0/3/25/26	0/3/3/3
88	MHW	A	1	88	-	0/2/2/4	0/1/1/1
84	P5P	r2	7	84	-	2/3/25/26	0/3/3/3
85	Y5P	r3	28	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	31	84	-	0/3/25/26	0/3/3/3
85	Y5P	r3	40	85	-	3/7/33/34	0/2/2/2
85	P5P	r3	23	85	-	0/3/25/26	0/3/3/3
85	Y5P	r3	53	85	-	3/7/33/34	0/2/2/2
85	Y5P	r3	36	85	-	3/7/33/34	0/2/2/2
85	P5P	r3	15	85	-	0/3/25/26	0/3/3/3
85	P5P	r3	68	85	-	0/3/25/26	0/3/3/3
83	Y5P	r1	46	83	-	4/7/33/34	0/2/2/2
84	Y5P	r2	48	84	-	2/7/33/34	0/2/2/2
85	P5P	r3	22	85	-	0/3/25/26	0/3/3/3
85	Y5P	r3	33	85	-	2/7/33/34	0/2/2/2
84	Y5P	r2	4	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	32	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	52	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	66	85	-	2/3/25/26	0/3/3/3
85	Y5P	r3	13	85	-	6/7/33/34	0/2/2/2
84	P5P	r2	29	84	-	0/3/25/26	0/3/3/3
84	Y5P	r2	47	84	-	3/7/33/34	0/2/2/2
84	P5P	r2	58	84	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	Y5P	r3	65	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	62	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	73	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	5	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	18	85	-	3/3/25/26	0/3/3/3
84	Y5P	r2	60	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	68	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	18	84	-	1/3/25/26	0/3/3/3
85	P5P	r3	71	85	-	0/3/25/26	0/3/3/3
85	P5P	r3	26	85	-	0/3/25/26	0/3/3/3
85	P5P	r3	55	85	-	2/3/25/26	0/3/3/3
84	P5P	r2	15	84	-	0/3/25/26	0/3/3/3
84	P5P	r2	26	84	-	0/3/25/26	0/3/3/3
85	P5P	r3	37	85	-	0/3/25/26	0/3/3/3
85	Y5P	r3	58	85	-	4/7/33/34	0/2/2/2
84	P5P	r2	14	84	-	2/3/25/26	0/3/3/3
85	Y5P	r3	24	85	-	1/7/33/34	0/2/2/2

The worst 5 of 346 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	r2	59	Y5P	C6-C5	10.61	1.52	1.33
84	r2	25	Y5P	C6-C5	10.58	1.52	1.33
84	r2	16	Y5P	C6-C5	10.58	1.52	1.33
85	r3	59	Y5P	C6-C5	10.57	1.52	1.33
84	r2	41	Y5P	C6-C5	10.56	1.52	1.33

The worst 5 of 233 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	A	1	MHW	O-C-CA	-8.04	116.60	124.22
84	r2	21	P5P	N1-C2-N3	-6.06	119.89	127.65
85	r3	35	P5P	N1-C2-N3	-6.04	119.92	127.65
85	r3	42	P5P	N1-C2-N3	-6.03	119.93	127.65
84	r2	26	P5P	N1-C2-N3	-6.01	119.96	127.65

There are no chirality outliers.

5 of 265 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	r1	46	Y5P	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
83	r1	46	Y5P	O4'-C1'-N1-C6
83	r1	47	Y5P	O4'-C4'-C5'-O5'
83	r1	47	Y5P	C3'-C4'-C5'-O5'
83	r1	55	Y5P	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A	7	004	2	0
88	A	5	MHU	2	0
88	A	1	MHW	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 204 ligands modelled in this entry, 202 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
92	GTP	AX	500	-	26,34,34	1.13	2 (7%)	32,54,54	1.50	6 (18%)
91	DOL	XA	5142	-	43,50,50	3.57	17 (39%)	51,70,70	2.61	9 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	GTP	AX	500	-	-	7/18/38/38	0/3/3/3
91	DOL	XA	5142	-	-	20/58/77/77	0/2/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	XA	5142	DOL	C28-C29	10.18	1.56	1.32
91	XA	5142	DOL	C22-C23	9.89	1.57	1.32
91	XA	5142	DOL	C19-C20	7.44	1.57	1.34
91	XA	5142	DOL	C26-N25	6.56	1.48	1.34
91	XA	5142	DOL	C6-N5	6.35	1.49	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	XA	5142	DOL	O40-S39-O41	-14.87	101.23	118.19
91	XA	5142	DOL	C24-N25-C26	-5.19	113.64	122.03
91	XA	5142	DOL	C23-C22-C20	-4.13	119.66	125.89
91	XA	5142	DOL	C32-O36-C37	-3.84	111.19	117.78
92	AX	500	GTP	PA-O3A-PB	-3.56	120.62	132.83

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	XA	5142	DOL	C3-C2-S39-C42
91	XA	5142	DOL	C1-C2-S39-O41
91	XA	5142	DOL	C1-C2-S39-O40
91	XA	5142	DOL	C1-C2-S39-C42
91	XA	5142	DOL	C43-C42-S39-C2

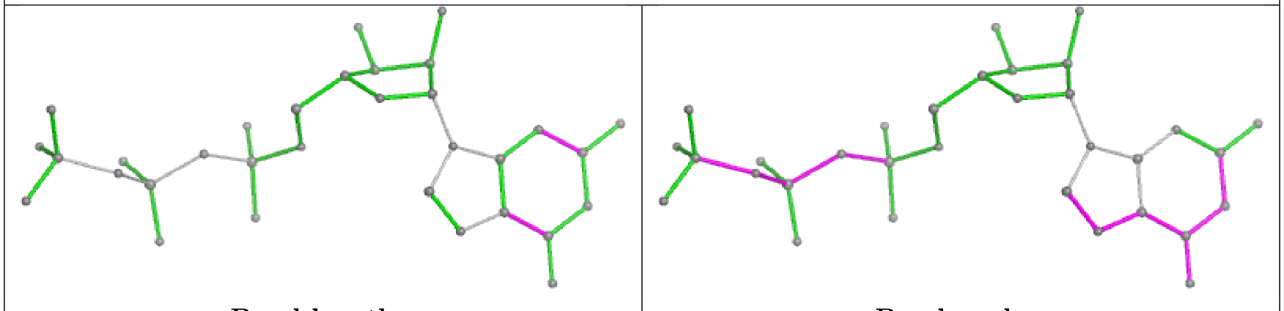
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	AX	500	GTP	1	0
91	XA	5142	DOL	1	0

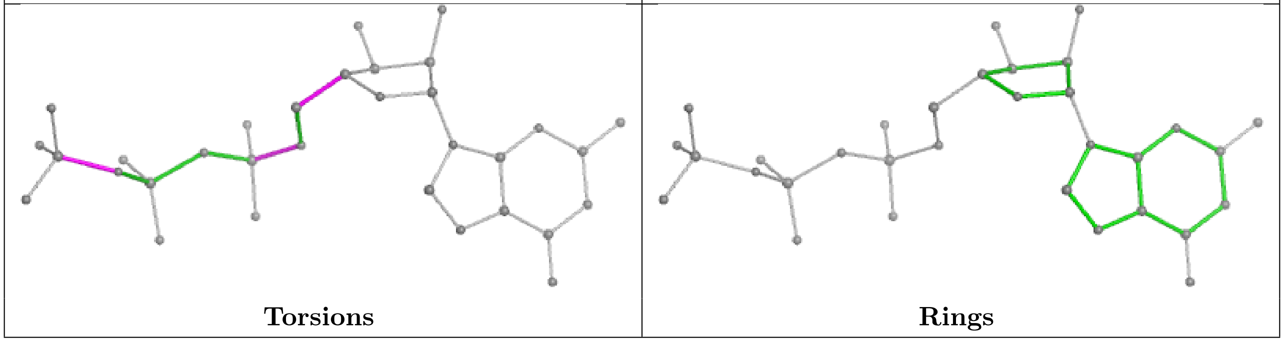
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand GTP AX 500



Bond lengths

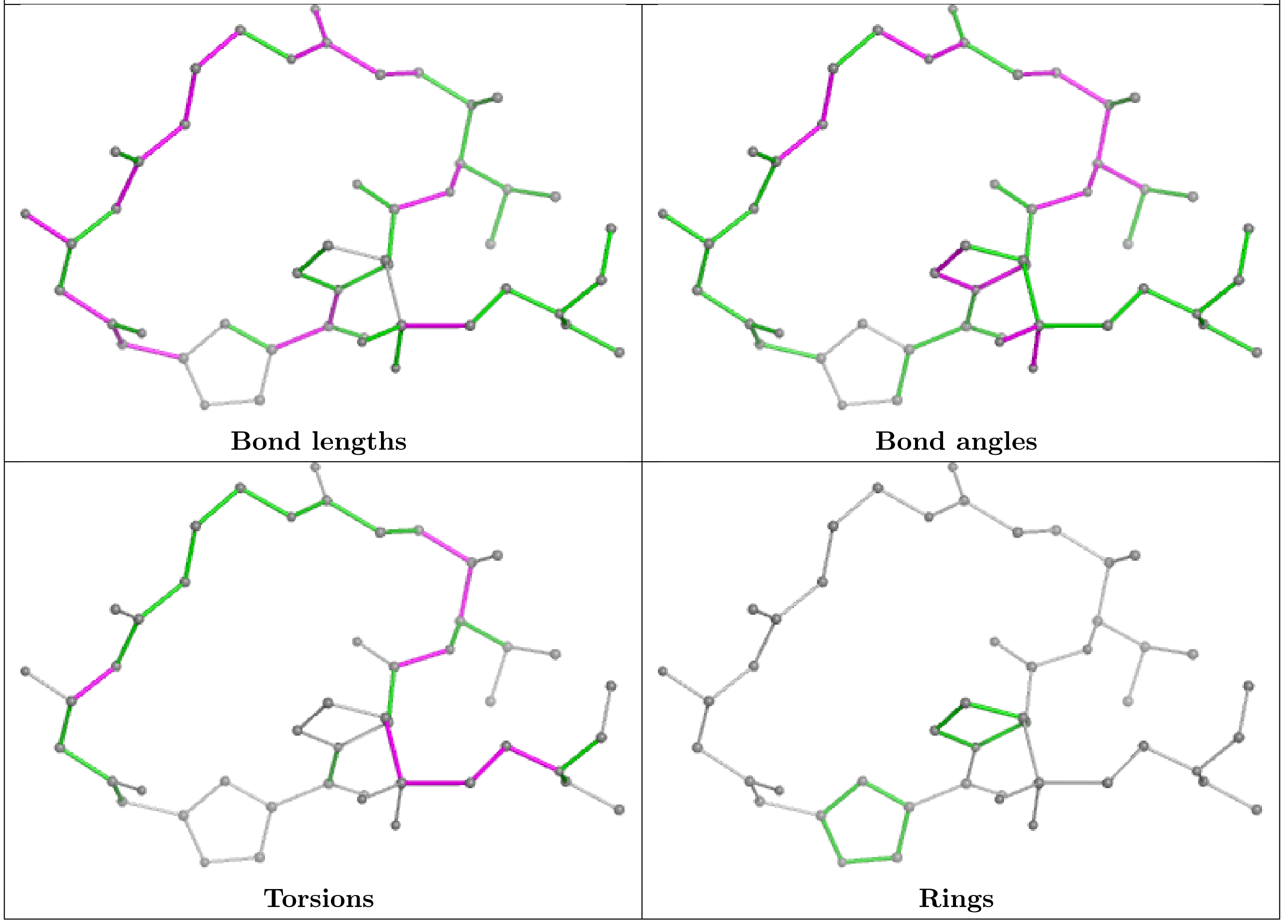
Bond angles



Torsions

Rings

Ligand DOL XA 5142



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	AA	7
8	7	3
16	A4	2
40	AX	2
82	r	1
85	r3	1
38	AV	1
7	6	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	955:A	O3’	965:C	P	31.06
1	AA	734:C	O3’	740:G	P	17.04
1	AA	1403:A	O3’	1407:U	P	14.09
1	AA	1115:U	O3’	1120:C	P	10.73
1	AA	928:A	O3’	931:C	P	9.83

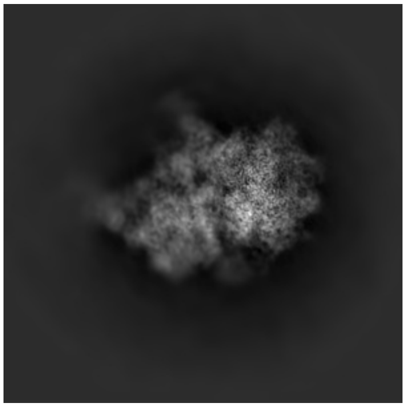
6 Map visualisation

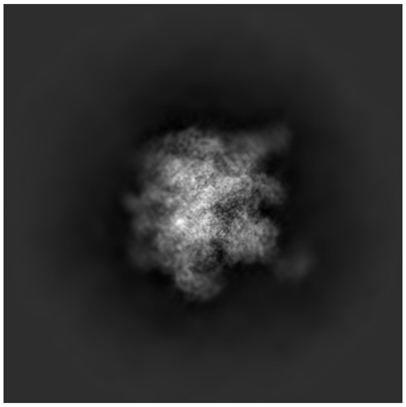
This section contains visualisations of the EMDB entry EMD-11395. These allow visual inspection of the internal detail of the map and identification of artifacts.

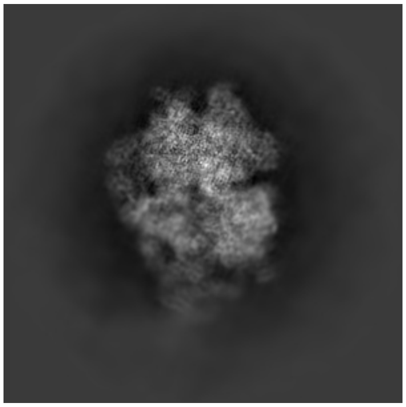
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

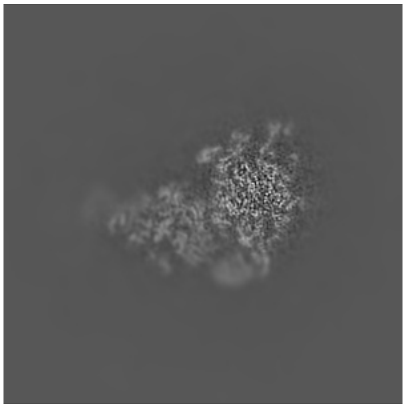

Y

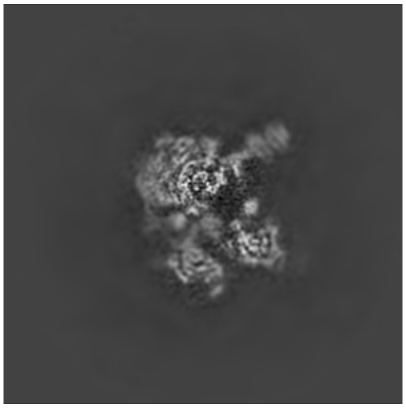

Z

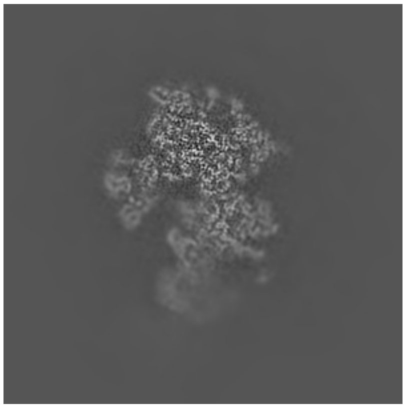
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 260

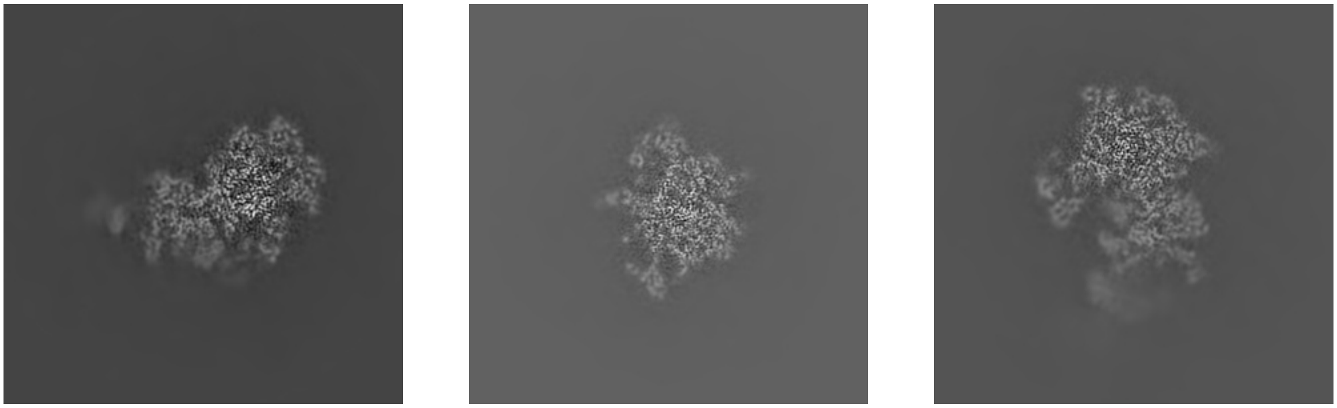

Y Index: 260


Z Index: 260

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

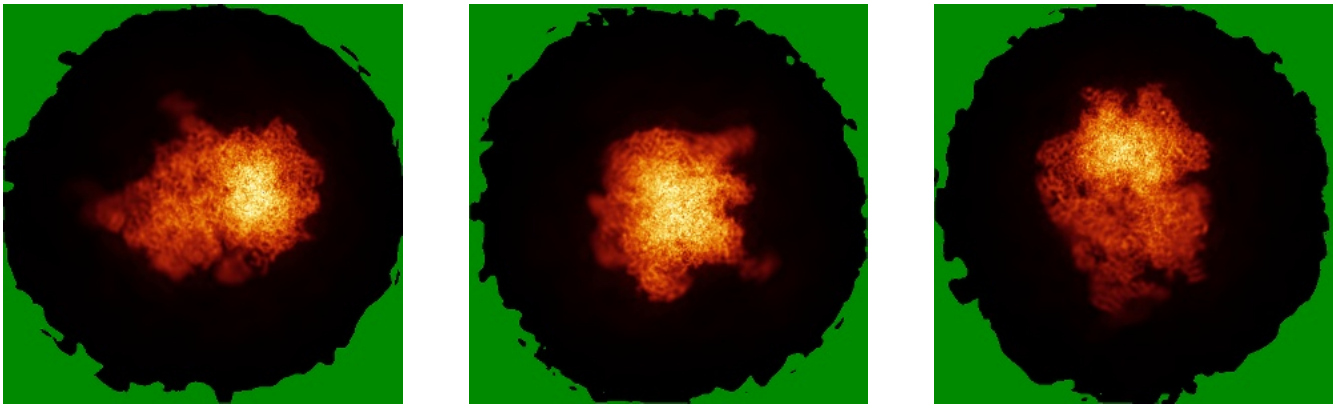


X Index: 277 Y Index: 333 Z Index: 265

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

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

6.4.1 Primary map

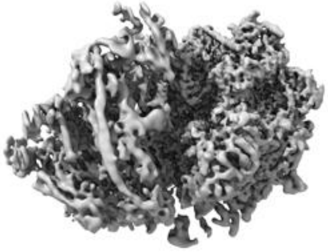


X Y Z

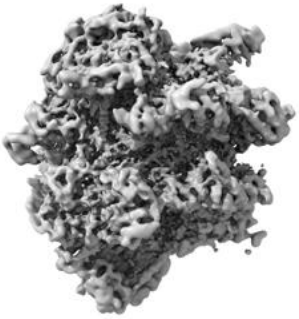
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

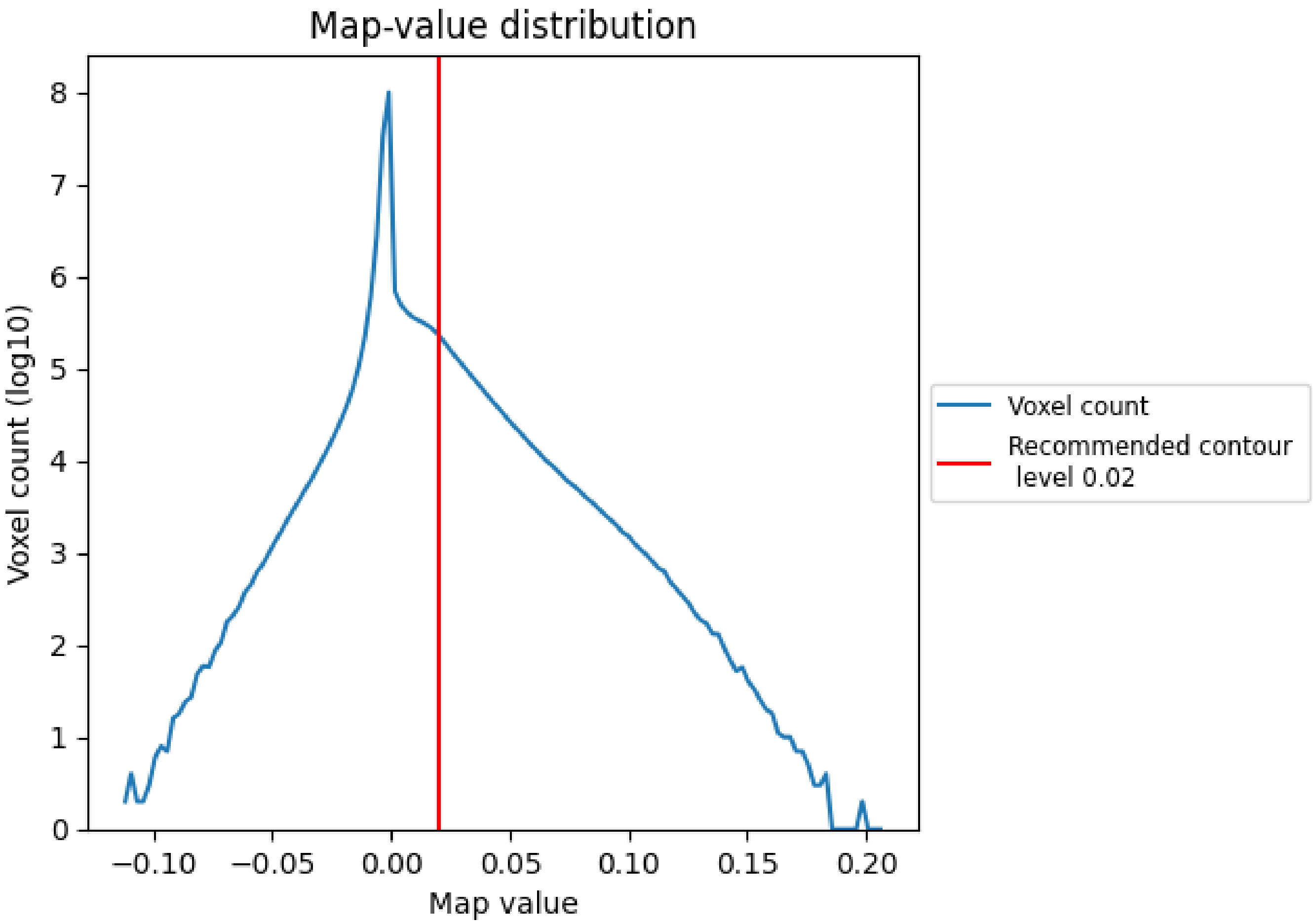
6.6 Mask visualisation

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

7 Map analysis ⓘ

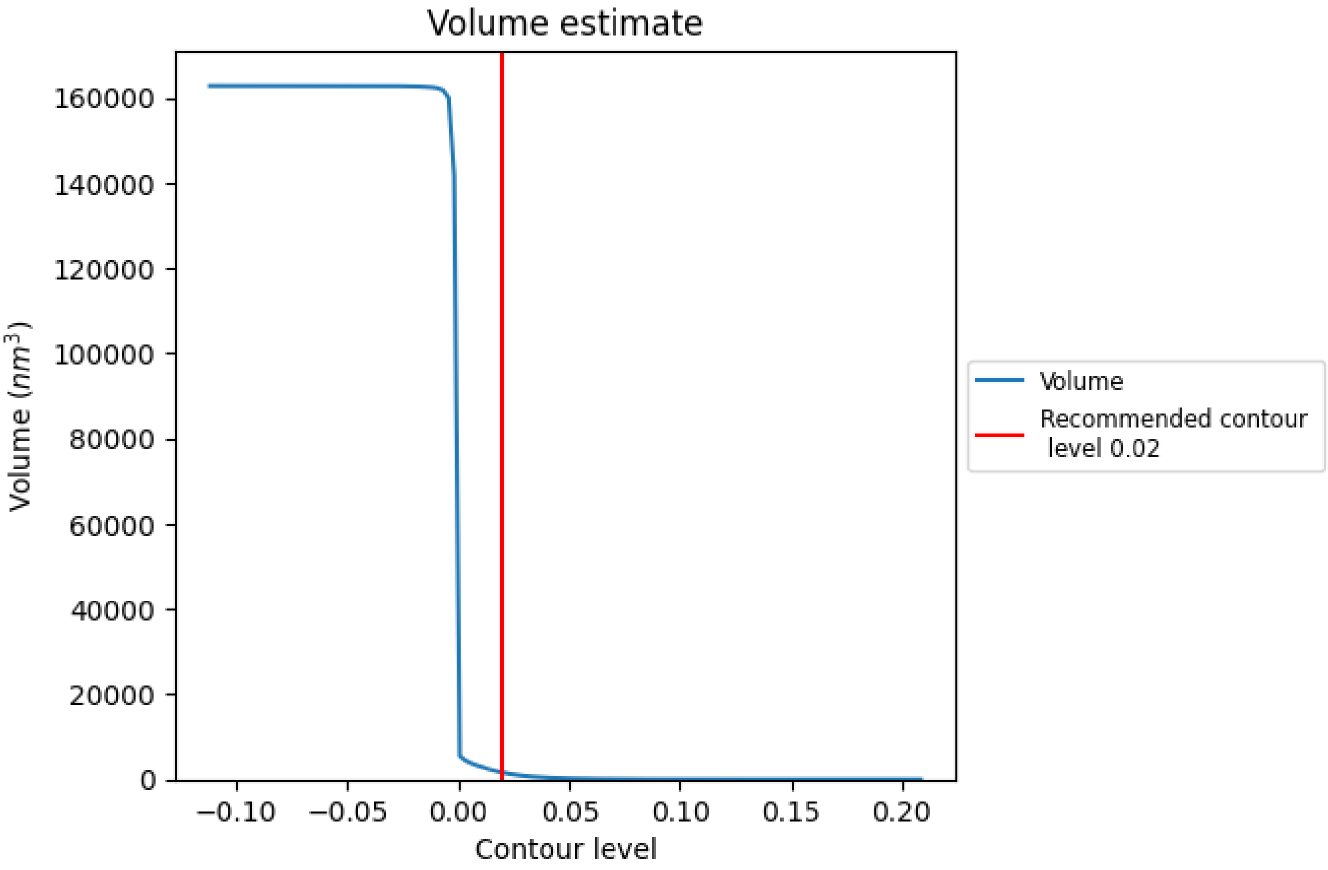
This section contains the results of statistical analysis of the map.

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.

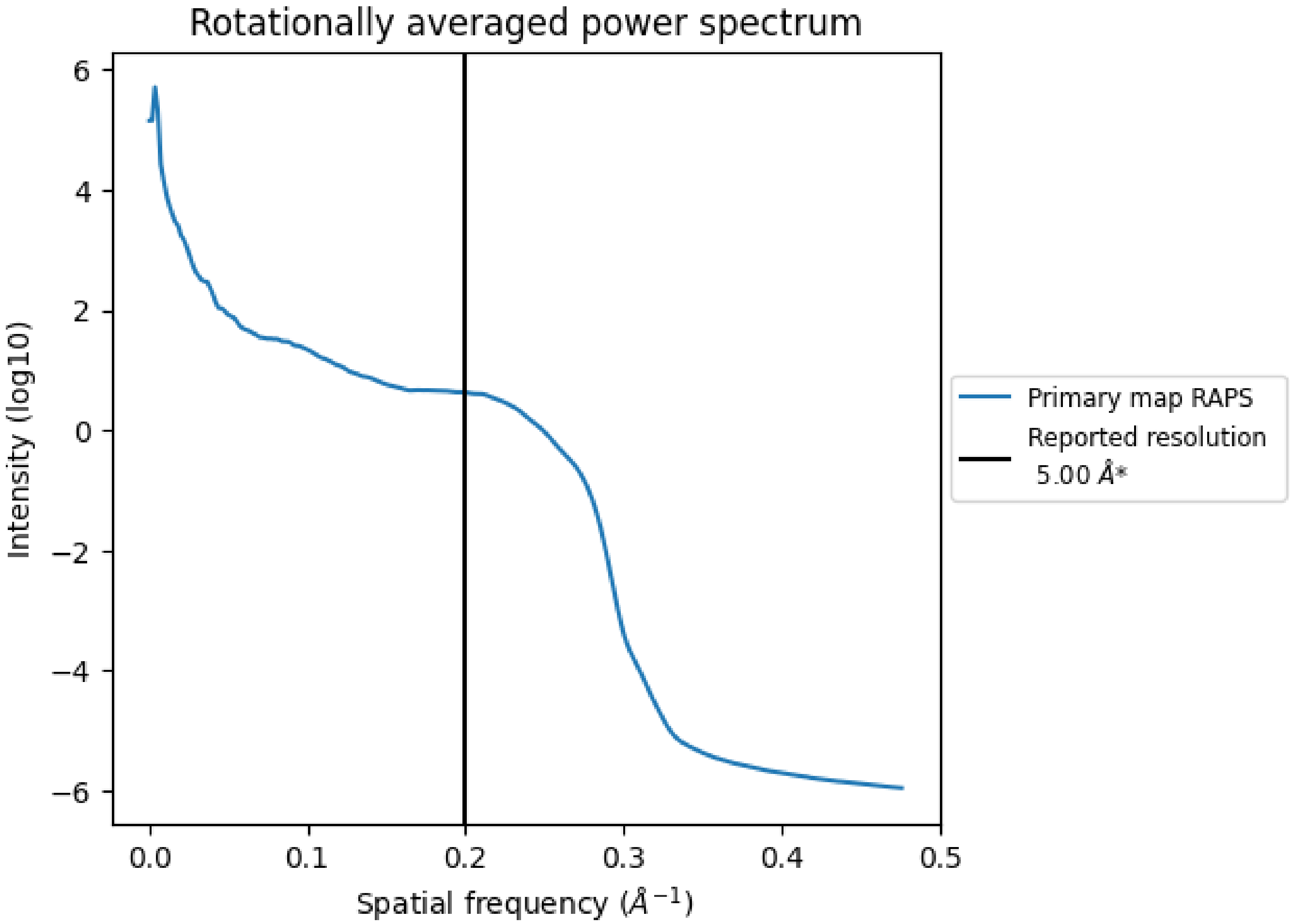
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1624 nm^3; this corresponds to an approximate mass of 1467 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 0.200 Å^{-1}

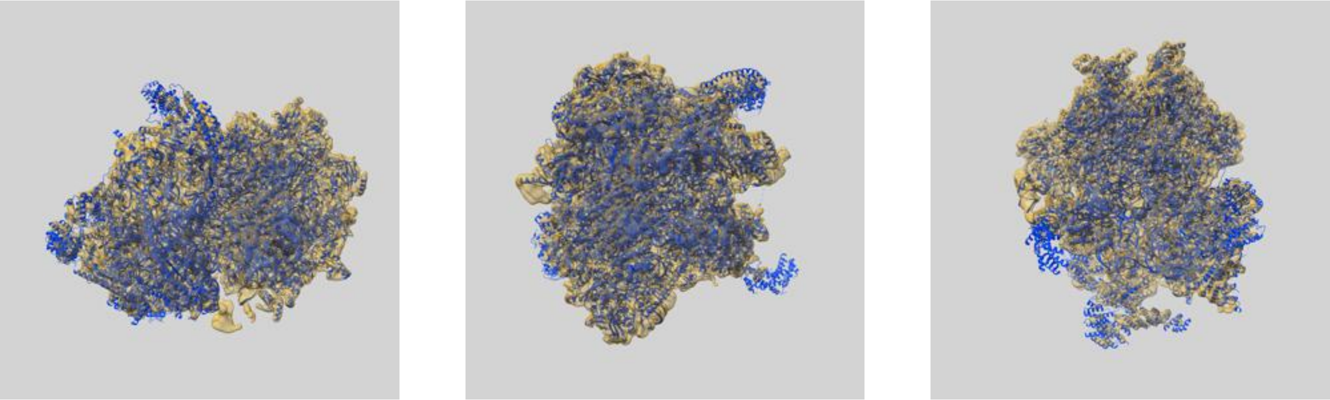
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11395 and PDB model 6ZSE. Per-residue inclusion information can be found in section 3 on page 22.

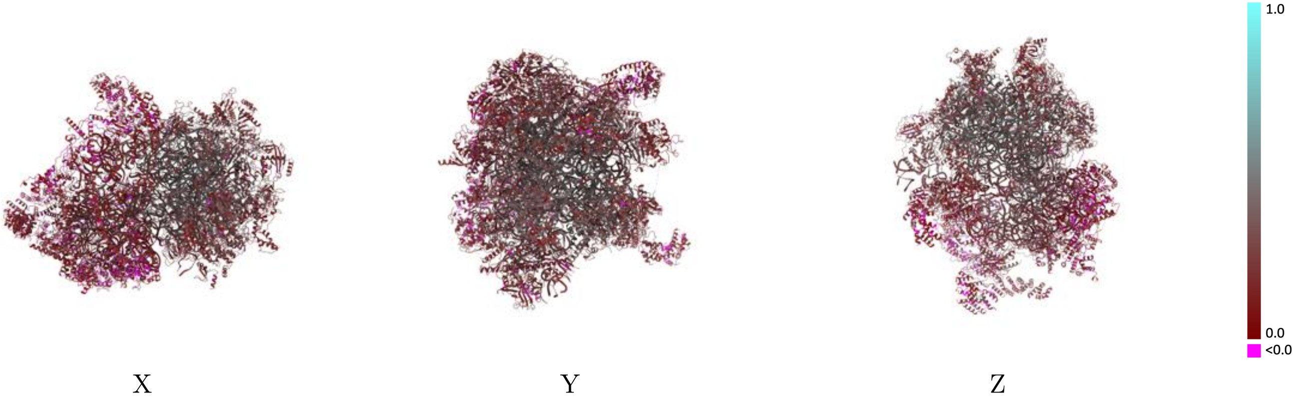
9.1 Map-model overlay ⓘ



X Y Z

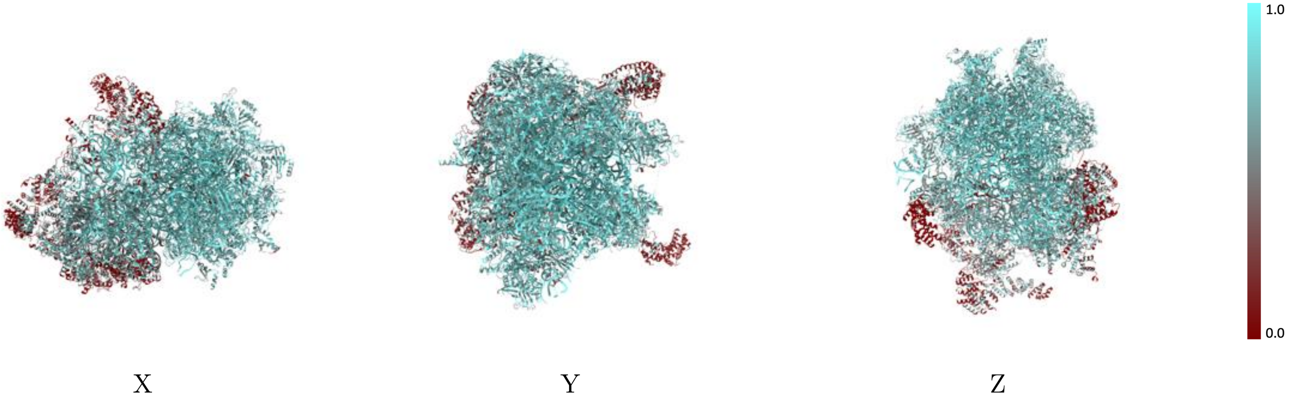
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



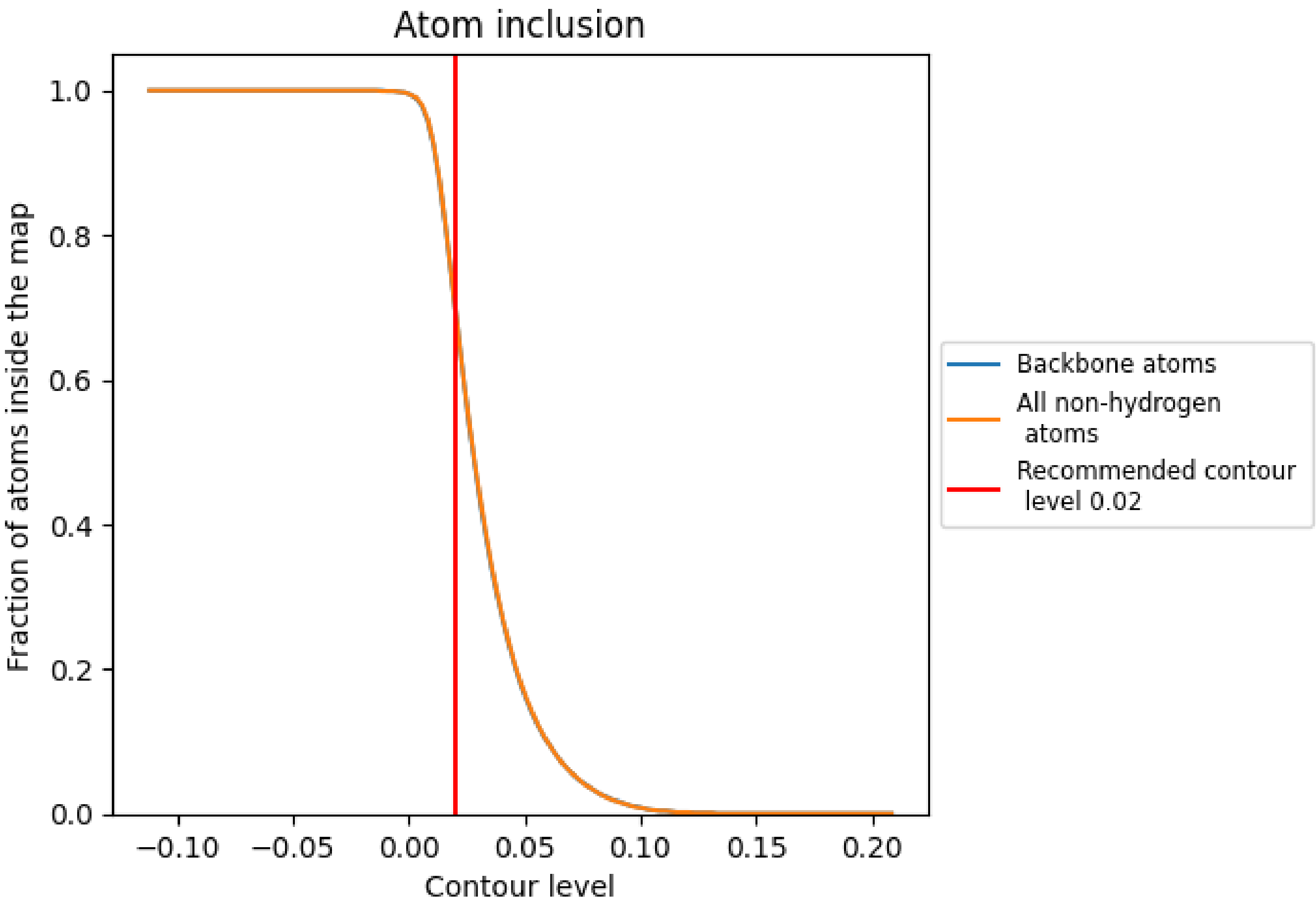
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7000	0.2530
0	0.7850	0.3180
1	0.7180	0.2780
2	0.8440	0.3950
3	0.8410	0.3950
4	0.7940	0.3320
5	0.7500	0.2530
6	0.7330	0.2450
7	0.7290	0.2560
8	0.5410	0.1860
9	0.7510	0.2860
A	0.8080	0.3540
A0	0.4340	0.1130
A1	0.2850	0.1000
A2	0.3800	0.1620
A3	0.7050	0.2760
A4	0.2690	0.1270
AA	0.8690	0.2190
AB	0.5830	0.1560
AC	0.5160	0.1450
AD	0.5530	0.1840
AE	0.4320	0.1380
AF	0.3730	0.1010
AG	0.4930	0.1390
AH	0.2820	0.0970
AI	0.4310	0.1040
AJ	0.6710	0.2200
AK	0.5100	0.0690
AL	0.5170	0.1400
AM	0.5000	0.1140
AN	0.5760	0.1320
AO	0.5710	0.1650
AP	0.4550	0.1270
AQ	0.5140	0.1640
AR	0.4700	0.1250

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Chain	Atom inclusion	Q-score
AS	0.5010	0.1550
AT	0.5910	0.1590
AU	0.5200	0.1510
AV	0.2660	0.1200
AW	0.4760	0.1330
AX	0.1910	0.0640
AY	0.2400	0.0880
AZ	0.4090	0.1160
XA	0.9340	0.3770
XB	0.9410	0.2600
XD	0.8010	0.3150
XE	0.8000	0.3390
XF	0.8350	0.3660
XH	0.7270	0.2790
XI	0.5390	0.1960
XJ	0.6010	0.1650
XK	0.8350	0.3660
XL	0.8080	0.3560
XM	0.8020	0.3440
XN	0.7780	0.3330
XO	0.7900	0.3170
XP	0.7410	0.2520
XQ	0.7130	0.2890
XR	0.8340	0.3650
XS	0.7860	0.3580
XT	0.8290	0.3730
XU	0.7950	0.3260
XV	0.7630	0.2730
XW	0.8170	0.3620
XX	0.7610	0.2840
XY	0.7940	0.2940
XZ	0.8260	0.3640
a	0.7450	0.3170
b	0.8410	0.3550
c	0.7630	0.2800
d	0.6810	0.2310
e	0.5970	0.1610
f	0.6050	0.1920
g	0.8090	0.3390
h	0.7230	0.2650
i	0.8450	0.3800
j	0.8030	0.3350

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Chain	Atom inclusion	Q-score
k	🟦 0.7000	🟥 0.2050
l	🟦 0.6420	🟥 0.1990
m	🟦 0.6930	🟥 0.1780
o	🟦 0.8530	🟫 0.3760
p	🟦 0.7210	🟥 0.2470
q	🟦 0.6190	🟥 0.2310
r	🟦 0.7920	🟥 0.2920
r1	🟦 0.6270	🟥 0.2510
r2	🟦 0.5370	🟥 0.1930
r3	🟦 0.6720	🟥 0.1550
s	🟦 0.7650	🟥 0.2790
t1	🟥 0.1730	🟥 0.1940
t2	🟥 0.2230	🟥 0.1700
t3	🟥 0.0000	🟥 0.1470
t4	🟥 0.0000	🟥 0.1300
t5	🟥 0.0000	🟥 0.1430
t6	🟥 0.0000	🟥 0.0830