Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 03:52 pm GMT

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

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

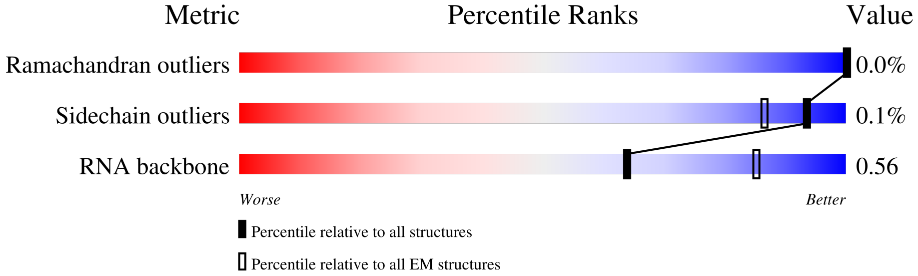
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

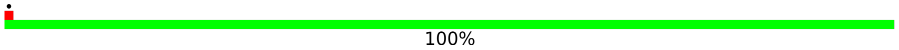
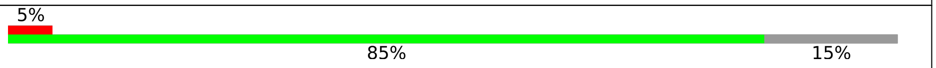
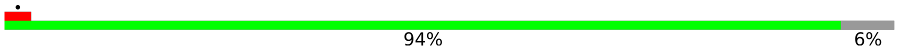
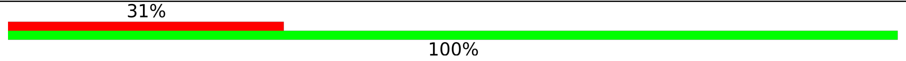
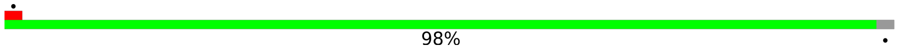
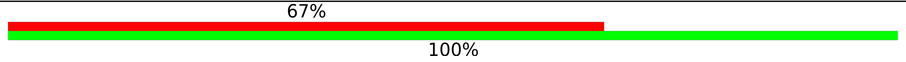
The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	Aa	278	
2	Ab	2314	
3	Ac	262	
4	Ad	439	
5	Ae	358	
6	Af	68	
7	Ag	179	
8	Ah	106	

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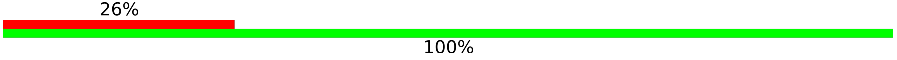
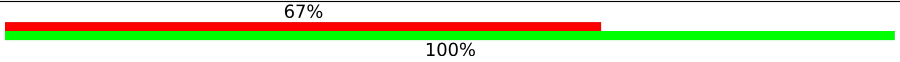
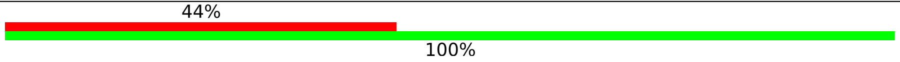
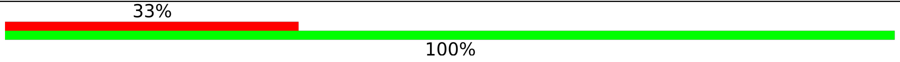
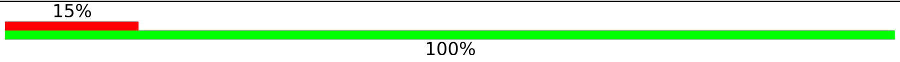
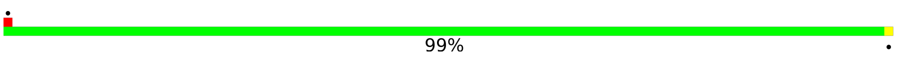
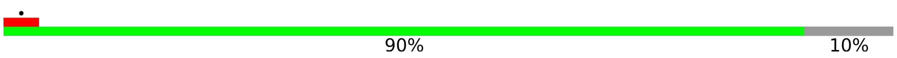
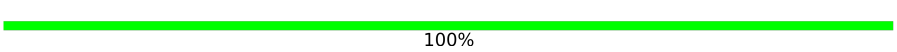
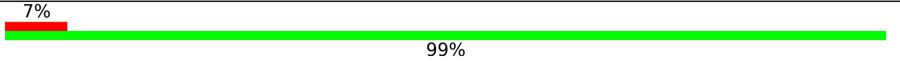
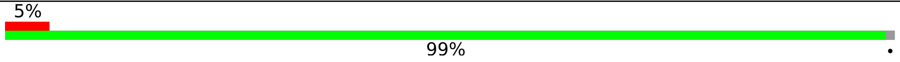
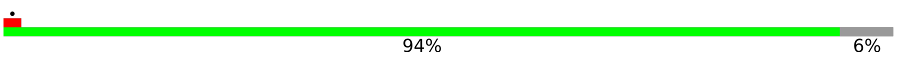
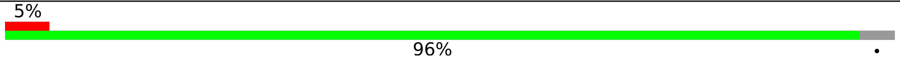
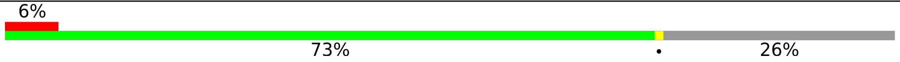
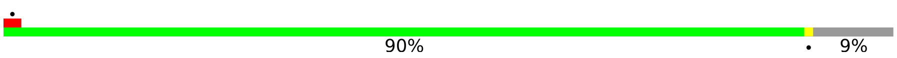
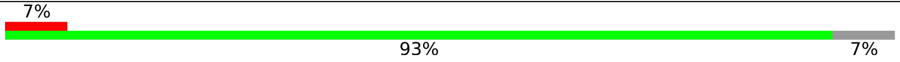
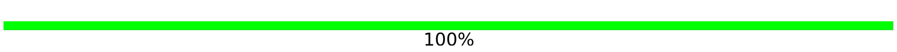
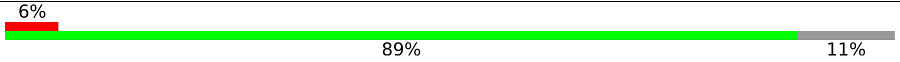
Mol	Chain	Length	Quality of chain
9	Ai	61	
10	Aj	69	
11	Ak	105	
12	Al	223	
13	Am	166	
14	An	158	
15	Ao	391	
16	Ap	119	
17	Aq	305	
18	Ar	143	
19	As	237	
20	At	242	
21	Au	170	
22	Av	235	
23	Aw	364	
24	Ax	138	
25	Ay	234	
26	Az	321	
27	AA	237	
28	AB	289	
29	AC	307	
30	AD	36	
31	AE	64	
32	AF	164	
33	AG	93	

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Mol	Chain	Length	Quality of chain
34	AH	199	31% 89% 11%
35	AI	155	• 79% 21%
36	AJ	179	• 99% ••
37	AK	309	47% 79% 21%
38	AL	145	100%
39	AM	184	• 68% 32%
40	AN	158	8% 61% 39%
41	AO	155	• 77% 23%
42	AP	386	5% 94% 6%
43	AQ	109	• 46% 54%
44	AR	348	26% 79% 21%
45	AS	764	18% 95% 5%
46	AT	299	18% 56% 44%
47	AU	499	5% 96% •
48	AV	160	• 80% • 19%
49	Ba	196	• 78% 22%
50	Bb	1395	• 81% 18% •
51	Bc	159	6% 100%
52	Bd	330	24% 100%
53	Be	405	• 100%
54	Bf	351	5% 95% • •
55	Bg	141	• 96% •
56	Bh	276	34% 92% 7%
57	Bi	737	15% 85% 15%
58	Bj	152	7% 100%

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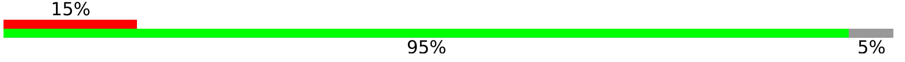
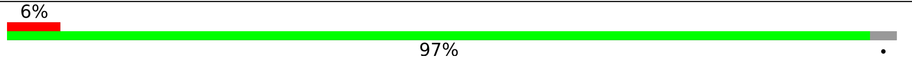
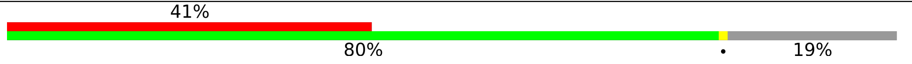
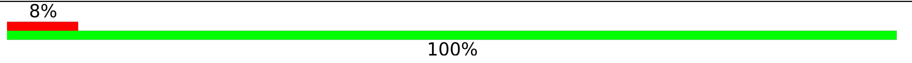
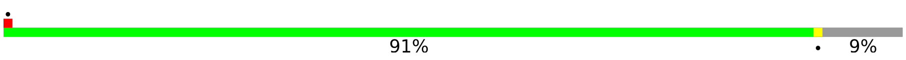
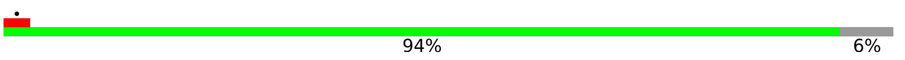
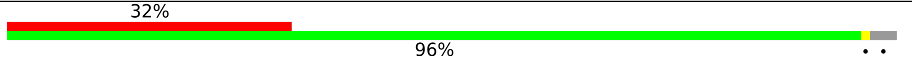
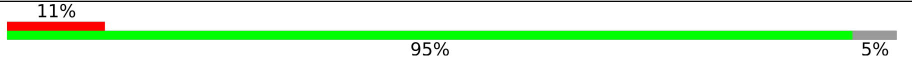
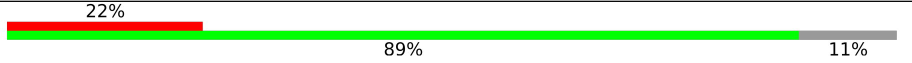
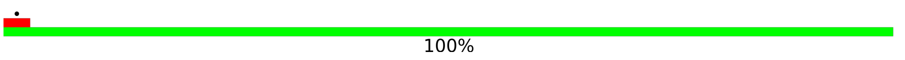
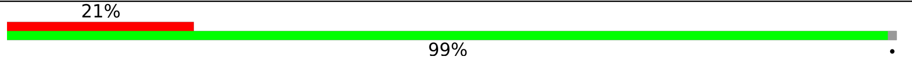
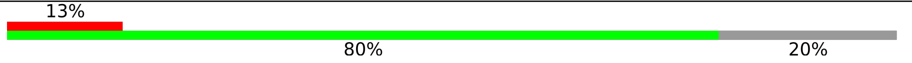
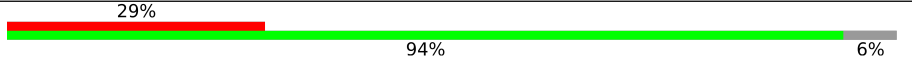
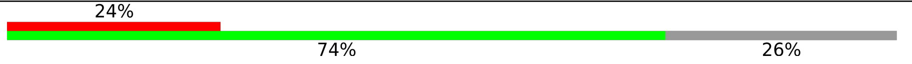
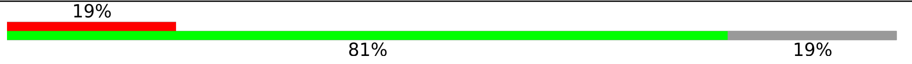
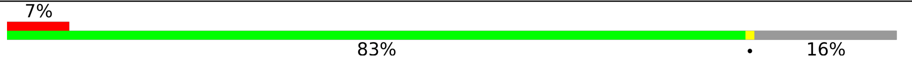
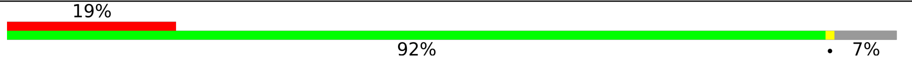
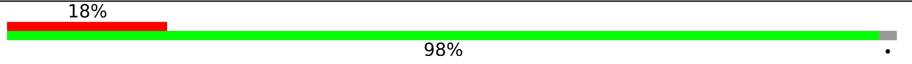
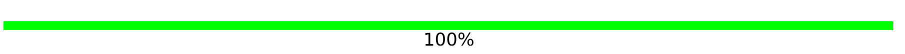
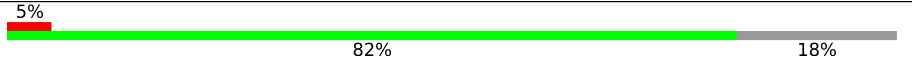
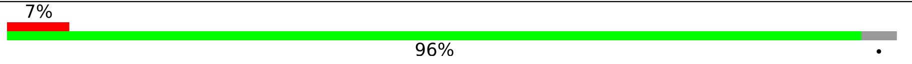
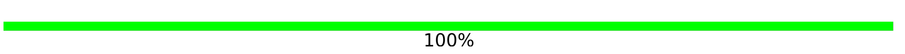
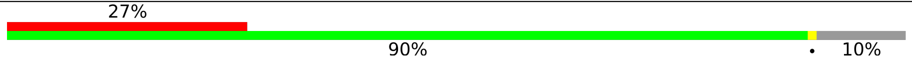
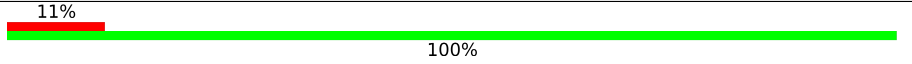
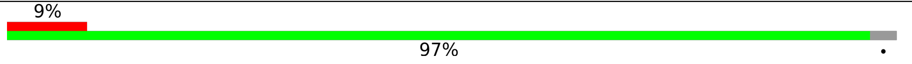
Mol	Chain	Length	Quality of chain
59	Bk	238	
60	Bl	133	
61	Bm	276	
62	Bn	101	
63	Bo	196	
64	Bp	437	
65	Bq	182	
66	Br	549	
67	Bs	98	
68	Bt	102	
69	Bu	567	
70	Bv	579	
71	Bw	703	
72	Bx	719	
73	By	132	
74	Bz	147	
75	BA	149	
76	BB	112	
77	BC	37	
78	BD	130	
79	BE	464	
80	BF	23	
81	BG	182	
82	BH	63	
83	BI	1451	

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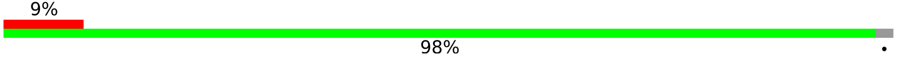
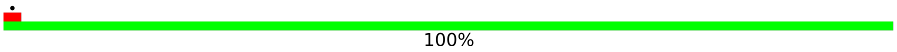
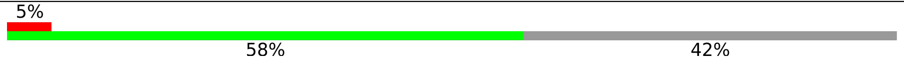
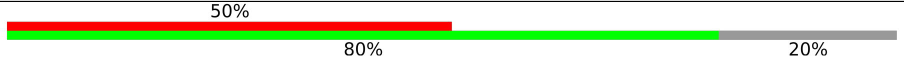
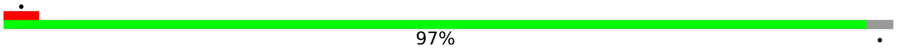
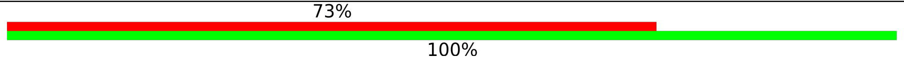
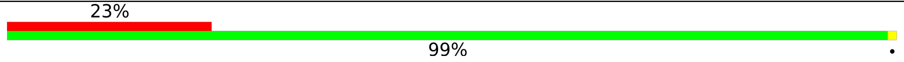
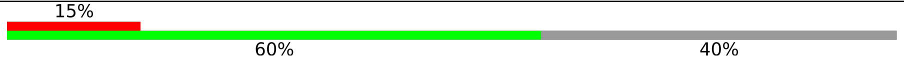
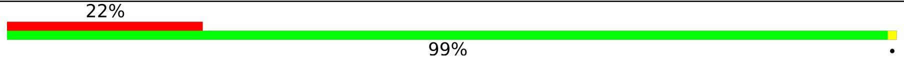
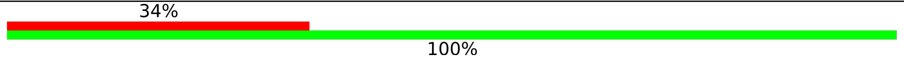
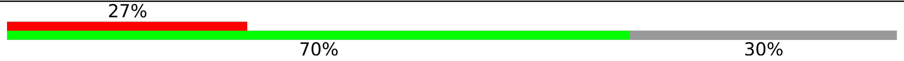
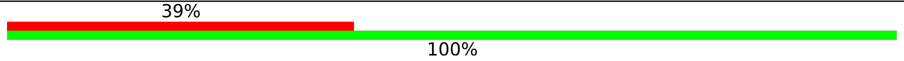
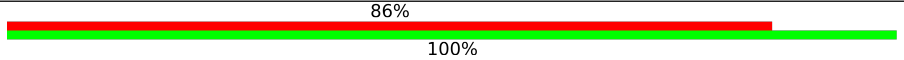
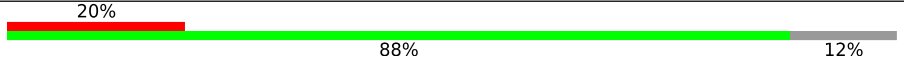
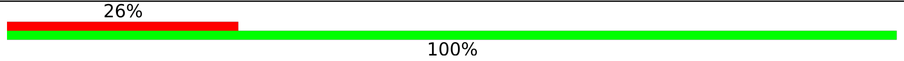
Mol	Chain	Length	Quality of chain
84	BJ	1539	
85	BK	267	
86	BL	310	
87	BM	355	
88	BN	283	
89	BO	142	
90	BP	100	
91	BQ	1032	
92	BR	143	
93	BS	1086	
94	BT	297	
95	BU	439	
96	BV	310	
97	BW	285	
98	BX	151	
99	BY	327	

2 Entry composition ⓘ

There are 103 unique types of molecules in this entry. The entry contains 518719 atoms, of which 235830 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called LSU rRNA_1.

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

- Molecule 2 is a RNA chain called LSU rRNA_2.

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

- Molecule 3 is a protein called Ribosomal protein L2.

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

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

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

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

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

- Molecule 6 is a protein called Ymf69.

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

- Molecule 7 is a protein called Ymf60.

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

- Molecule 8 is a protein called bL7/L12m.

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 13 is a protein called Ymf74.

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

There are 9 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- Molecule 16 is a protein called Ribosomal protein L14.

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

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

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

- Molecule 18 is a protein called Ribosomal protein L16.

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

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

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

- Molecule 20 is a protein called bL19m.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called bL25m.

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

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

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

- Molecule 28 is a protein called Ribosomal protein L28.

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

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

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

- Molecule 30 is a protein called bL32m.

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

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

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

- Molecule 32 is a protein called bL35m.

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

- Molecule 33 is a protein called Ribosomal protein.

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

- Molecule 34 is a protein called mL40.

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

- Molecule 35 is a protein called Ribosomal protein L27.

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

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

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

- Molecule 37 is a protein called mL46.

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

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

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

- Molecule 39 is a protein called mL53.

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

- Molecule 40 is a protein called mL54.

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

- Molecule 41 is a protein called mL64.

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

- Molecule 42 is a protein called mL101.

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

- Molecule 43 is a protein called mL102.

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

- Molecule 44 is a protein called mL103.

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

- Molecule 45 is a protein called mL104.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 47 is a protein called mL106.

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

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

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

- Molecule 49 is a RNA chain called SSU rRNA_1.

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

There are 11 discrepancies between the modelled and reference sequences:

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

- Molecule 50 is a RNA chain called SSU rRNA_2.

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

- Molecule 51 is a protein called Ymf73.

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

- Molecule 52 is a protein called Ymf64.

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

- Molecule 53 is a protein called Ymf76.

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

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

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

- Molecule 55 is a protein called Ribosomal protein S6.

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

- Molecule 56 is a protein called Ymf63.

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

- Molecule 57 is a protein called Ribosomal protein S9.

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

- Molecule 58 is a protein called Ymf59.

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

- Molecule 59 is a protein called Ymf61.

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

- Molecule 60 is a protein called Ribosomal protein S12.

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

- Molecule 61 is a protein called Ribosomal protein S13.

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

- Molecule 62 is a protein called Ribosomal protein S14.

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 66 is a protein called Ribosomal protein S18.

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

- Molecule 67 is a protein called Ribosomal protein S19.

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

- Molecule 68 is a protein called bS21m.

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

- Molecule 69 is a protein called mS23.

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

- Molecule 70 is a protein called mS26.

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

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

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

- Molecule 72 is a protein called mS31.

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

- Molecule 73 is a protein called mS33.

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

- Molecule 74 is a protein called mS34.

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

- Molecule 75 is a protein called Ribosomal subunit protein.

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

- Molecule 76 is a protein called mS37.

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

- Molecule 77 is a protein called mS38.

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

- Molecule 78 is a protein called IGR motif protein.

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

- Molecule 79 is a protein called mS45.

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

- Molecule 80 is a protein called mS75.

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

- Molecule 81 is a protein called mS76.

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

- Molecule 82 is a protein called mS77.

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

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

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

- Molecule 84 is a protein called mS78.

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

- Molecule 85 is a protein called mS79.

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

- Molecule 86 is a protein called SelR domain protein.

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

- Molecule 87 is a protein called mS81.

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

- Molecule 88 is a protein called mS82.

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

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

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

- Molecule 90 is a protein called mS84,mS84.

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

- Molecule 91 is a protein called mS85.

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

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

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

- Molecule 93 is a protein called mS87.

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

- Molecule 94 is a protein called mS88.

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

- Molecule 95 is a protein called mS89.

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

- Molecule 96 is a protein called mS90.

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

- Molecule 97 is a protein called mS91.

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

- Molecule 98 is a protein called Ribosomal protein S3.

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

- Molecule 99 is a protein called mS93.

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

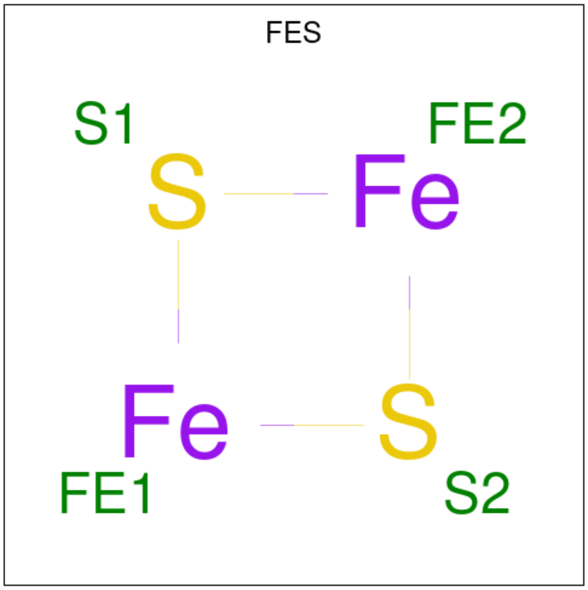
- Molecule 100 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 101 is ZINC ION (three-letter code: ZN) (formula: Zn).

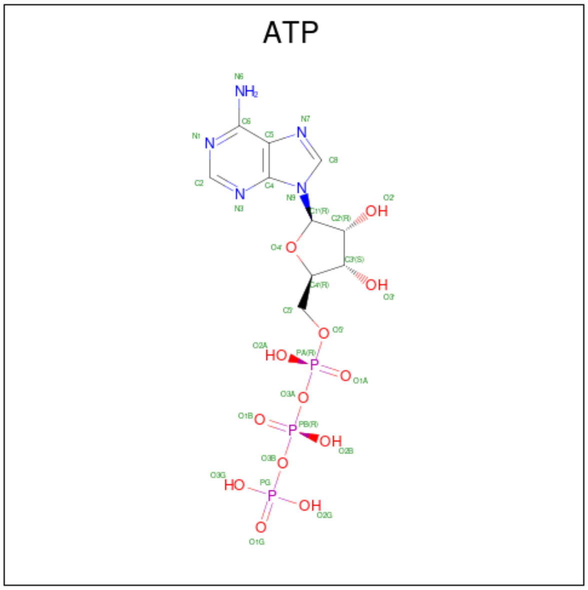
Mol	Chain	Residues	Atoms	AltConf
101	AG	1	Total Zn 1 1	0
101	BL	1	Total Zn 1 1	0

- Molecule 102 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
102	AV	1	Total Fe S 8 4 4	0
102	AV	1	Total Fe S 8 4 4	0

- Molecule 103 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



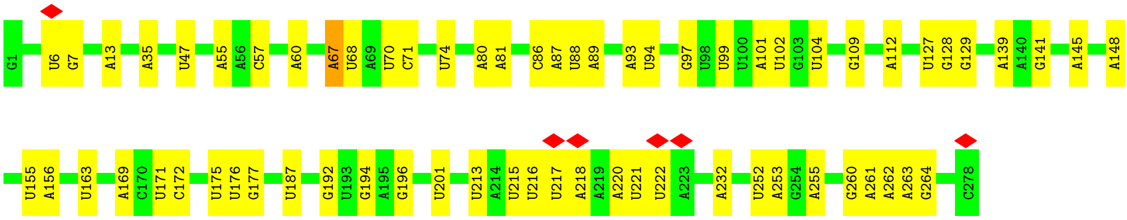
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
103	Bw	1	35	10	4	5	13	3	0

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.

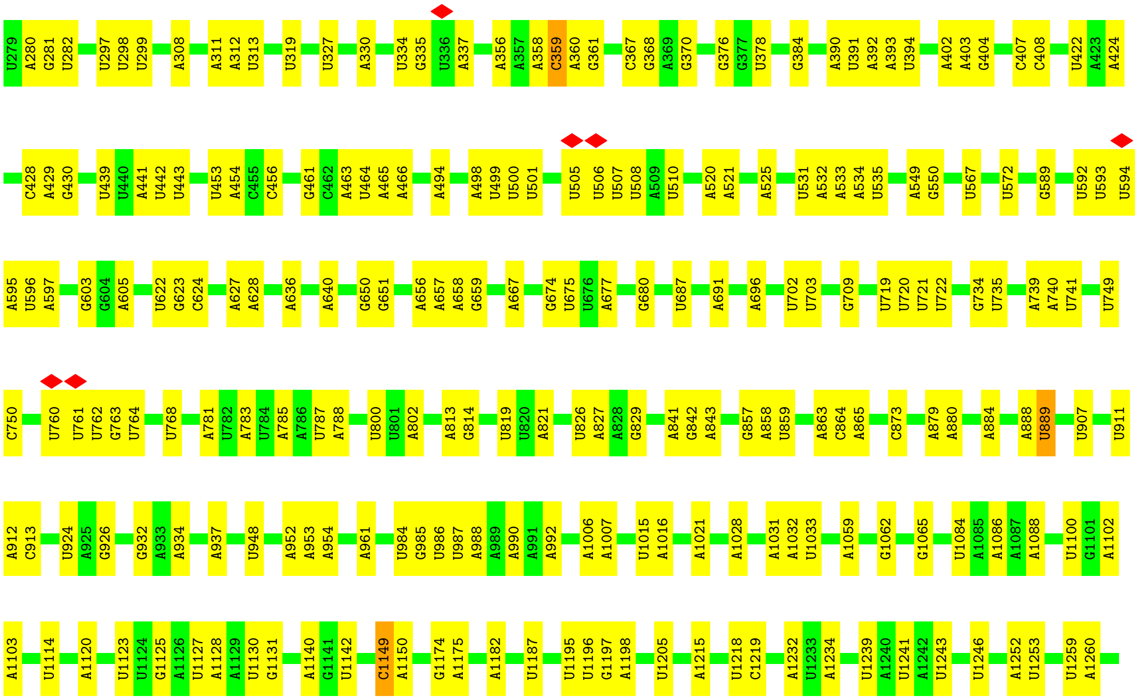
- Molecule 1: LSU rRNA_1

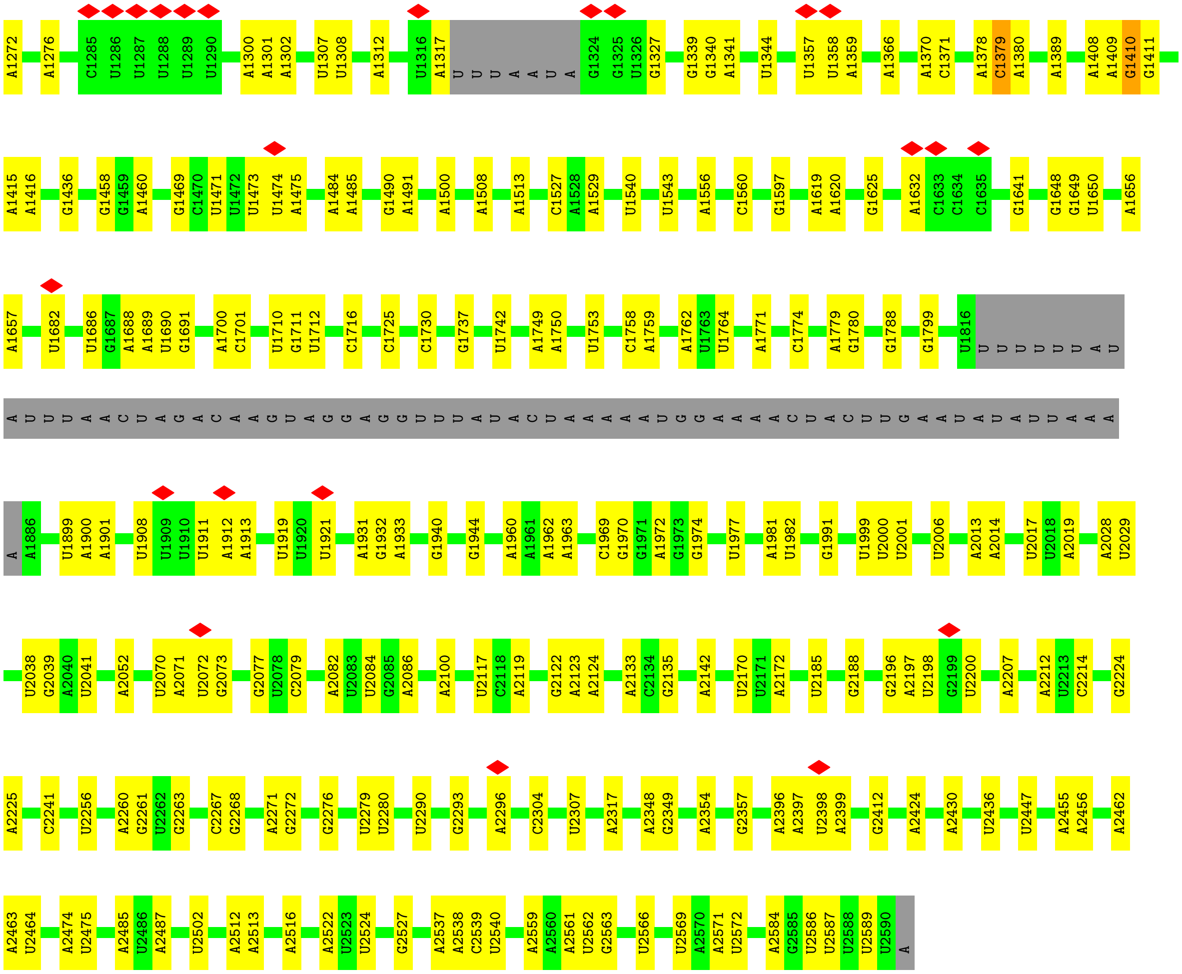
Chain Aa:



- Molecule 2: LSU rRNA_2

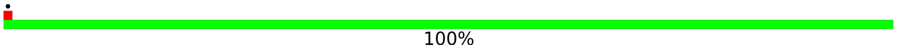
Chain Ab:

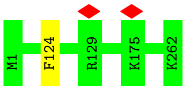




- Molecule 3: Ribosomal protein L2

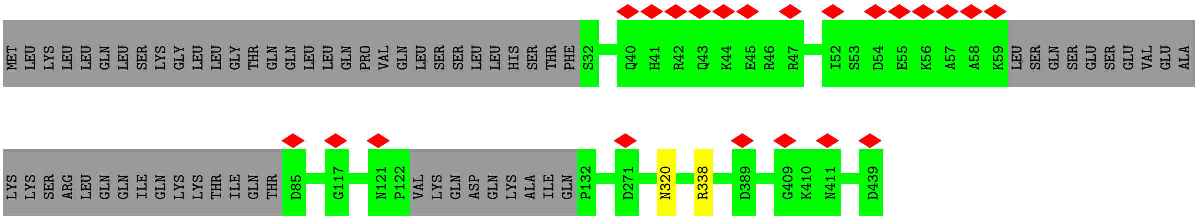
Chain Ac:





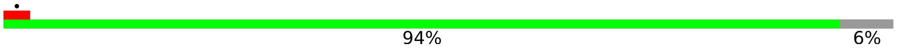
- Molecule 4: 50S ribosomal protein L3

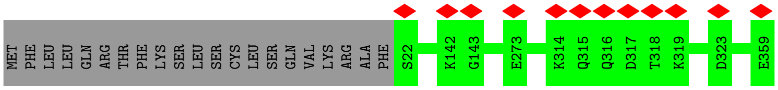
Chain Ad:



- Molecule 5: 50S ribosomal protein L4

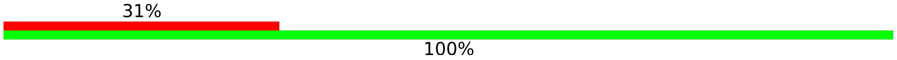
Chain Ae:

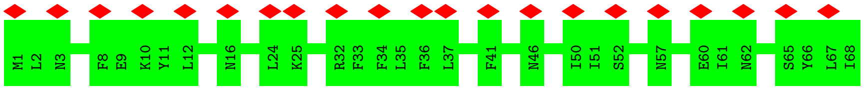




- Molecule 6: Ymf69

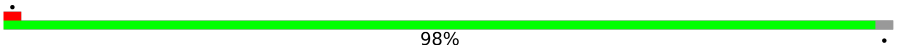
Chain Af:

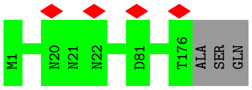




- Molecule 7: Ymf60

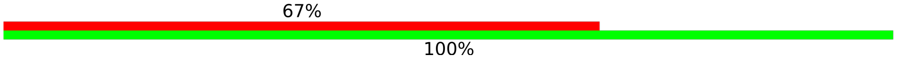
Chain Ag:

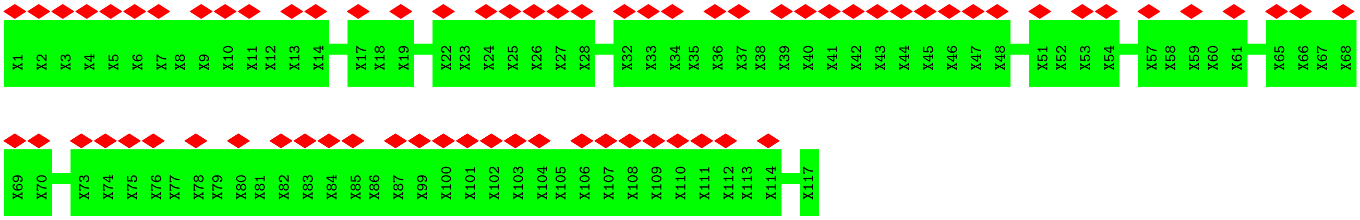




- Molecule 8: bL7/L12m

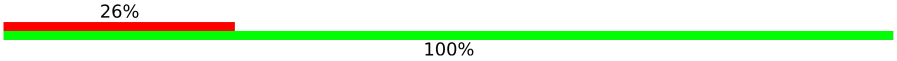
Chain Ah:

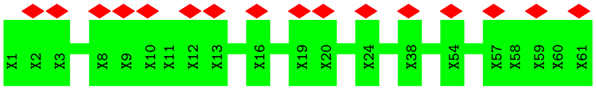




- Molecule 9: bL7/12m

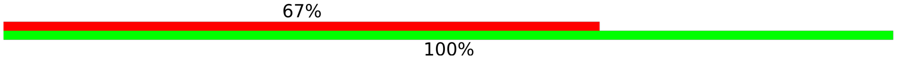
Chain Ai:

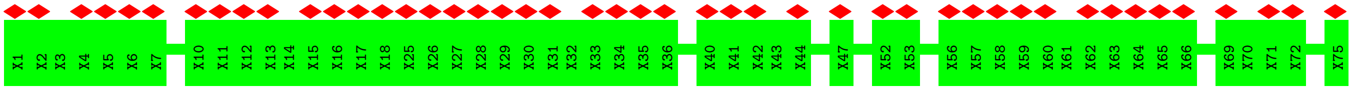




- Molecule 10: bL7/12m

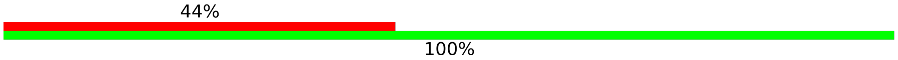
Chain Aj:

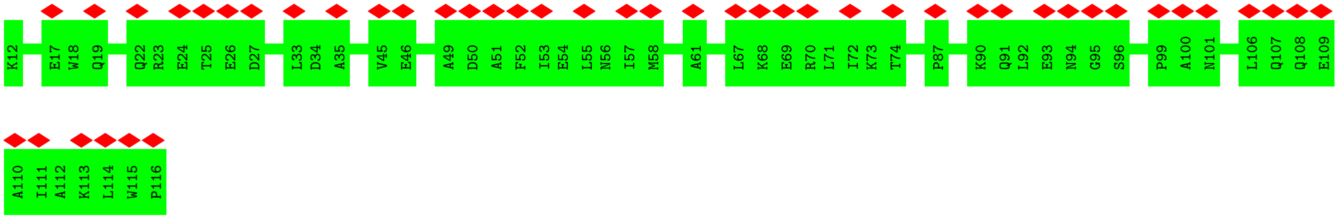




- Molecule 11: Ribosomal protein L7/L12 carboxy-terminal domain protein

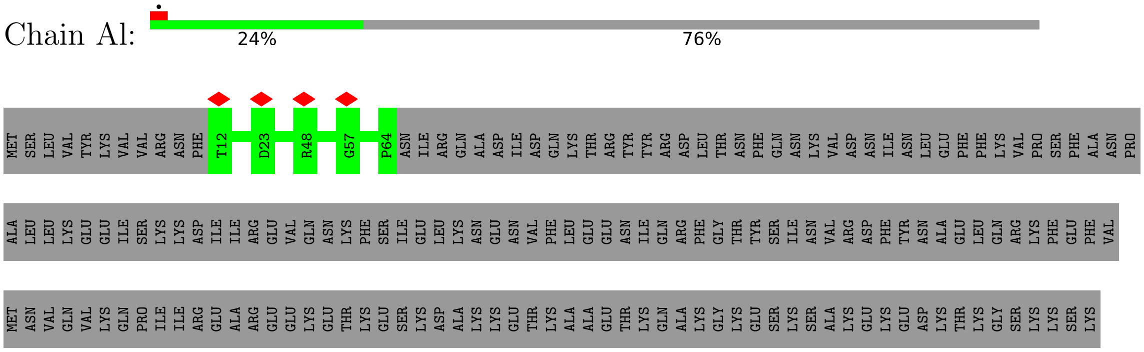
Chain Ak:





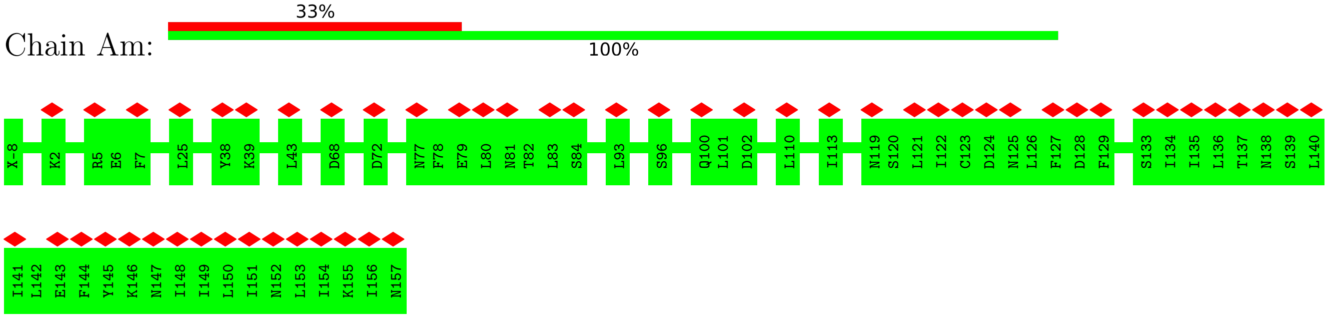
- Molecule 12: Ribosomal protein L9, amine-terminal domain protein

Chain Al:



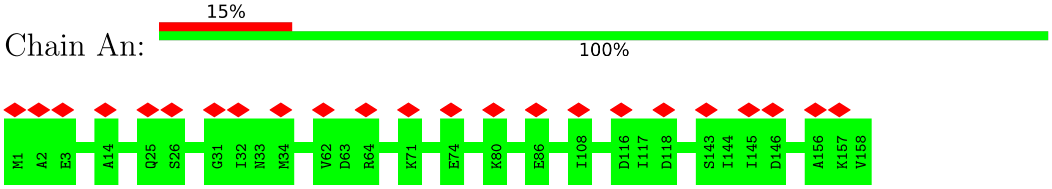
- Molecule 13: Ymf74

Chain Am:



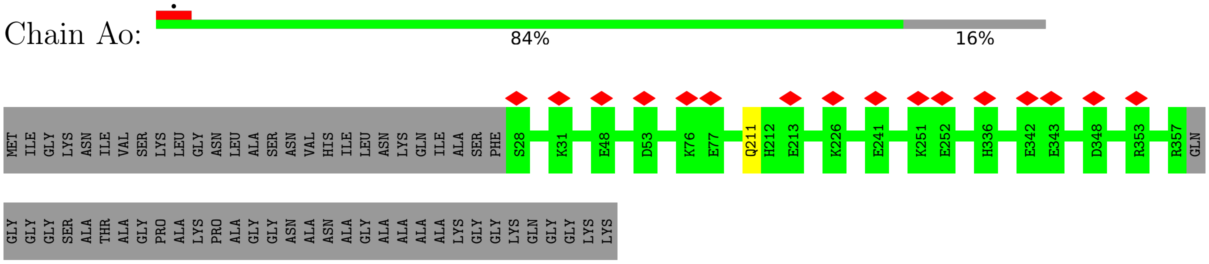
- Molecule 14: Ribosomal protein L11, amine-terminal domain protein

Chain An:



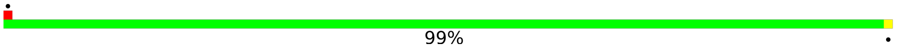
- Molecule 15: 50S ribosomal protein L13

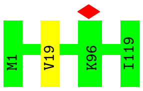
Chain Ao:



- Molecule 16: Ribosomal protein L14

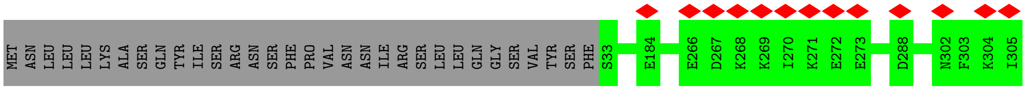
Chain Ap:





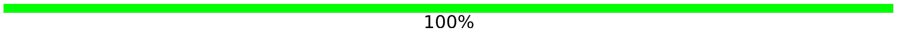
- Molecule 17: Ribosomal protein L15, putative

Chain Aq:



- Molecule 18: Ribosomal protein L16

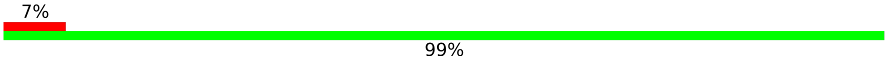
Chain Ar:

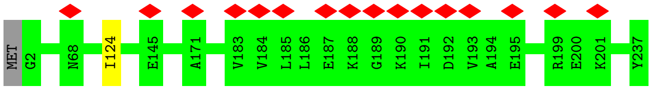


There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L17

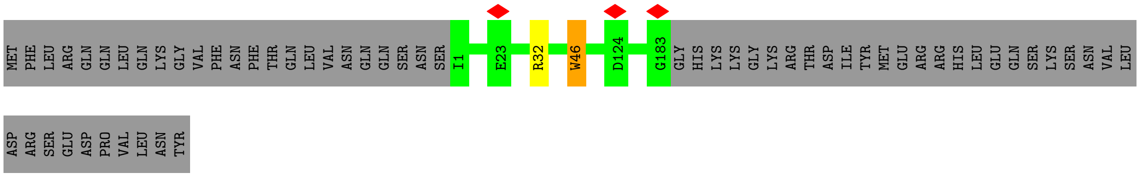
Chain As:





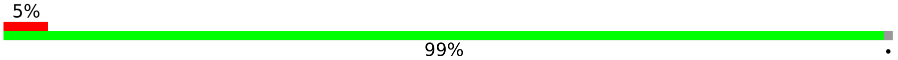
- Molecule 20: bL19m

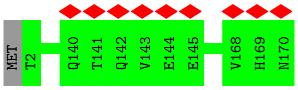
Chain At:



- Molecule 21: 50S ribosomal protein L20

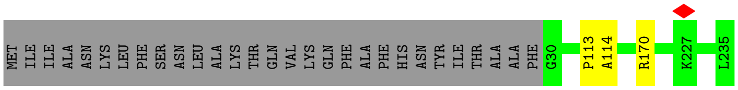
Chain Au:





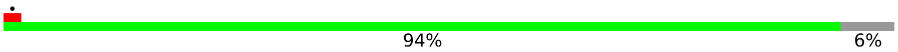
- Molecule 22: 50S ribosomal protein L21

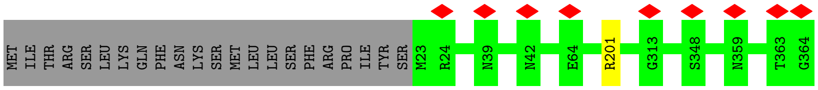
Chain Av:



- Molecule 23: Ribosomal protein L22/L17e

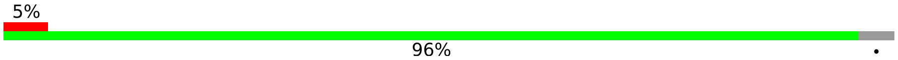
Chain Aw:

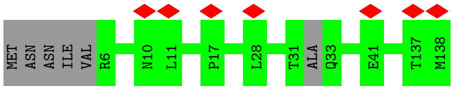




- Molecule 24: Ribosomal protein L23, putative

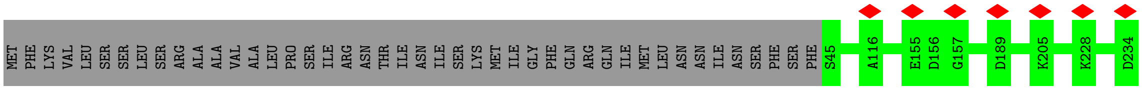
Chain Ax:





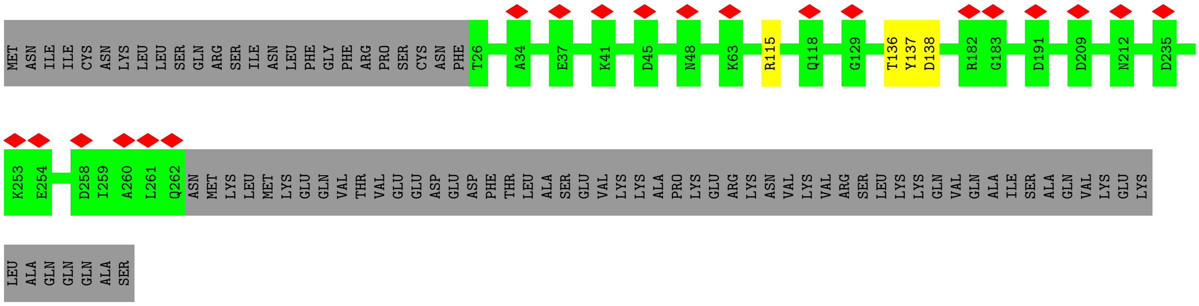
- Molecule 25: 50S ribosomal protein L24

Chain Ay:



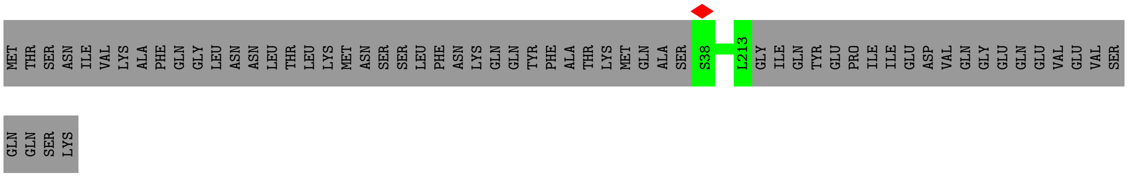
- Molecule 26: bL25m

Chain Az:



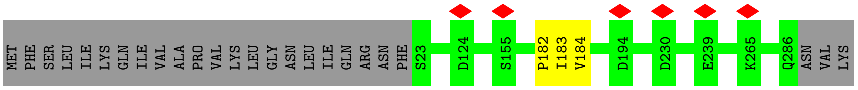
- Molecule 27: 50S ribosomal protein L27

Chain AA:



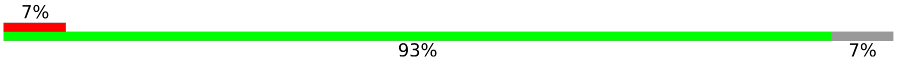
- Molecule 28: Ribosomal protein L28

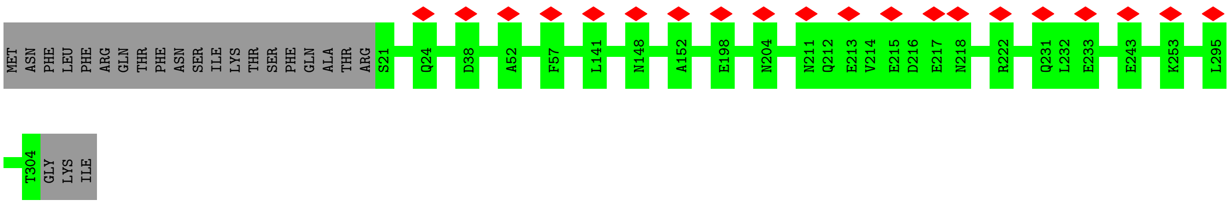
Chain AB:



- Molecule 29: 39-S ribosomal protein L47

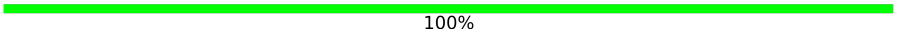
Chain AC:





- Molecule 30: bL32m

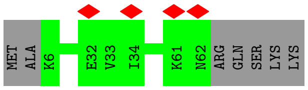
Chain AD:



There are no outlier residues recorded for this chain.

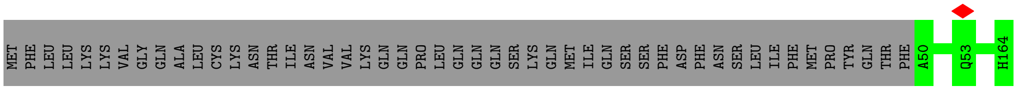
- Molecule 31: 50S ribosomal protein L33

Chain AE:



- Molecule 32: bL35m

Chain AF:

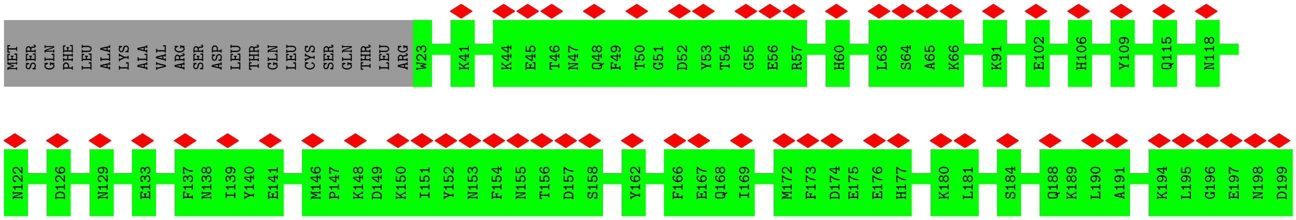


- Molecule 33: Ribosomal protein

Chain AG:

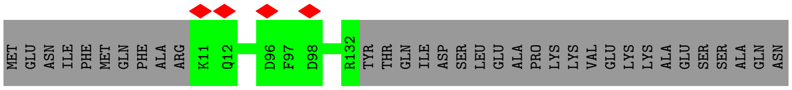
- Molecule 34: mL40

Chain AH:



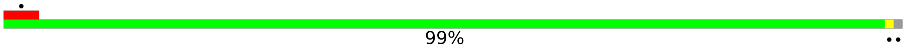
- Molecule 35: Ribosomal protein L27

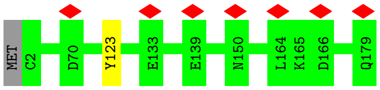
Chain AI:



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

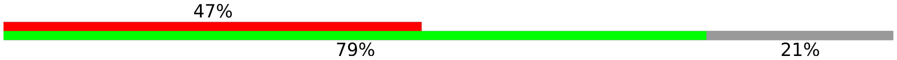
Chain AJ:

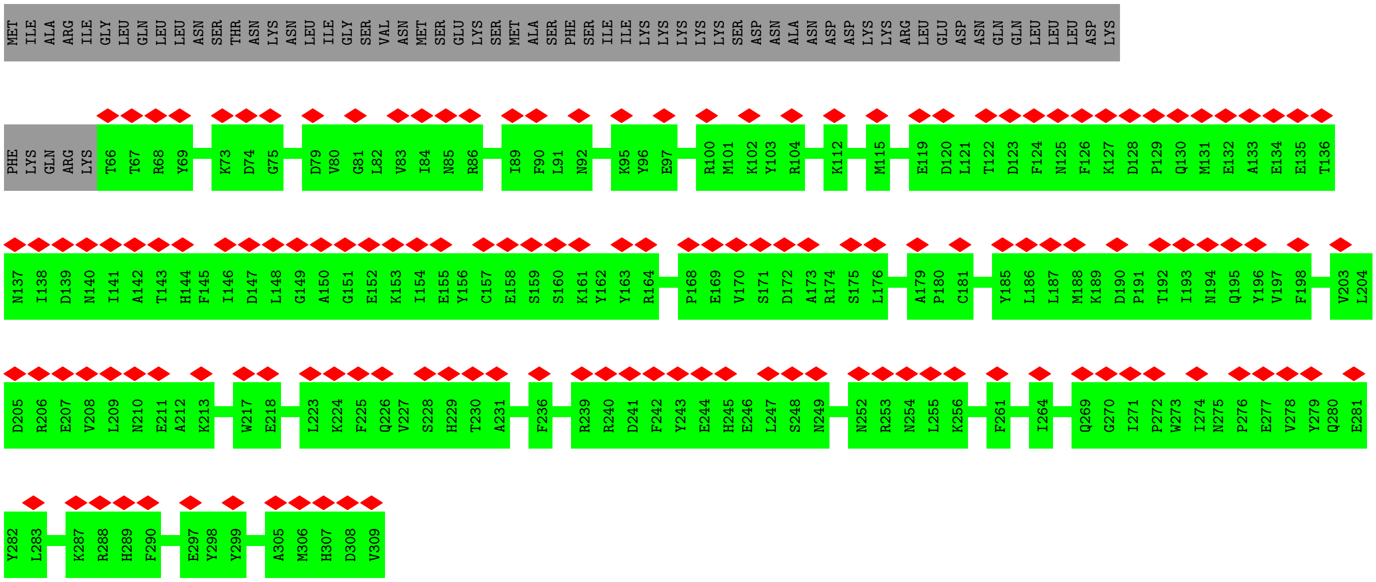




- Molecule 37: mL46

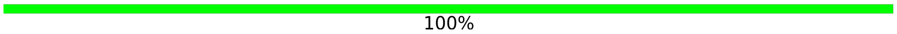
Chain AK:





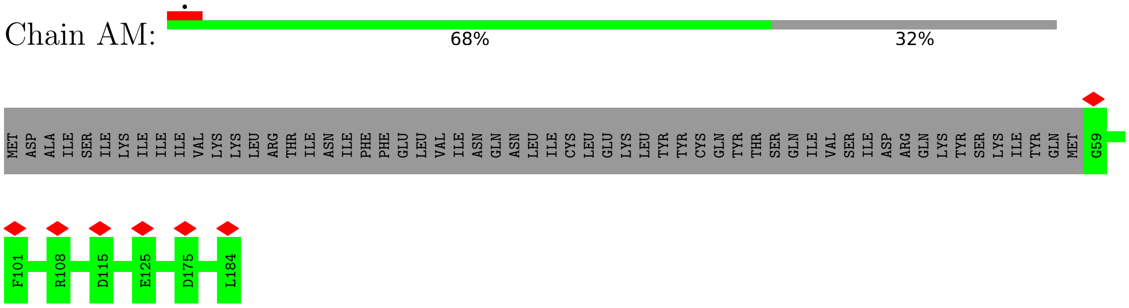
- Molecule 38: Large subunit ribosomal protein

Chain AL:

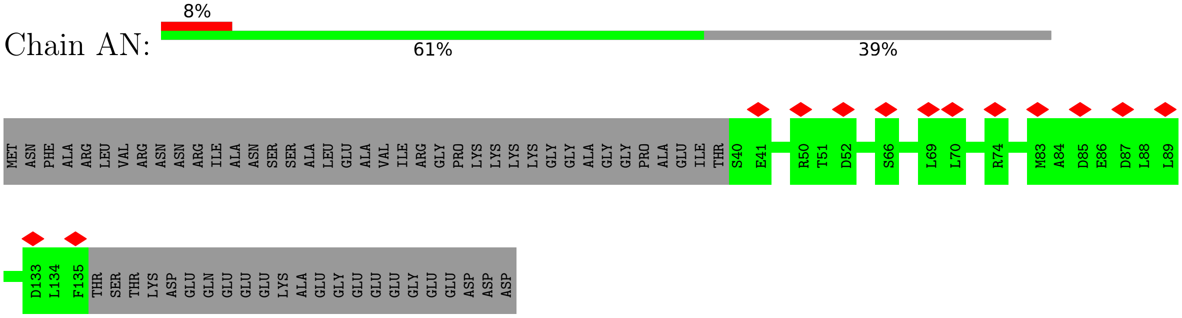


There are no outlier residues recorded for this chain.

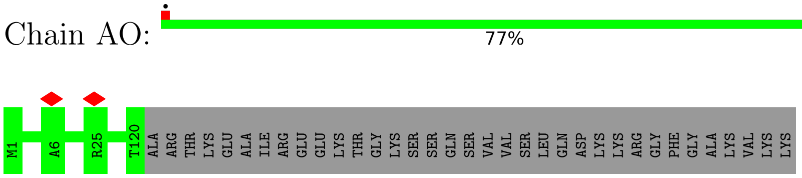
- Molecule 39: mL53



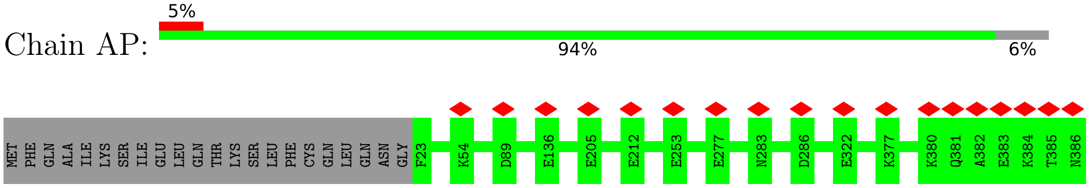
- Molecule 40: mL54



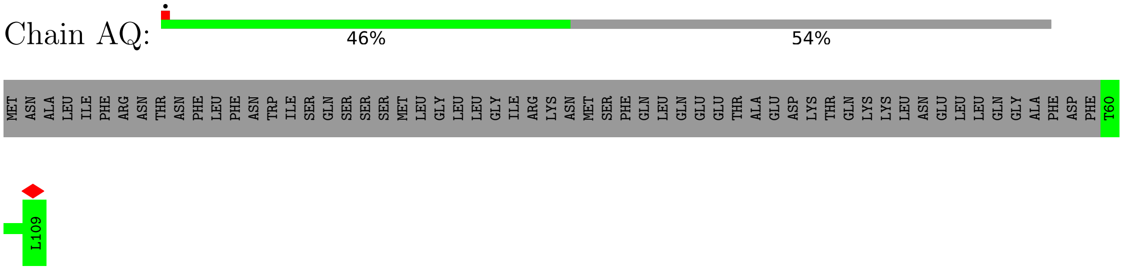
- Molecule 41: mL64



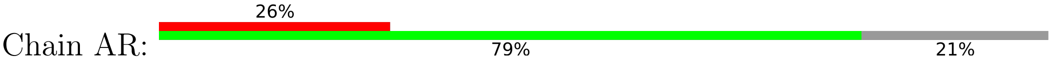
- Molecule 42: mL101

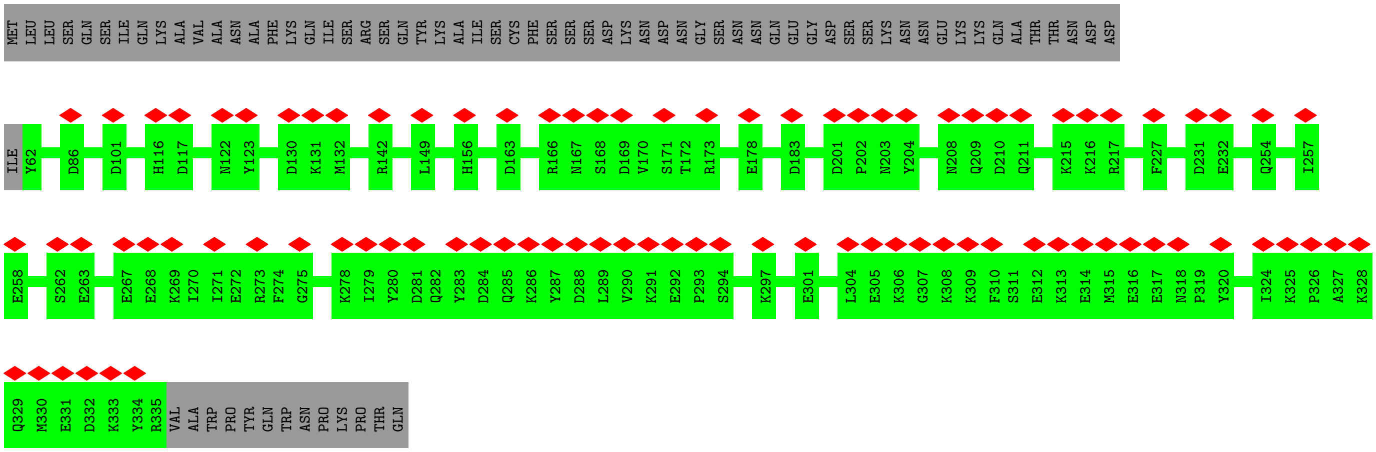


- Molecule 43: mL102



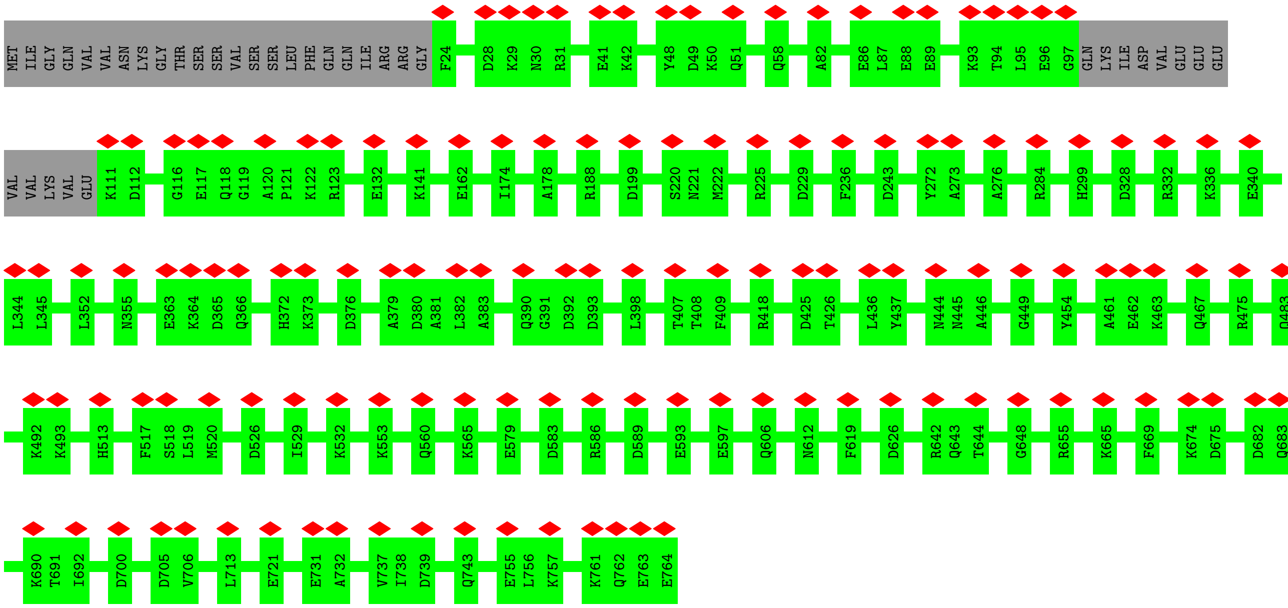
- Molecule 44: mL103





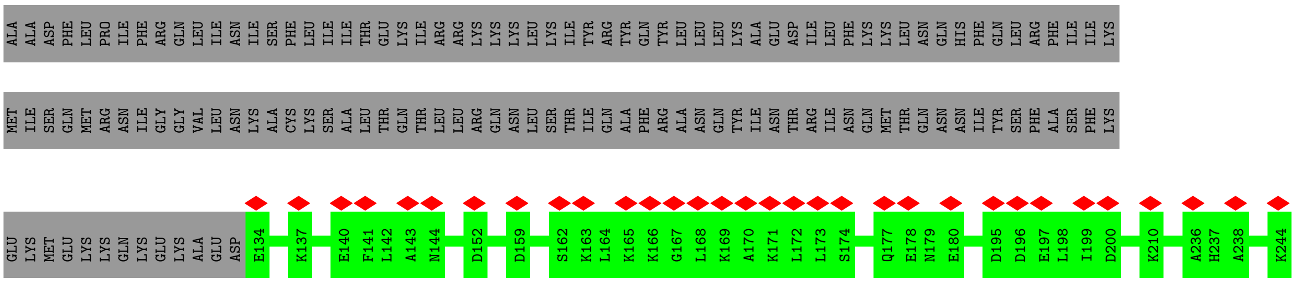
- Molecule 45: mL104

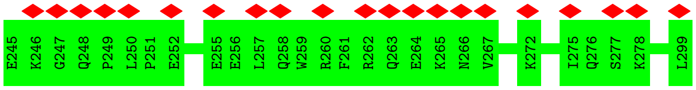
Chain AS:



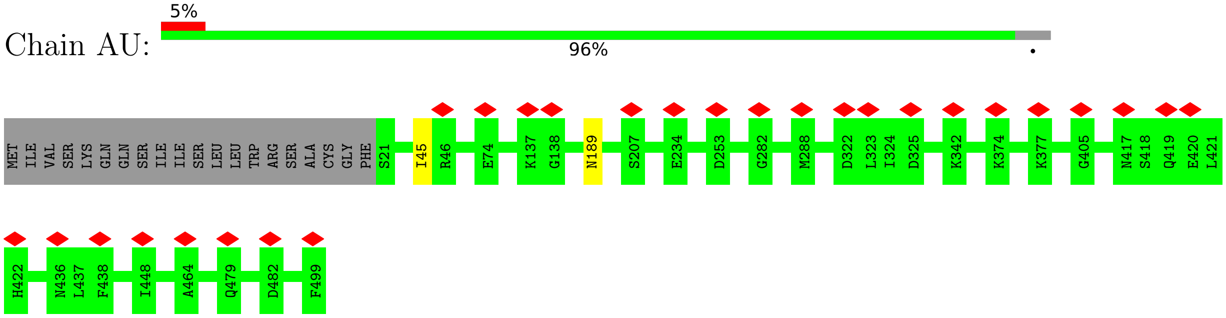
- Molecule 46: Signal peptide-binding domain protein

Chain AT:

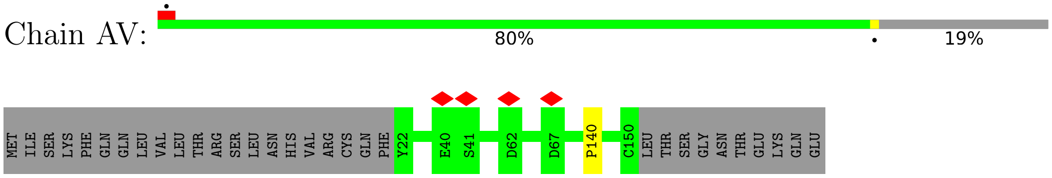




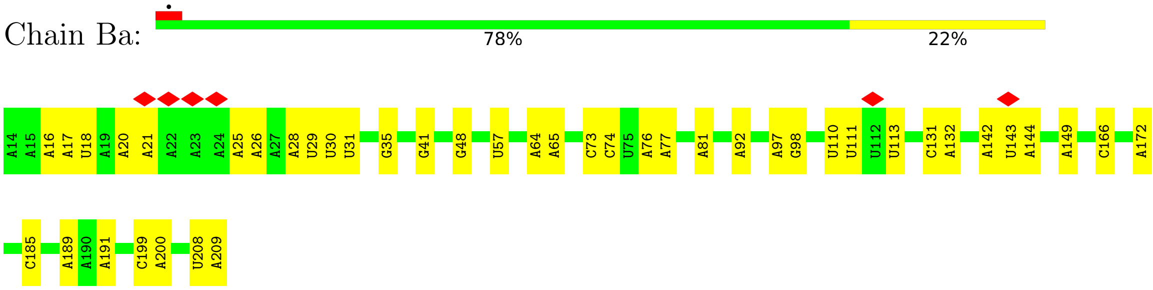
- Molecule 47: mL106



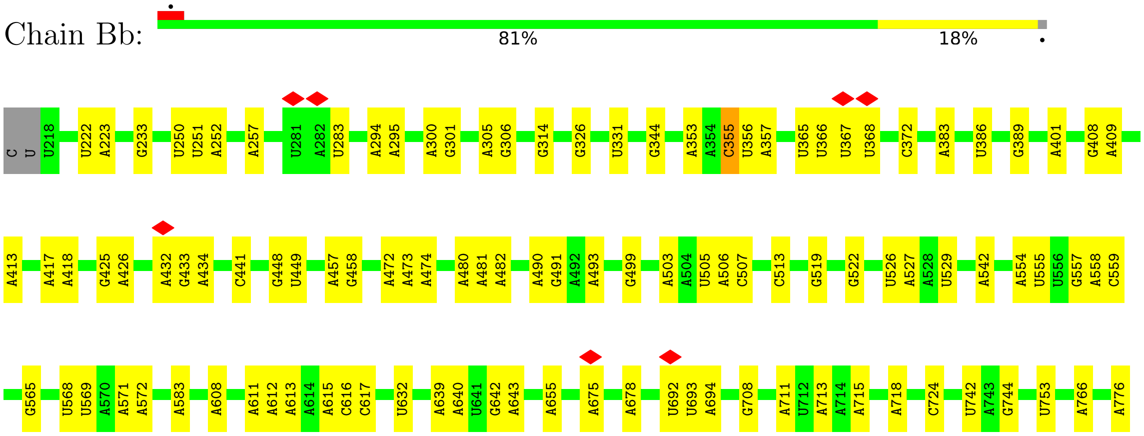
- Molecule 48: Iron-binding zinc finger CDGSH type protein

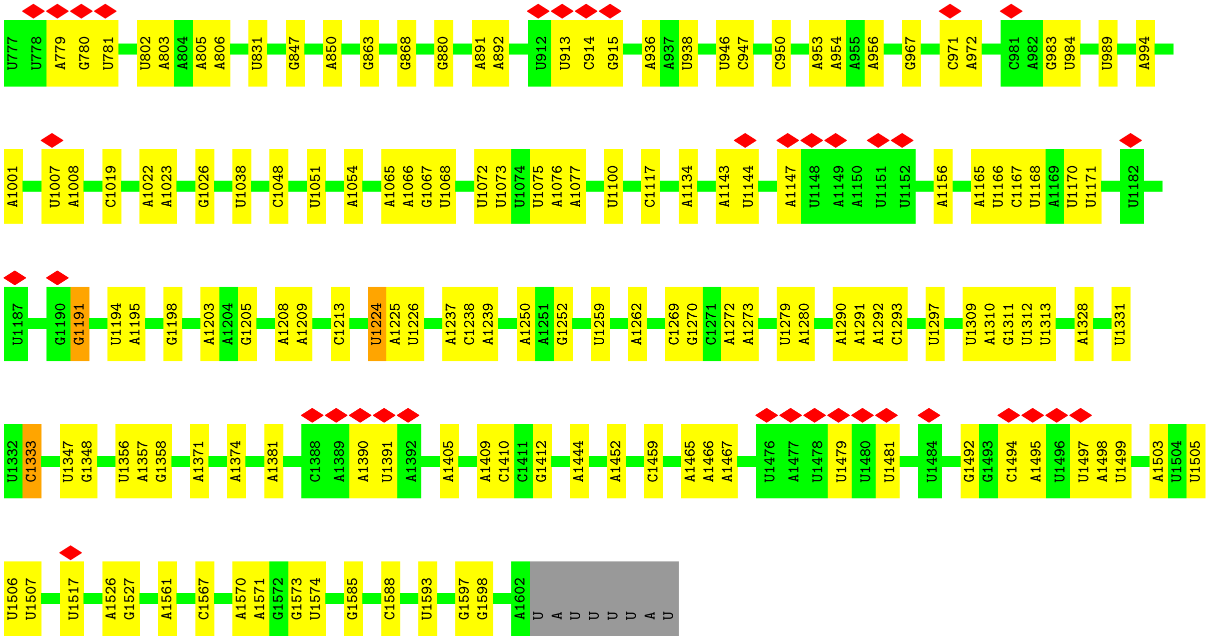


- Molecule 49: SSU rRNA_1



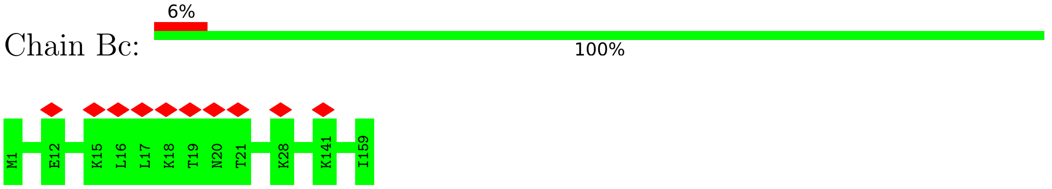
- Molecule 50: SSU rRNA_2





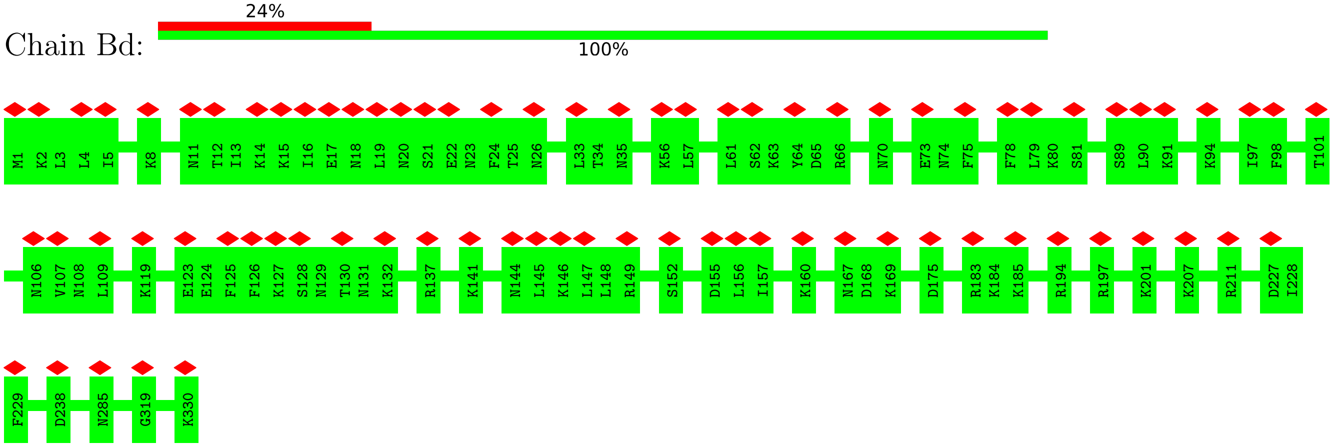
- Molecule 51: Ymf73

Chain Bc:



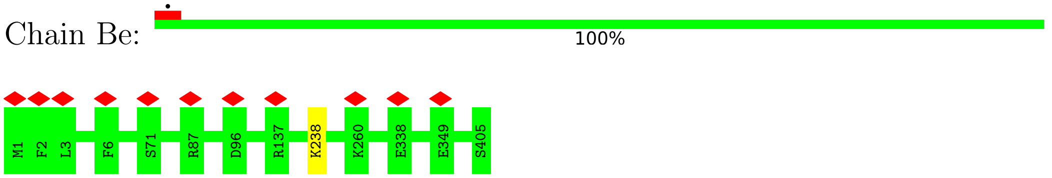
- Molecule 52: Ymf64

Chain Bd:

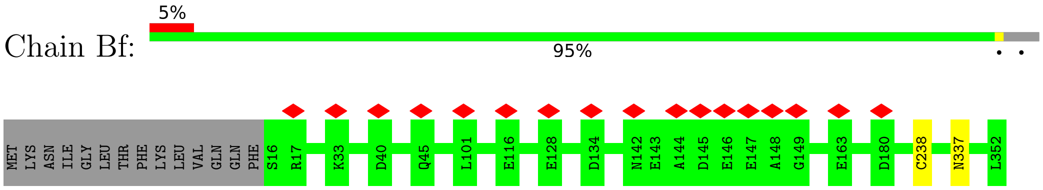


- Molecule 53: Ymf76

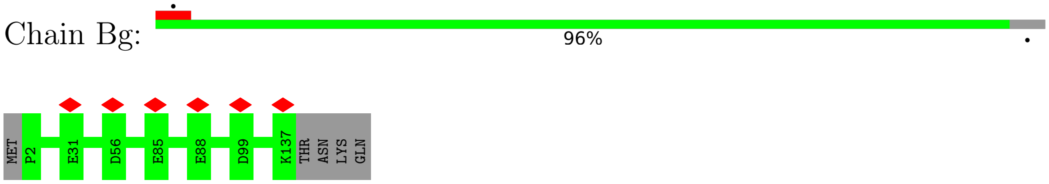
Chain Be:



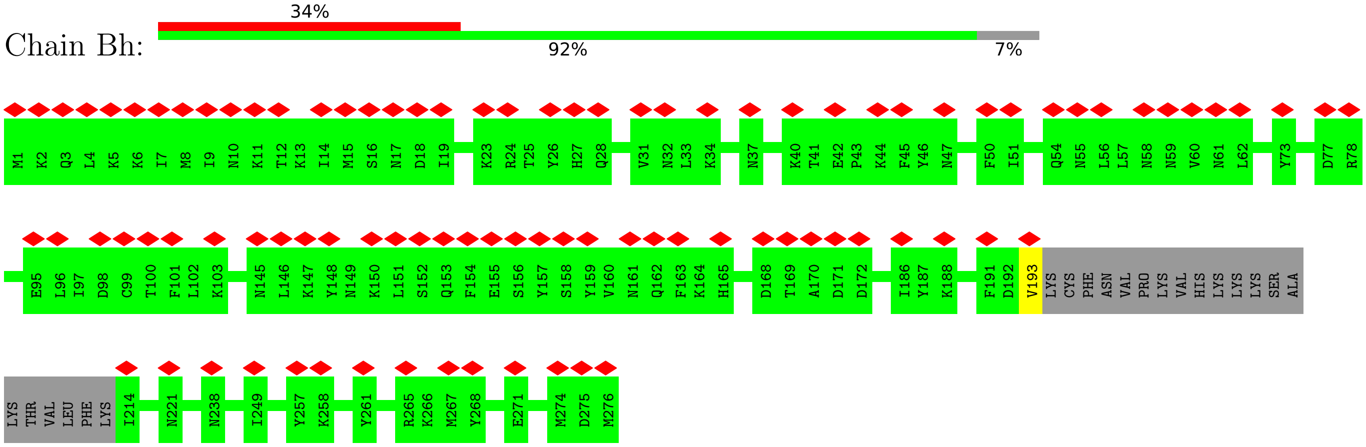
- Molecule 54: 30S ribosomal protein S5



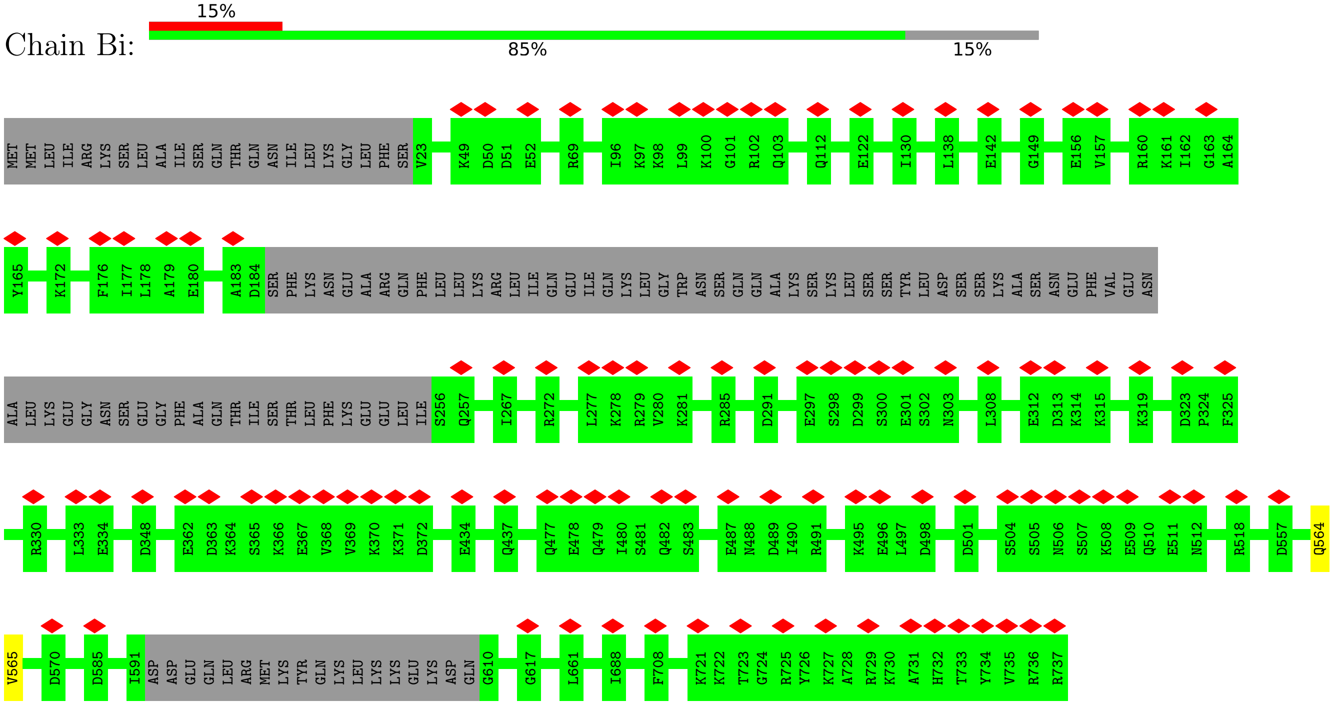
- Molecule 55: Ribosomal protein S6



- Molecule 56: Ymf63

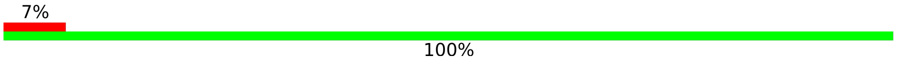


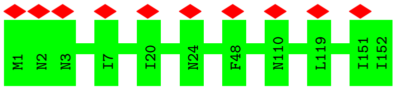
- Molecule 57: Ribosomal protein S9



- Molecule 58: Ymf59

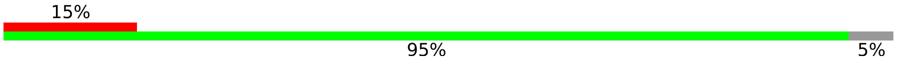
Chain Bj:

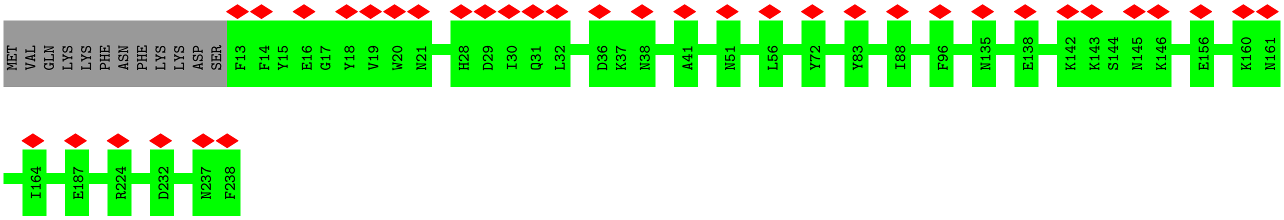




- Molecule 59: Ymf61

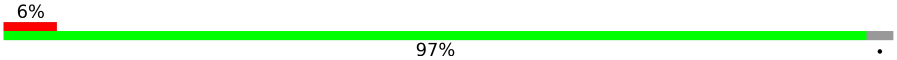
Chain Bk:

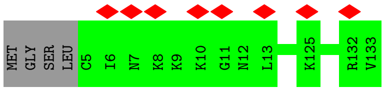




- Molecule 60: Ribosomal protein S12

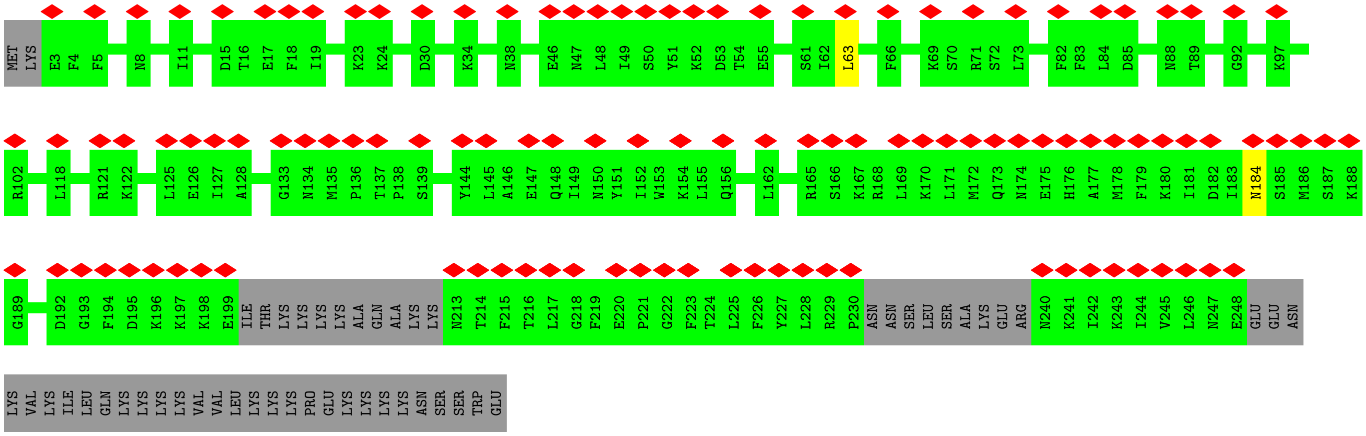
Chain Bl:





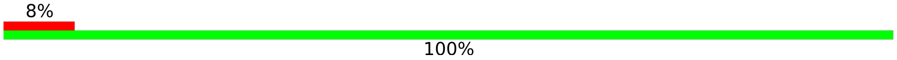
- Molecule 61: Ribosomal protein S13

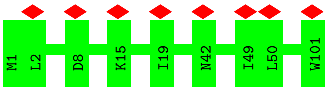
Chain Bm:



- Molecule 62: Ribosomal protein S14

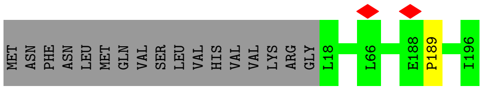
Chain Bn:





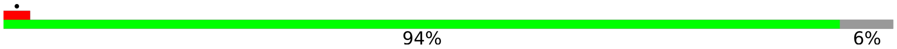
- Molecule 63: 30S ribosomal protein S15

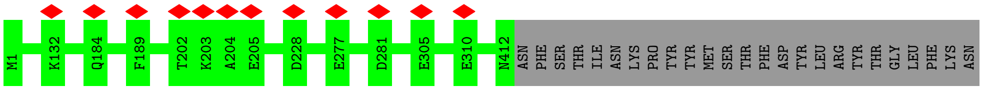
Chain Bo:



- Molecule 64: 30S ribosomal protein S16

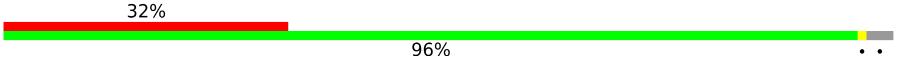
Chain Bp:

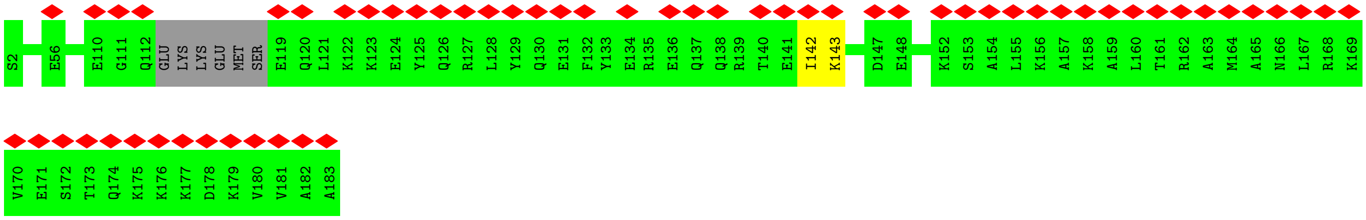




- Molecule 65: 30S ribosomal protein S17

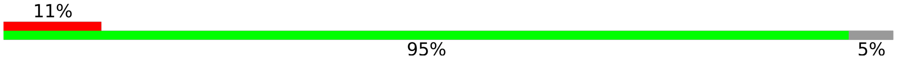
Chain Bq:

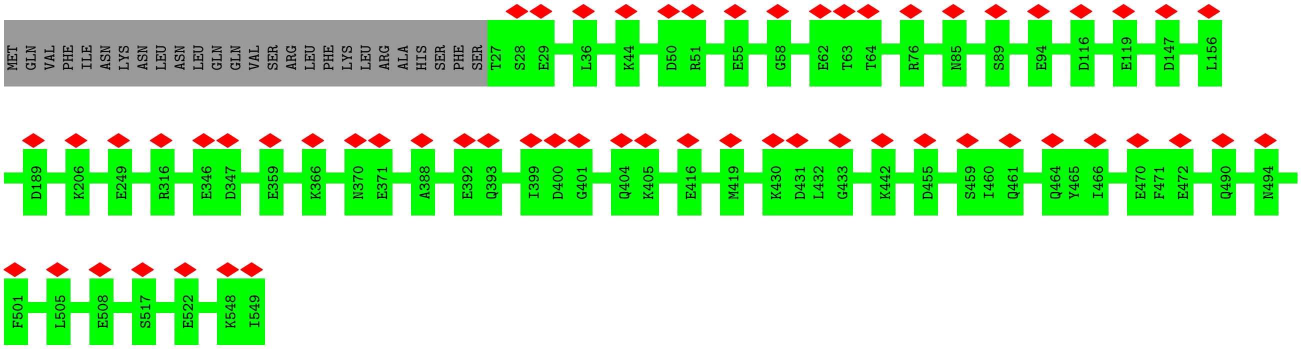




- Molecule 66: Ribosomal protein S18

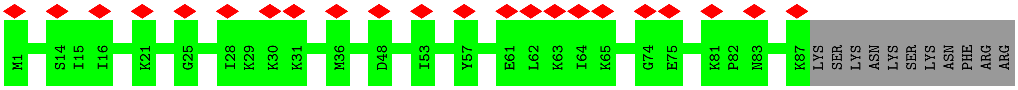
Chain Br:





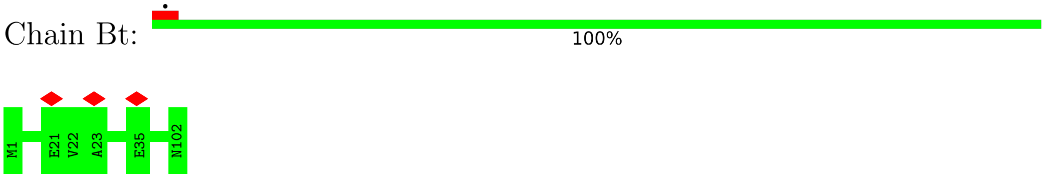
- Molecule 67: Ribosomal protein S19

Chain Bs:



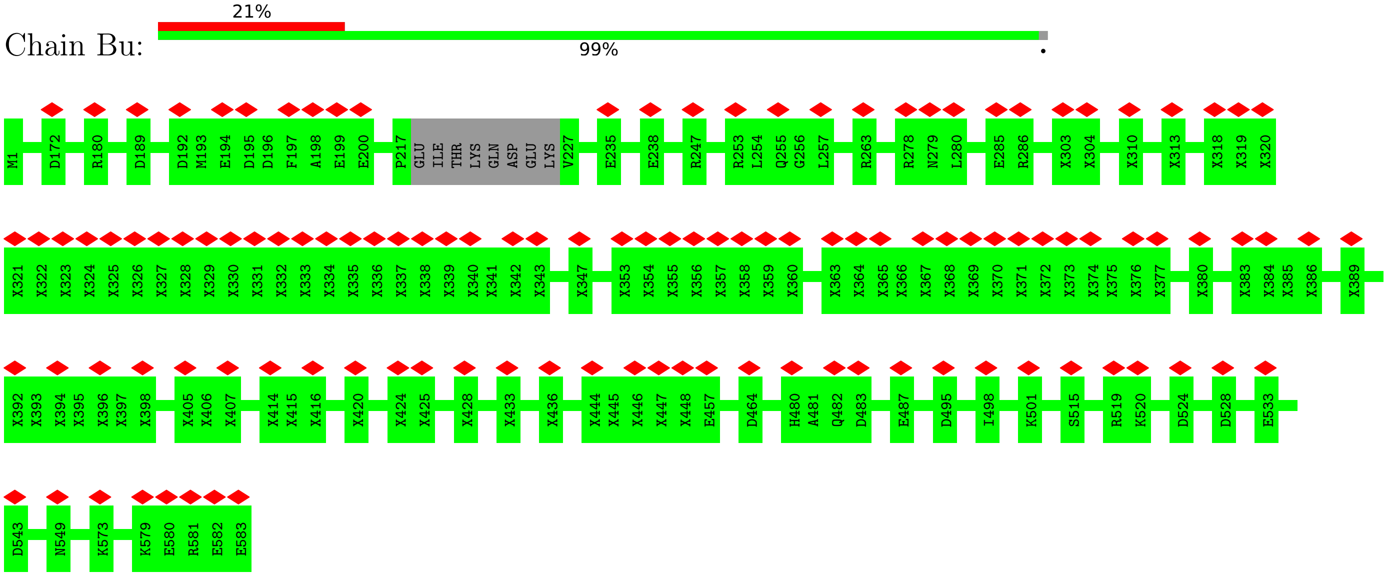
- Molecule 68: bS21m

Chain Bt:



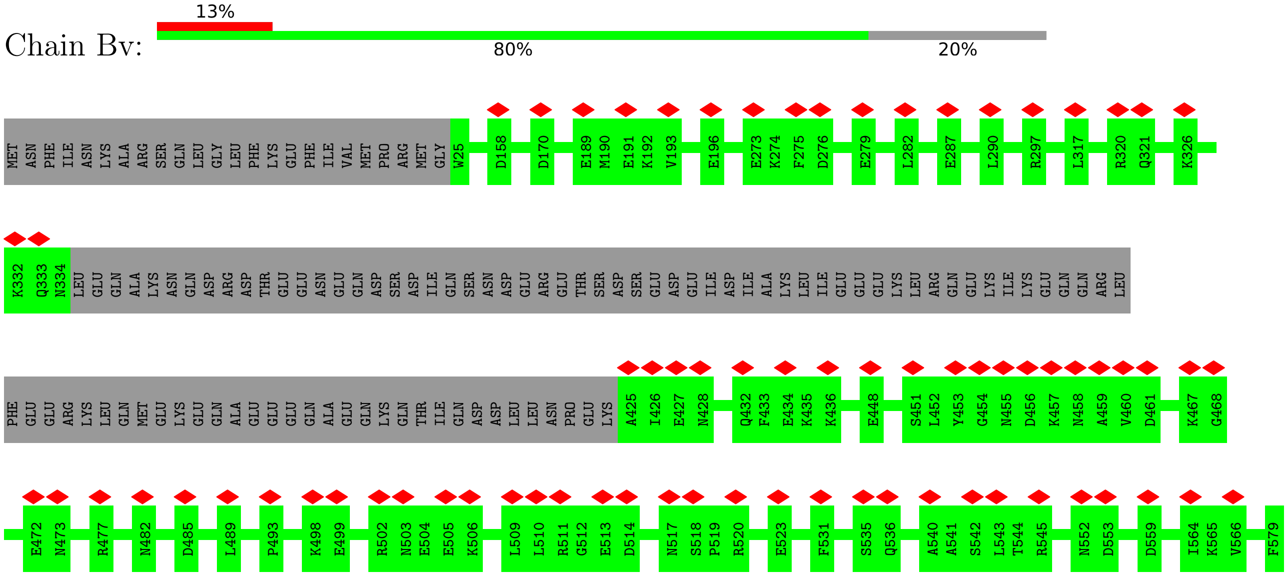
- Molecule 69: mS23

Chain Bu:



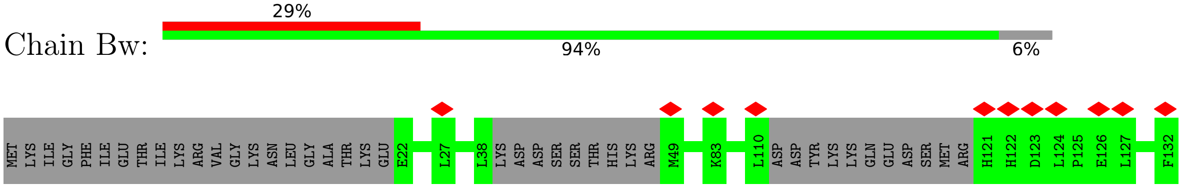
- Molecule 70: mS26

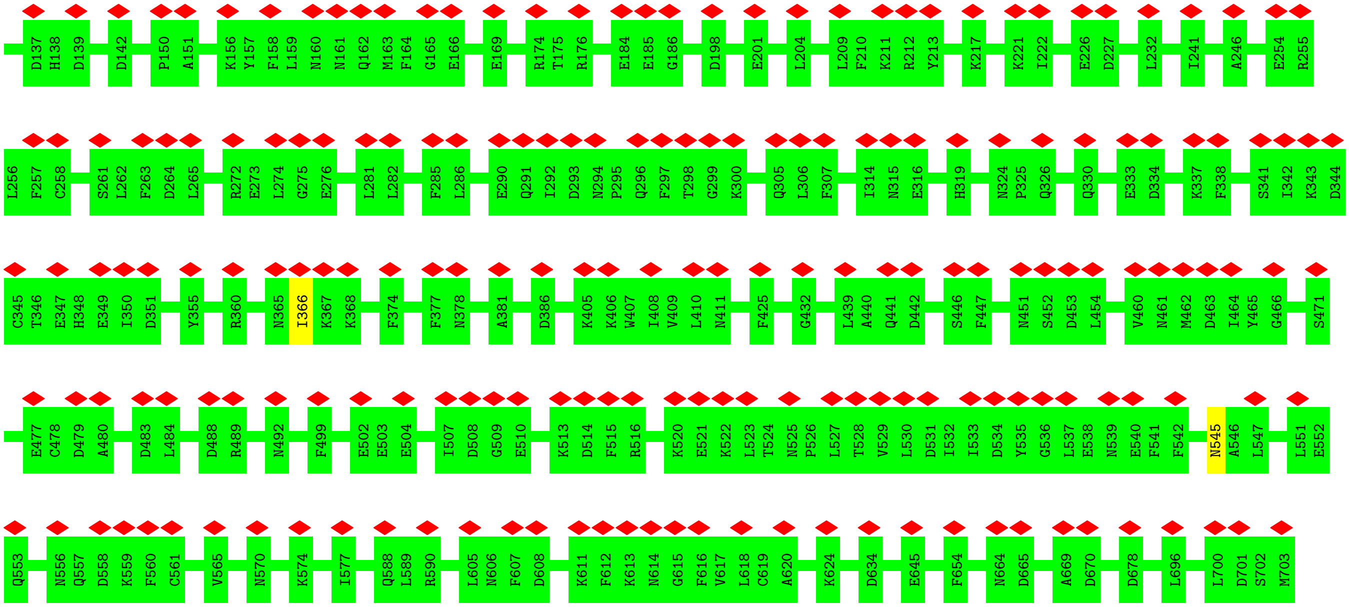
Chain Bv:



- Molecule 71: Ribosomal death-associated protein

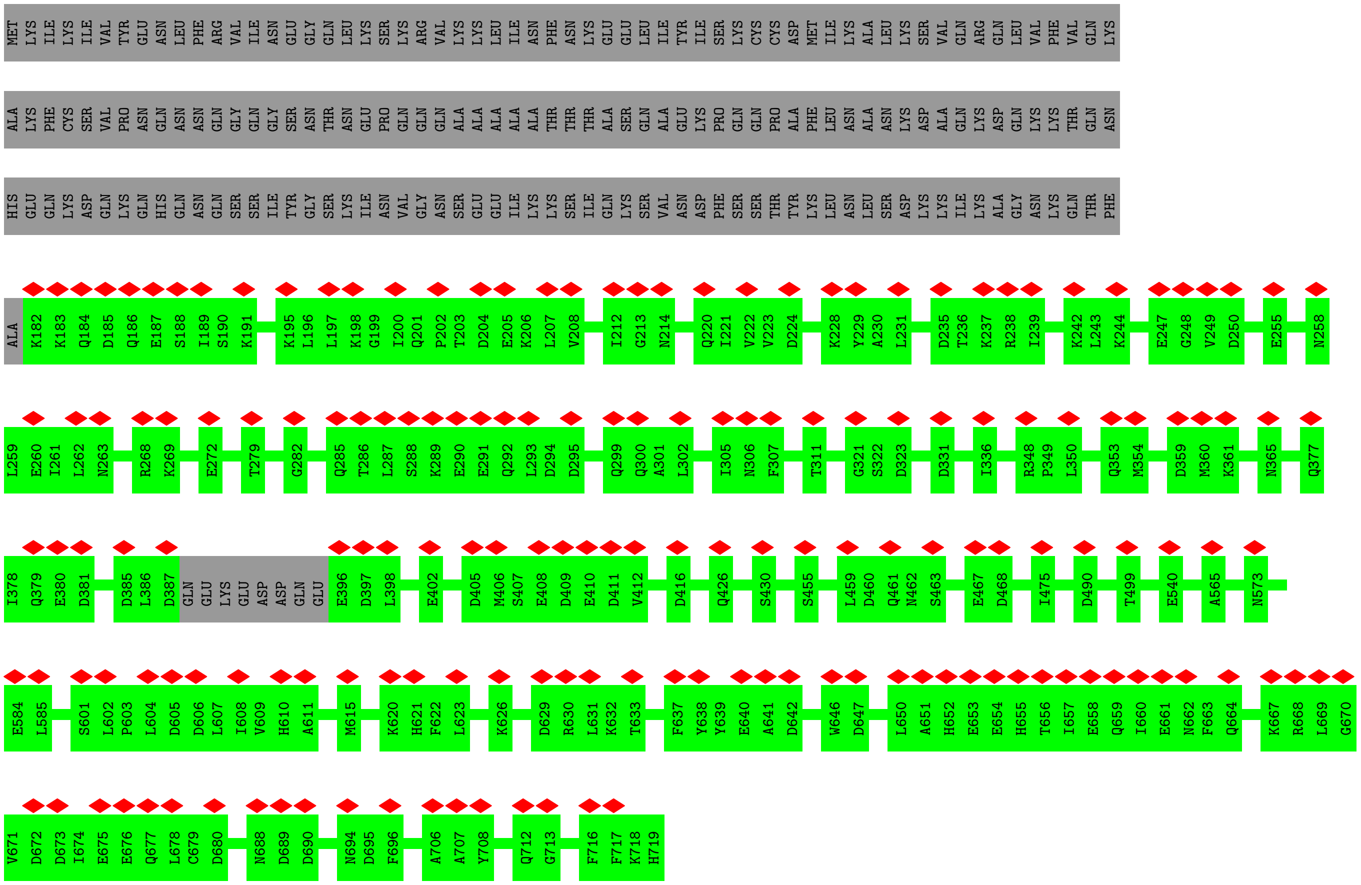
Chain Bw:





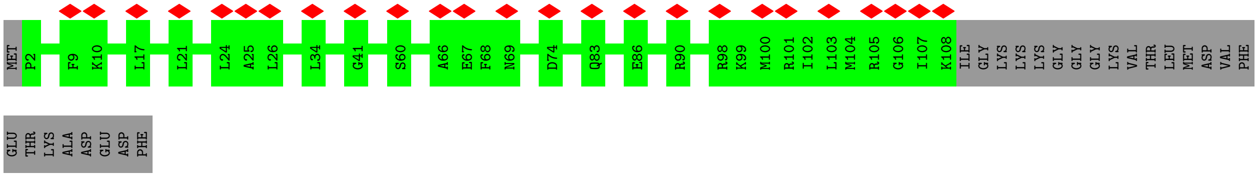
- Molecule 72: mS31

Chain Bx:



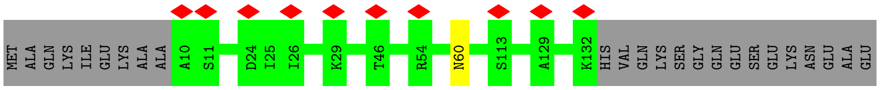
- Molecule 73: mS33

Chain By:



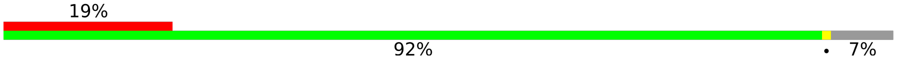
- Molecule 74: mS34

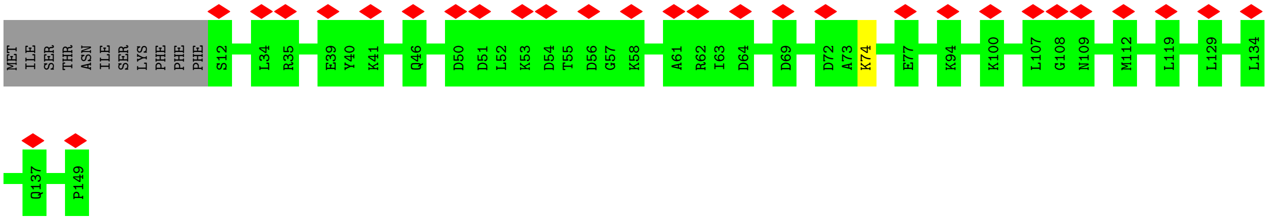
Chain Bz:



- Molecule 75: Ribosomal subunit protein

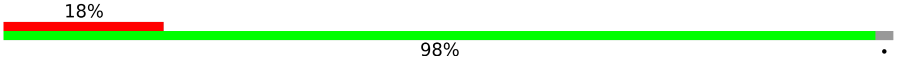
Chain BA:

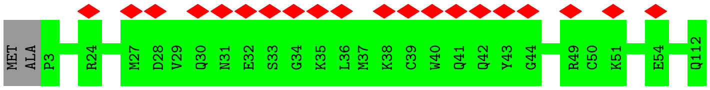




- Molecule 76: mS37

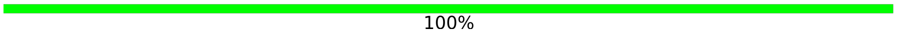
Chain BB:





- Molecule 77: mS38

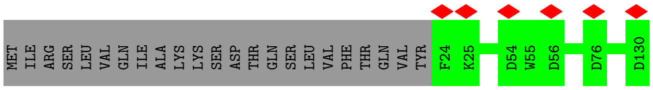
Chain BC:



There are no outlier residues recorded for this chain.

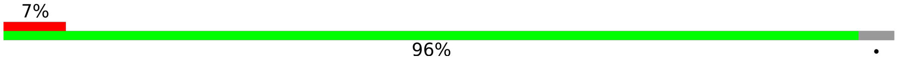
- Molecule 78: IGR motif protein

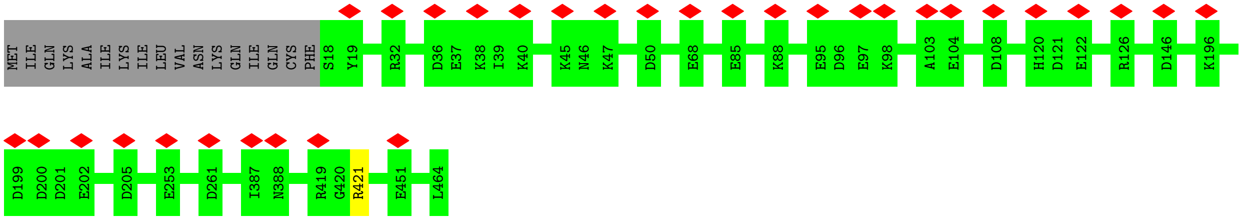
Chain BD:



- Molecule 79: mS45

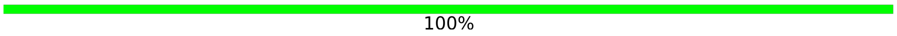
Chain BE:





- Molecule 80: mS75

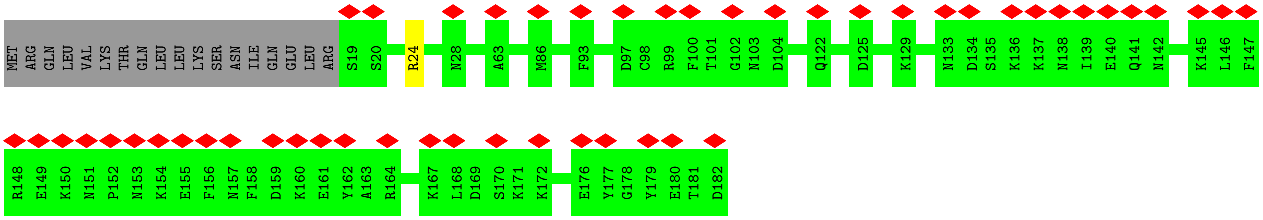
Chain BF:



There are no outlier residues recorded for this chain.

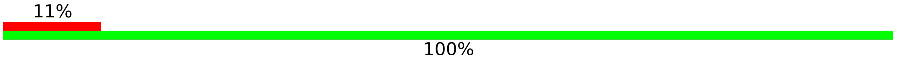
- Molecule 81: mS76

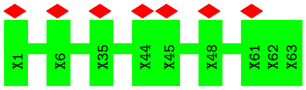
Chain BG:



- Molecule 82: mS77

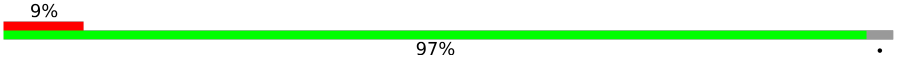
Chain BH:

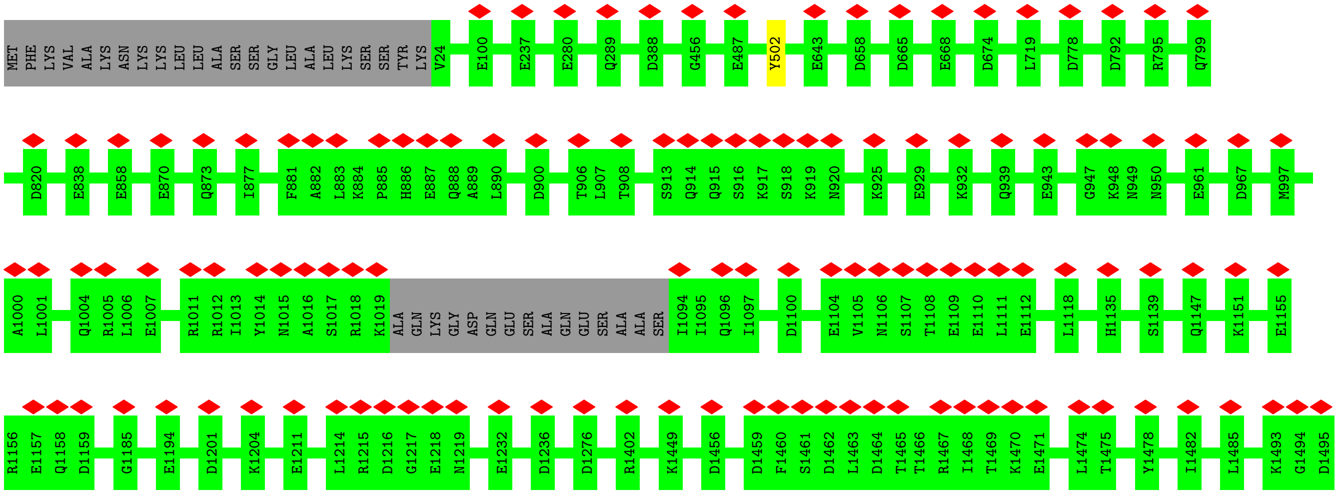


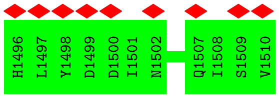


- Molecule 83: Enoyl-CoA hydratase/isomerase

Chain BI:

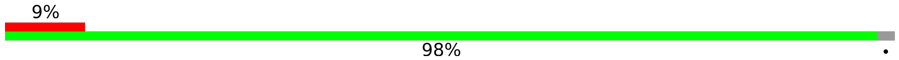


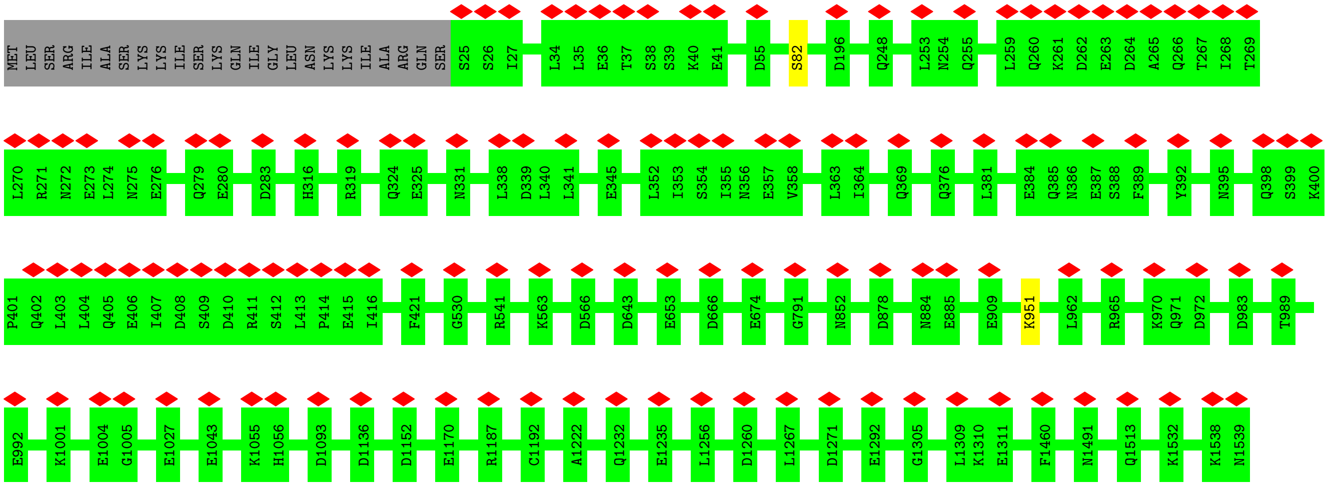




- Molecule 84: mS78

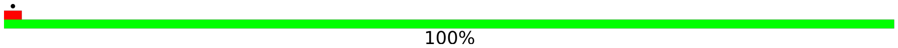
Chain BJ:

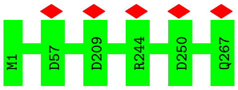




- Molecule 85: mS79

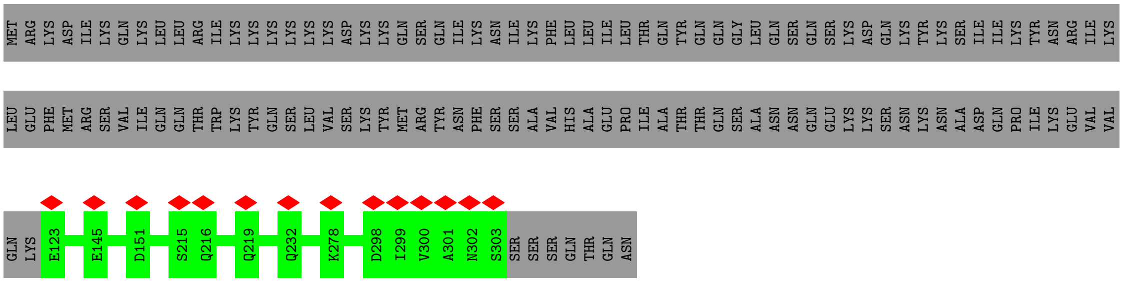
Chain BK:





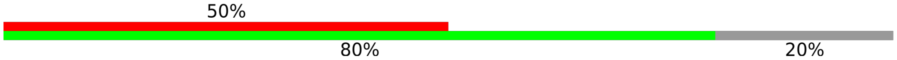
- Molecule 86: SelR domain protein

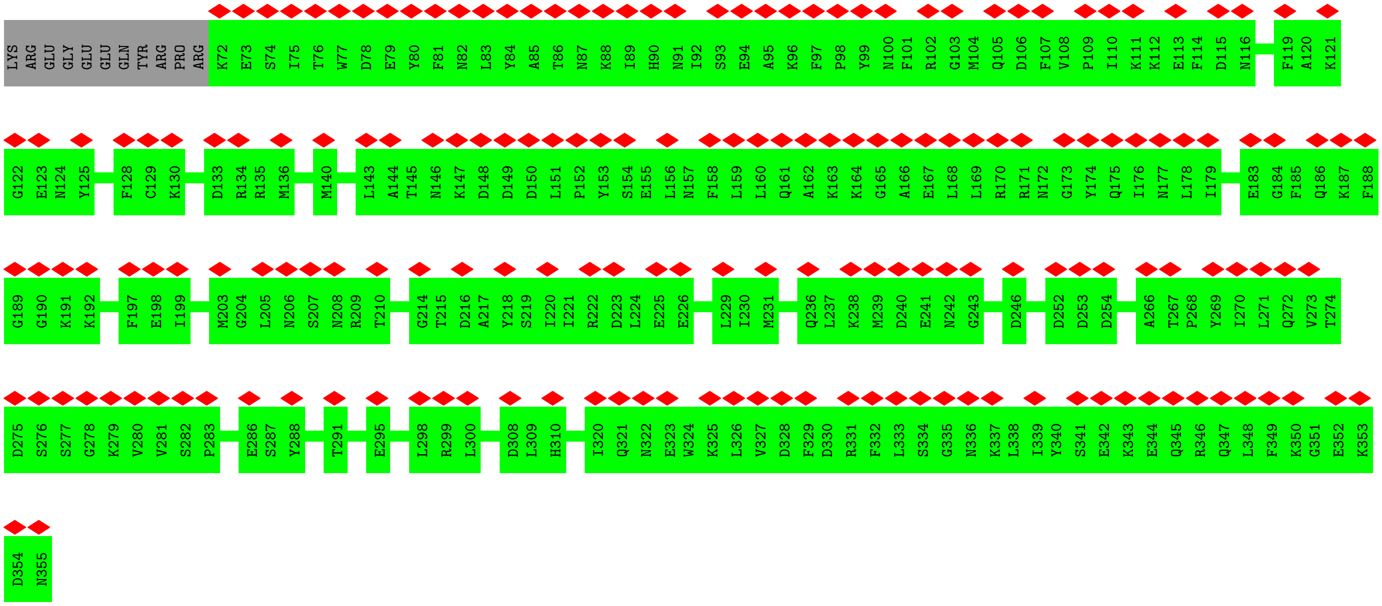
Chain BL:



- Molecule 87: mS81

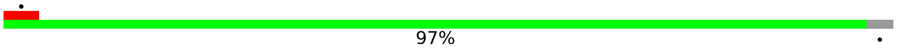
Chain BM:

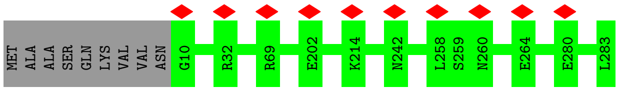




- Molecule 88: mS82

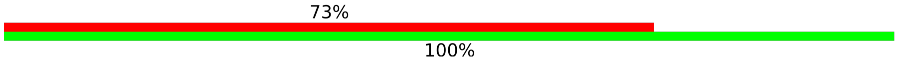
Chain BN:





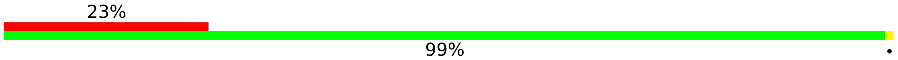
- Molecule 89: PARP alpha-helical domain-containing protein,mS83

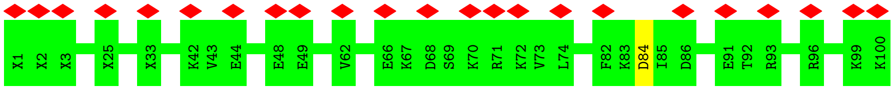
Chain BO:



- Molecule 90: mS84,mS84

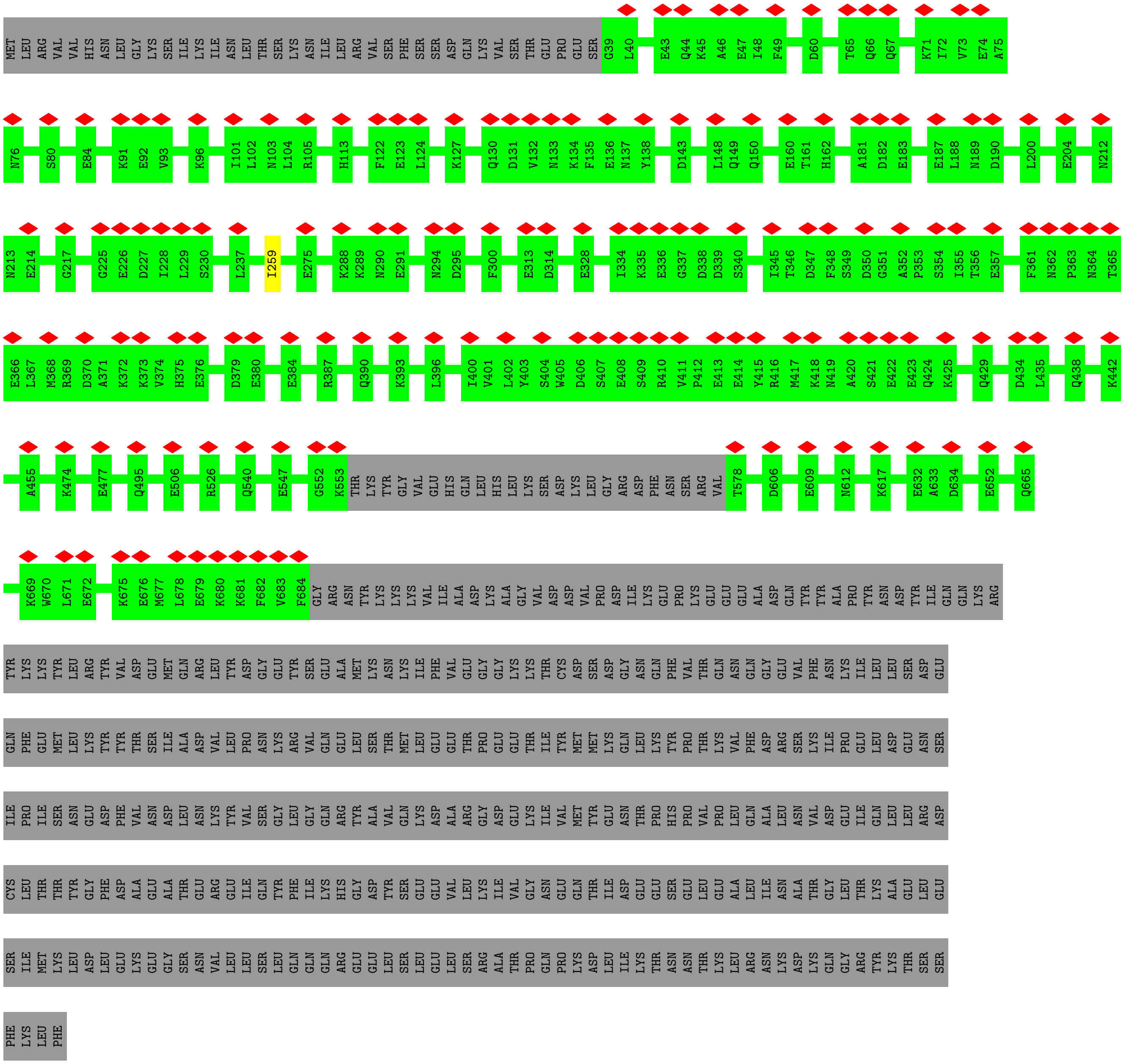
Chain BP:





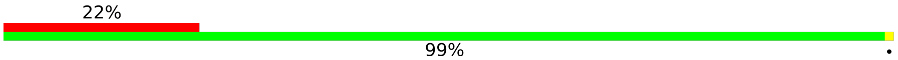
- Molecule 91: mS85

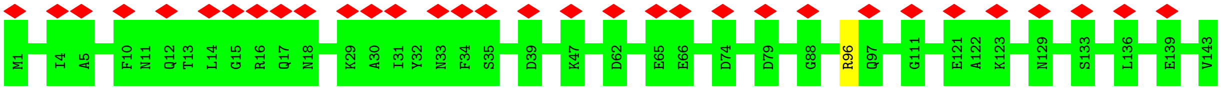
Chain BQ:



- Molecule 92: Iron donor protein CyaY

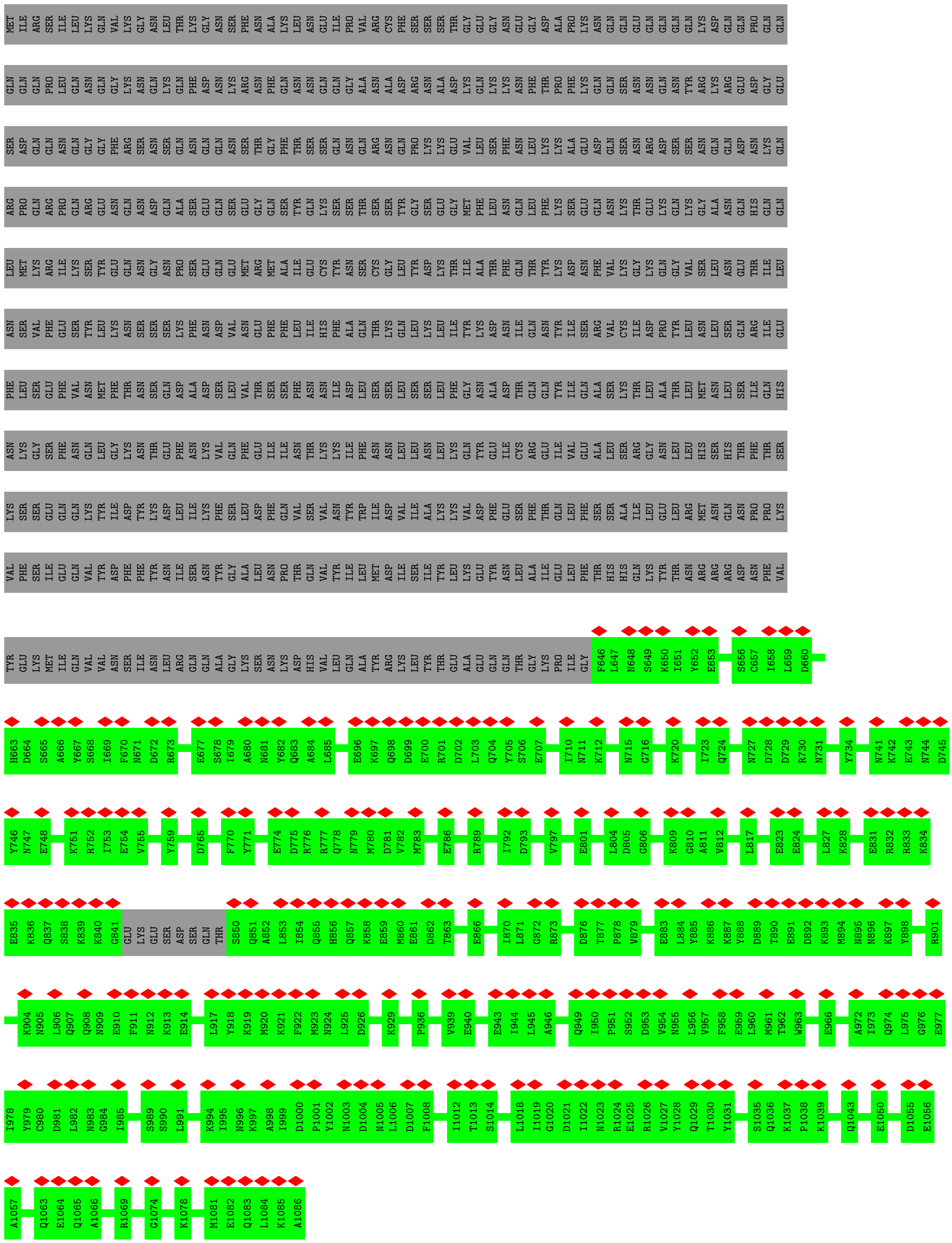
Chain BR:



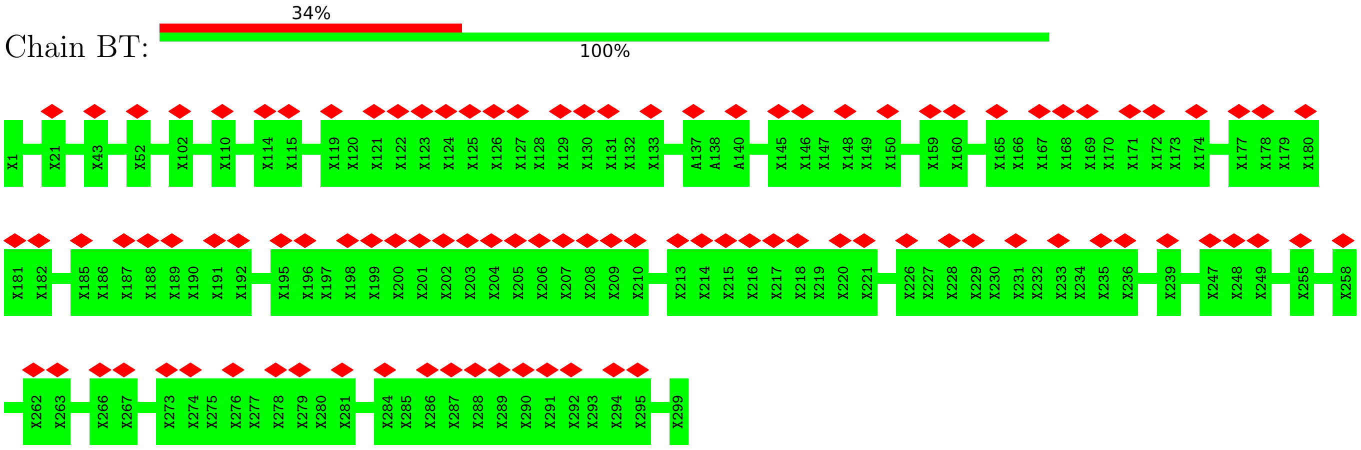


- Molecule 93: mS87

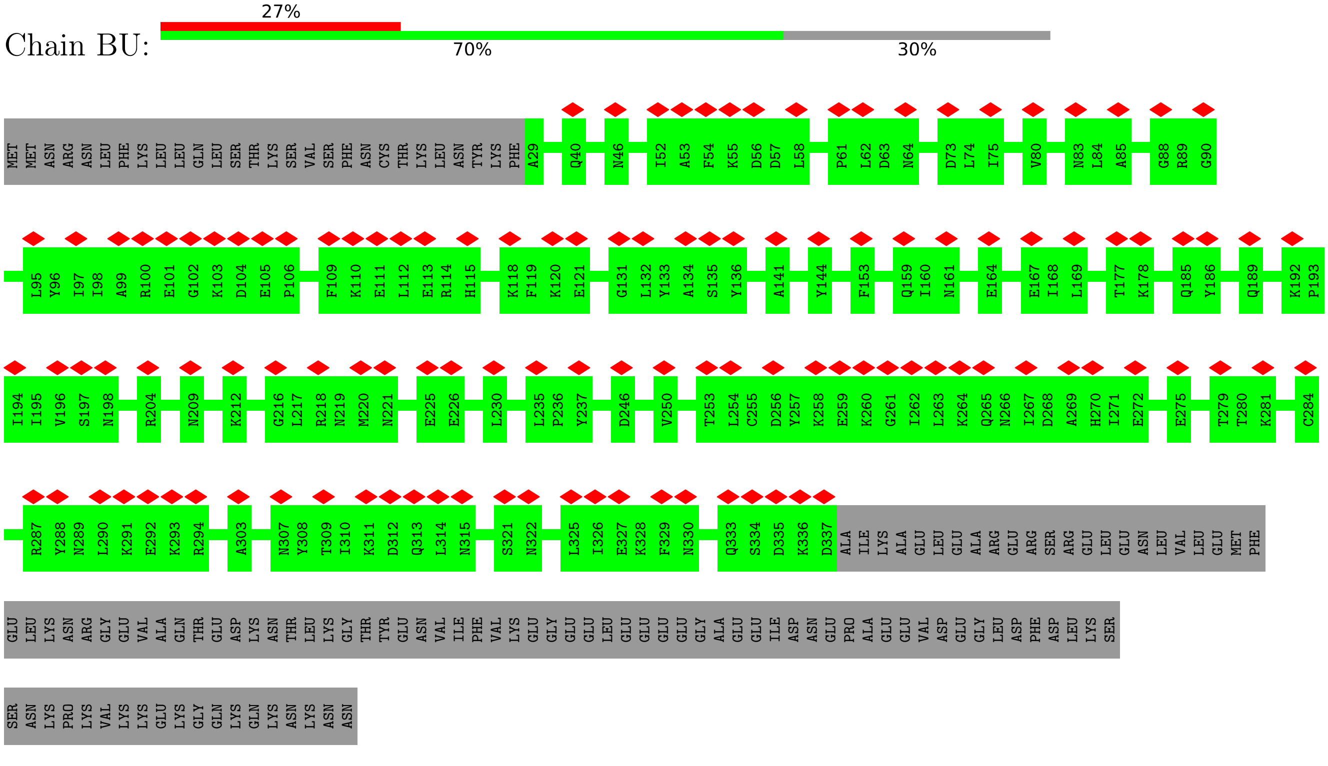
Chain BS:


MET ILE ARG SER ILE LEU LYS GLN VAL LYS GLY ASN LEU THR LYS GLY ASN SER PHE ASN ALA LYS LEU ASN GLU ILE PRO VAL ARG CYS PHE SER SER SER THR GLY GLU GLY ASN GLU GLY ASP ALA PRO LYS ASN GLN GLN GLU GLN GLN GLN GLN LYS ASP GLN GLN PRO GLN GLN
GLN GLN GLN PRO LEU GLN ASN GLN GLY LYS ASN GLN LYS GLN PHE ASP ASN LYS ARG ASN PHE GLN ASN ASN GLN GLN GLY ALA ASN ALA ASP ARG ASN ALA ASP LYS GLN LYS LYS ASN PHE THR PRO PHE LYS GLN GLN SER ASN ASN GLN ASN TYR ARG LYS ARG GLU ASP GLY GLU
SER ASP GLN GLN ASN GLN GLY GLY PHE ARG SER ASN SER GLN ASN GLN GLN ASN SER THR GLY PHE THR SER SER GLN ASN GLN ARG ASN GLN PRO LYS LYS GLU VAL LEU SER PHE ASN LEU LYS LYS ALA GLU ASP GLN SER ASN ARG ASP SER SER ASN GLN GLN ASP ASN LYS GLN
ARG PRO GLN ARG PRO GLN ARG GLU ASN GLN ASN ASP GLN ALA SER GLU GLN SER GLU GLY GLN SER TYR GLN LYS SER SER THR SER SER TYR GLY SER GLU GLY MET PHE LEU ASN GLN LEU PHE LYS SER GLU GLN ASN LYS THR GLU LYS GLN LYS GLY ALA ASN GLN HIS GLN GLN
LEU MET LYS ARG ILE LYS SER TYR GLU GLN ASN GLY ASN PRO SER GLU GLN GLU MET ARG MET ALA ILE GLU CYS TYR ASN SER CYS GLY LEU TYR ASP LYS THR ILE ALA THR PHE GLN THR TYR LYS ASP ASN PHE VAL LYS GLY LYS GLN GLY VAL SER LEU ASN GLU THR ILE LEU
ASN SER VAL PHE GLU SER TYR LEU LYS ASN SER SER SER LYS PHE ASN ASP VAL ASN GLU PHE PHE LEU ILE HIS PHE ALA GLN THR LYS GLN LEU LYS LEU ILE TYR LYS ASP ASN ILE GLN ASN TYR ILE SER ARG VAL CYS ILE ASP PRO TYR LEU ASN LEU SER GLN ARG ILE GLU
PHE LEU SER GLU PHE VAL ASN MET PHE THR ASN SER GLN ASP ALA ASP SER LEU VAL THR SER SER PHE ASN ASN ILE ASP LEU SER SER LEU SER SER LEU PHE GLY ASN ALA ASP THR GLN GLN TYR ILE GLN ALA SER LYS THR LEU ALA THR LEU MET ASN LEU SER ILE GLN HIS
ASN LYS GLY SER PHE ASN GLN LEU GLY LYS ASN THR GLU PHE ASN LYS VAL GLN PHE GLU ILE ILE ASN THR LYS LYS ILE PHE ASN ASN LEU LEU ASN LEU LYS GLN TYR GLU ILE CYS ARG GLU ILE VAL GLU ALA LEU SER ARG GLY ASN LEU LEU HIS SER HIS THR PHE THR SER
LYS SER SER GLU GLN GLN LYS TYR ILE ASP TYR LYS ASP LEU ILE ILE LYS PHE SER LEU ASP PHE GLN VAL SER VAL ASN TYR TRP ILE ASP VAL ILE ALA LYS LYS VAL ASP PHE GLU SER PHE THR GLN LEU PHE SER SER ALA ILE LEU GLU LEU ARG MET ASN GLN ASN PRO LYS
VAL PHE SER ILE GLU GLN VAL TYR ASP PHE PHE TYR ASN ILE SER ASN TYR GLY ALA LEU ASN PRO THR GLN VAL TYR ILE LEU MET ASP ILE SER ILE TYR LEU LYS GLU TYR ASN LEU ALA ILE GLU LEU PHE THR HIS HIS GLN LYS TYR THR ASN ARG ARG ARG ASP ASN PHE VAL
TYR GLU LYS MET ILE GLN VAL VAL ASN SER ILE ASN LEU ARG GLN GLN ALA GLY LYS SER ASN LYS ASP HIS VAL LEU GLN ALA TYR ARG LYS LEU TYR THR GLU ALA GLU GLN GLN THR GLY LYS PRO ILE GLY F646 L647 N648 S649 K650 I651 Y652 E653 S656 C657 I658 L659 D660
H663 D664 S665 A666 Y667 S668 I669 F670 N671 D672 R673 E677 S678 I679 A680 N681 Y682 Q683 A684 L685 E696 K697 Q698 D699 E700 R701 D702 L703 Q704 Y705 S706 E707 I710 N711 K712 N715 G716 K720 I723 Q724 N727 D728 D729 R730 N731 Y734 N741 K742 E743 N744 D745
Y746 N747 E748 K751 R752 I753 E754 V755 Y759 D765 F770 Y771 E774 D775 R776 R777 Q778 N779 M780 D781 V782 M783 E786 R789 I792 D793 V797 E801 L804 D805 G806 K809 G810 A811 V812 L817 E823 E824 L827 K828 E831 R832 R833 K834
E835 K836 Q837 S838 K839 K840 G841 GLU LYS GLU ASP SER GLN THR S850 Q851 A852 L853 I854 Q855 H856 Q857 K858 E859 M860 E861 D862 T863 E866 I870 L871 G872 R873 D876 T877 P878 V879 E883 L884 Y885 K886 K887 Y888 D889 T890 E891 D892 K893 M894 N895 N896 K897 Y898 R901
K904 N905 L906 Q907 Q908 N909 E910 F911 N912 K913 E914 L917 Y918 K919 M920 K921 F922 M923 N924 L925 D926 K929 P936 V939 E940 E943 I944 L945 A946 Q949 I950 P951 S952 D953 V954 N955 L956 V957 F958 E959 L960 M961 T962 W963 E966 A972 I973 Q974 L975 G976 E977
I978 Y979 C980 D981 L982 N983 G984 I985 S989 S990 L991 K994 I995 N996 K997 A998 I999 D1000 P1001 Y1002 N1003 D1004 N1005 L1006 D1007 F1008 I1012 T1013 S1014 L1018 I1019 G1020 D1021 I1022 N1023 R1024 E1025 R1026 V1027 Y1028 Q1029 T1030 Y1031 S1035 Q1036 K1037 P1038 K1039 Q1043 E1050 D1055 E1056
A1057 Q1063 E1064 Q1065 A1066 R1069 G1074 K1078 M1081 E1082 Q1083 L1084 K1085 A1086

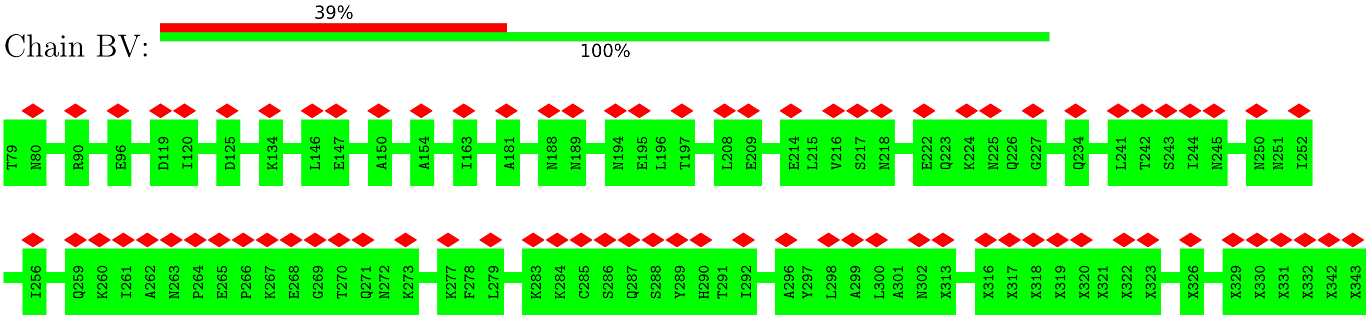
- Molecule 94: mS88

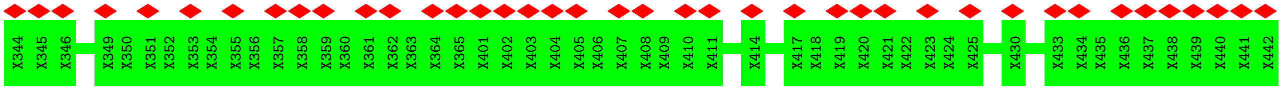


- Molecule 95: mS89



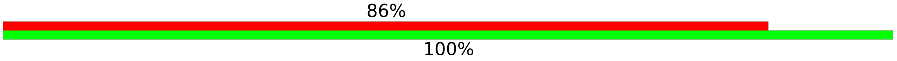
- Molecule 96: mS90

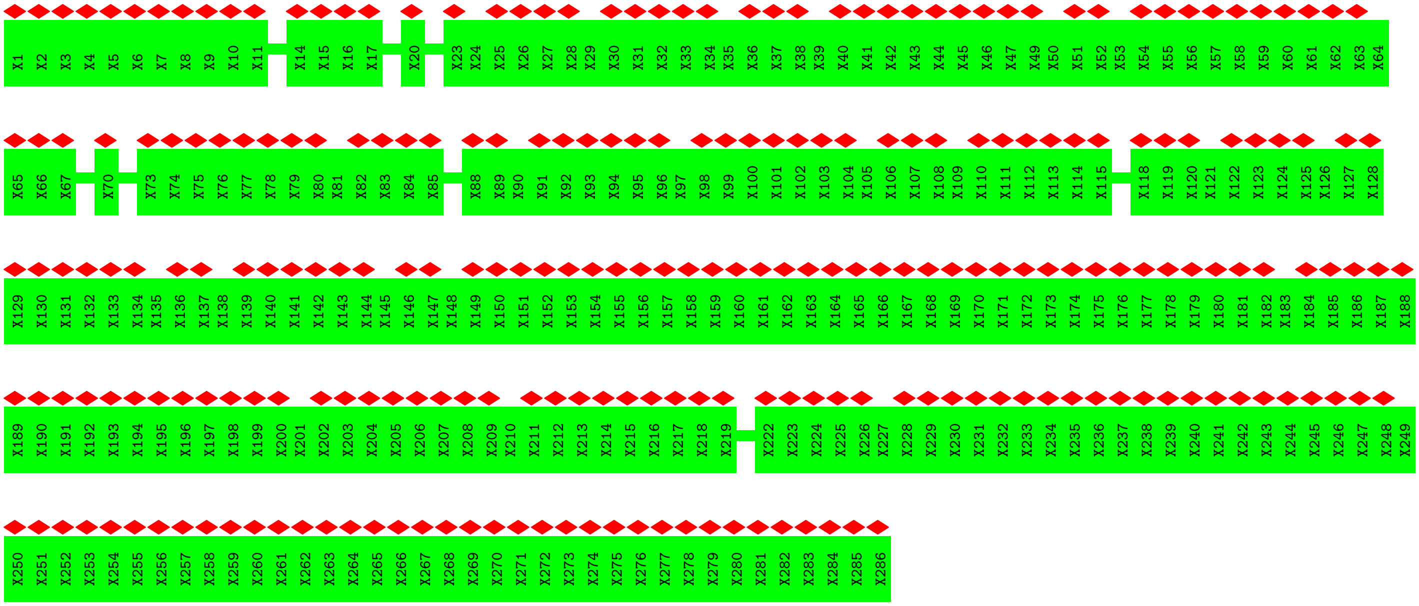




- Molecule 97: mS91

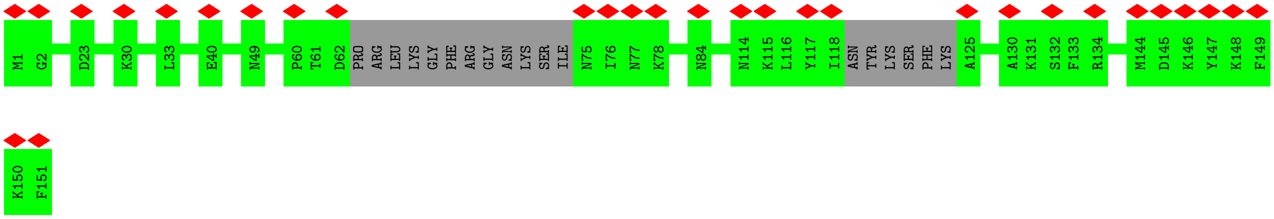
Chain BW:





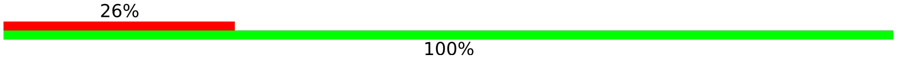
- Molecule 98: Ribosomal protein S3

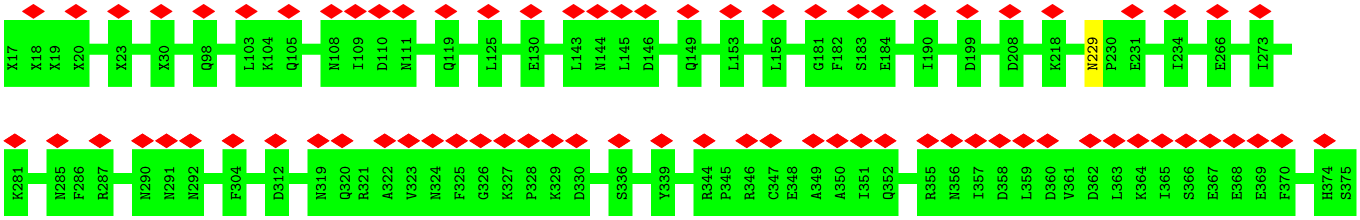
Chain BX:

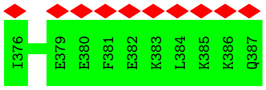


- Molecule 99: mS93

Chain BY:






I376
E379
E380
F381
E382
K383
L384
K385
K386
Q387

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	99300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	92000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	588.5, 588.5, 588.5	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Aa	0.71	0/6630	0.87	3/10321 (0.0%)
2	Ab	0.74	0/53260	0.87	22/82922 (0.0%)
3	Ac	0.49	0/2161	0.64	0/2897
4	Ad	0.49	0/3051	0.60	0/4097
5	Ae	0.50	0/2836	0.60	0/3817
6	Af	0.39	0/608	0.50	0/811
7	Ag	0.48	0/1553	0.61	0/2081
11	Ak	0.35	0/890	0.52	0/1205
12	Al	0.45	0/440	0.61	0/596
13	Am	0.43	0/1389	0.53	0/1861
14	An	0.41	0/1268	0.54	0/1709
15	Ao	0.49	0/2842	0.58	0/3820
16	Ap	0.53	1/975 (0.1%)	0.66	0/1303
17	Aq	0.49	0/2232	0.61	0/2998
18	Ar	0.51	0/1261	0.65	0/1682
19	As	0.44	0/1964	0.59	0/2620
20	At	0.53	1/1579 (0.1%)	0.63	0/2128
21	Au	0.54	0/1449	0.64	0/1949
22	Av	0.51	0/1744	0.64	0/2350
23	Aw	0.46	0/2866	0.59	1/3840 (0.0%)
24	Ax	0.47	0/1115	0.59	0/1498
25	Ay	0.45	0/1548	0.63	0/2068
26	Az	0.46	0/1984	0.60	1/2680 (0.0%)
27	AA	0.48	0/1482	0.62	0/2003
28	AB	0.48	0/2304	0.60	0/3082
29	AC	0.45	0/2416	0.56	0/3227
31	AE	0.47	0/459	0.63	0/612
32	AF	0.49	0/997	0.70	0/1321
33	AG	0.54	0/320	0.58	0/418
34	AH	0.37	0/1520	0.47	0/2038
35	AI	0.48	0/1059	0.56	0/1416
36	AJ	0.52	0/1513	0.58	0/2031

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	AK	0.35	0/2136	0.56	0/2895
38	AL	0.50	0/1208	0.58	0/1630
39	AM	0.51	0/1083	0.52	0/1458
40	AN	0.45	0/833	0.61	0/1129
41	AO	0.47	0/1037	0.60	0/1403
42	AP	0.48	0/3125	0.54	0/4220
43	AQ	0.57	0/428	0.64	0/567
44	AR	0.40	0/2415	0.54	0/3250
45	AS	0.41	0/6212	0.53	0/8373
46	AT	0.34	0/1398	0.49	0/1867
47	AU	0.40	0/3979	0.50	0/5353
48	AV	0.57	0/1067	0.58	0/1439
49	Ba	0.52	0/4674	0.80	0/7275
50	Bb	0.52	0/32970	0.80	8/51341 (0.0%)
51	Bc	0.47	0/1403	0.58	0/1880
52	Bd	0.35	0/2883	0.53	0/3843
53	Be	0.46	0/3693	0.55	0/4907
54	Bf	0.45	1/2814 (0.0%)	0.56	0/3788
55	Bg	0.39	0/1095	0.62	0/1471
56	Bh	0.32	0/2259	0.49	0/3043
57	Bi	0.38	0/5344	0.53	0/7174
58	Bj	0.43	0/1339	0.60	0/1801
59	Bk	0.37	0/2006	0.51	0/2685
60	Bl	0.41	0/1062	0.70	0/1415
61	Bm	0.38	0/1983	0.54	1/2661 (0.0%)
62	Bn	0.44	0/881	0.55	0/1168
63	Bo	0.42	0/1519	0.56	0/2038
64	Bp	0.42	0/3537	0.53	0/4761
65	Bq	0.41	0/1480	0.54	0/1982
66	Br	0.37	0/4353	0.54	0/5860
67	Bs	0.42	0/739	0.56	0/983
68	Bt	0.42	0/891	0.52	0/1195
69	Bu	0.38	0/3548	0.54	0/4746
70	Bv	0.35	0/3981	0.48	0/5335
71	Bw	0.40	0/5700	0.52	0/7694
72	Bx	0.36	0/4504	0.49	0/6108
73	By	0.36	0/887	0.47	0/1185
74	Bz	0.37	0/1025	0.54	0/1388
75	BA	0.40	0/1193	0.57	0/1601
76	BB	0.39	0/959	0.52	0/1290
78	BD	0.38	0/903	0.59	0/1214
79	BE	0.42	0/3795	0.53	0/5084
81	BG	0.37	0/1402	0.50	0/1878

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
83	BI	0.41	0/12014	0.53	0/16144
84	BJ	0.40	0/12675	0.48	0/17091
85	BK	0.42	0/2176	0.54	0/2937
86	BL	0.39	0/1542	0.53	0/2078
87	BM	0.34	0/2428	0.51	0/3263
88	BN	0.40	0/2359	0.50	0/3168
89	BO	0.36	0/306	0.48	0/414
90	BP	0.38	0/489	0.56	0/647
91	BQ	0.35	0/5264	0.49	0/7086
92	BR	0.35	0/1204	0.52	0/1623
93	BS	0.31	0/3682	0.44	0/4953
94	BT	0.22	0/19	0.46	0/25
95	BU	0.37	0/2655	0.50	0/3578
96	BV	0.30	0/1868	0.44	0/2523
98	BX	0.42	0/1189	0.54	0/1591
99	BY	0.30	0/2465	0.48	0/3331
All	All	0.51	3/289793 (0.0%)	0.67	36/410231 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	Ac	0	1
15	Ao	0	1
19	As	0	1
20	At	0	1
22	Av	0	1
26	Az	0	2
28	AB	0	2
36	AJ	0	1
47	AU	0	1
48	AV	0	1
53	Be	0	1
56	Bh	0	1
57	Bi	0	1
63	Bo	0	1
65	Bq	0	1
71	Bw	0	1
75	BA	0	1
83	BI	0	1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	At	32	ARG	C-N	-5.63	1.21	1.34
54	Bf	238	CYS	CB-SG	-5.26	1.73	1.81
16	Ap	19	VAL	CB-CG2	-5.03	1.42	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Ab	1015	U	C2-N1-C1’	8.29	127.65	117.70
2	Ab	1149	C	N1-C2-O2	7.27	123.26	118.90
2	Ab	624	C	N1-C2-O2	7.14	123.18	118.90
2	Ab	359	C	C2-N1-C1’	7.07	126.58	118.80
2	Ab	1410	G	O4’-C1’-N9	6.66	113.53	108.20
2	Ab	1149	C	N3-C2-O2	-6.58	117.30	121.90
50	Bb	1333	C	N1-C2-O2	6.57	122.84	118.90
2	Ab	1015	U	N3-C2-O2	-6.53	117.63	122.20
2	Ab	1015	U	N1-C2-O2	6.46	127.32	122.80
2	Ab	359	C	N1-C2-O2	6.44	122.76	118.90
2	Ab	1379	C	C6-N1-C2	-6.28	117.79	120.30
50	Bb	1191	G	C4-N9-C1’	6.23	134.60	126.50
50	Bb	1333	C	C2-N1-C1’	6.22	125.64	118.80
2	Ab	1149	C	C6-N1-C2	-6.21	117.82	120.30
2	Ab	624	C	N3-C2-O2	-6.12	117.61	121.90
2	Ab	508	U	C2-N1-C1’	5.88	124.75	117.70
50	Bb	1333	C	N3-C2-O2	-5.58	117.99	121.90
2	Ab	1149	C	C2-N1-C1’	5.57	124.93	118.80
2	Ab	359	C	N3-C2-O2	-5.56	118.01	121.90
50	Bb	1191	G	C8-N9-C1’	-5.53	119.81	127.00
50	Bb	616	C	C6-N1-C2	-5.41	118.14	120.30
61	Bm	63	LEU	CA-CB-CG	5.41	127.74	115.30
2	Ab	1015	U	C6-N1-C1’	-5.33	113.74	121.20
26	Az	115	ARG	NE-CZ-NH2	5.30	122.95	120.30
2	Ab	624	C	C2-N1-C1’	5.30	124.63	118.80
2	Ab	407	C	C6-N1-C2	-5.27	118.19	120.30
1	Aa	67	A	P-O3’-C3’	5.24	125.99	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Ab	986	U	C2-N1-C1'	5.24	123.99	117.70
1	Aa	88	U	C2-N1-C1'	5.22	123.97	117.70
2	Ab	889	U	N1-C2-O2	5.22	126.45	122.80
1	Aa	86	C	C2-N1-C1'	5.14	124.46	118.80
50	Bb	1224	U	P-O3'-C3'	5.09	125.81	119.70
2	Ab	359	C	C6-N1-C1'	-5.08	114.71	120.80
50	Bb	355	C	C6-N1-C2	-5.05	118.28	120.30
23	Aw	201	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	Ab	889	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	AB	182	PRO	Peptide
28	AB	183	ILE	Peptide
36	AJ	123	TYR	Peptide
47	AU	45	ILE	Peptide
48	AV	140	PRO	Peptide
3	Ac	124	PHE	Mainchain
15	Ao	211	GLN	Peptide
19	As	124	ILE	Peptide
20	At	46	TRP	Peptide
22	Av	170	ARG	Peptide
26	Az	136	THR	Peptide
26	Az	137	TYR	Peptide
75	BA	74	LYS	Peptide
83	BI	502	TYR	Peptide
84	BJ	82	SER	Peptide
84	BJ	951	LYS	Peptide
90	BP	84	ASP	Peptide
91	BQ	259	ILE	Peptide
53	Be	238	LYS	Peptide
56	Bh	193	VAL	Peptide
57	Bi	564	GLN	Peptide
63	Bo	189	PRO	Peptide
65	Bq	142	ILE	Peptide
71	Bw	366	ILE	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ac	260/262 (99%)	244 (94%)	16 (6%)	0	100	100
4	Ad	368/439 (84%)	344 (94%)	24 (6%)	0	100	100
5	Ae	335/358 (94%)	319 (95%)	16 (5%)	0	100	100
6	Af	66/68 (97%)	63 (96%)	3 (4%)	0	100	100
7	Ag	174/179 (97%)	165 (95%)	9 (5%)	0	100	100
11	Ak	102/105 (97%)	96 (94%)	6 (6%)	0	100	100
12	Al	51/223 (23%)	49 (96%)	2 (4%)	0	100	100
13	Am	156/166 (94%)	145 (93%)	11 (7%)	0	100	100
14	An	156/158 (99%)	150 (96%)	6 (4%)	0	100	100
15	Ao	328/391 (84%)	309 (94%)	19 (6%)	0	100	100
16	Ap	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
17	Aq	271/305 (89%)	251 (93%)	20 (7%)	0	100	100
18	Ar	141/143 (99%)	126 (89%)	15 (11%)	0	100	100
19	As	234/237 (99%)	215 (92%)	19 (8%)	0	100	100
20	At	181/242 (75%)	170 (94%)	10 (6%)	1 (1%)	25	62
21	Au	167/170 (98%)	161 (96%)	6 (4%)	0	100	100
22	Av	204/235 (87%)	193 (95%)	9 (4%)	2 (1%)	15	51
23	Aw	340/364 (93%)	323 (95%)	17 (5%)	0	100	100
24	Ax	130/138 (94%)	124 (95%)	6 (5%)	0	100	100
25	Ay	188/234 (80%)	180 (96%)	8 (4%)	0	100	100
26	Az	235/321 (73%)	223 (95%)	11 (5%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	AA	174/237 (73%)	162 (93%)	12 (7%)	0	100	100
28	AB	262/289 (91%)	247 (94%)	14 (5%)	1 (0%)	34	69
29	AC	282/307 (92%)	269 (95%)	13 (5%)	0	100	100
31	AE	55/64 (86%)	51 (93%)	4 (7%)	0	100	100
32	AF	113/164 (69%)	110 (97%)	3 (3%)	0	100	100
33	AG	36/93 (39%)	35 (97%)	1 (3%)	0	100	100
34	AH	175/199 (88%)	169 (97%)	6 (3%)	0	100	100
35	AI	120/155 (77%)	113 (94%)	7 (6%)	0	100	100
36	AJ	176/179 (98%)	165 (94%)	11 (6%)	0	100	100
37	AK	242/309 (78%)	230 (95%)	12 (5%)	0	100	100
38	AL	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
39	AM	124/184 (67%)	121 (98%)	3 (2%)	0	100	100
40	AN	94/158 (60%)	91 (97%)	3 (3%)	0	100	100
41	AO	118/155 (76%)	117 (99%)	1 (1%)	0	100	100
42	AP	362/386 (94%)	351 (97%)	11 (3%)	0	100	100
43	AQ	48/109 (44%)	41 (85%)	7 (15%)	0	100	100
44	AR	272/348 (78%)	256 (94%)	16 (6%)	0	100	100
45	AS	724/764 (95%)	696 (96%)	28 (4%)	0	100	100
46	AT	164/299 (55%)	155 (94%)	9 (6%)	0	100	100
47	AU	477/499 (96%)	454 (95%)	23 (5%)	0	100	100
48	AV	127/160 (79%)	116 (91%)	11 (9%)	0	100	100
51	Bc	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
52	Bd	328/330 (99%)	316 (96%)	12 (4%)	0	100	100
53	Be	403/405 (100%)	387 (96%)	16 (4%)	0	100	100
54	Bf	335/351 (95%)	314 (94%)	21 (6%)	0	100	100
55	Bg	134/141 (95%)	124 (92%)	10 (8%)	0	100	100
56	Bh	254/276 (92%)	237 (93%)	17 (7%)	0	100	100
57	Bi	620/737 (84%)	593 (96%)	26 (4%)	1 (0%)	47	78
58	Bj	150/152 (99%)	143 (95%)	7 (5%)	0	100	100
59	Bk	224/238 (94%)	208 (93%)	16 (7%)	0	100	100
60	Bl	127/133 (96%)	115 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	Bm	218/276 (79%)	205 (94%)	13 (6%)	0	100	100
62	Bn	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
63	Bo	177/196 (90%)	170 (96%)	7 (4%)	0	100	100
64	Bp	410/437 (94%)	386 (94%)	24 (6%)	0	100	100
65	Bq	172/182 (94%)	164 (95%)	7 (4%)	1 (1%)	25	62
66	Br	521/549 (95%)	498 (96%)	23 (4%)	0	100	100
67	Bs	85/98 (87%)	78 (92%)	7 (8%)	0	100	100
68	Bt	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
69	Bu	400/567 (70%)	385 (96%)	15 (4%)	0	100	100
70	Bv	461/579 (80%)	450 (98%)	11 (2%)	0	100	100
71	Bw	656/703 (93%)	630 (96%)	26 (4%)	0	100	100
72	Bx	526/719 (73%)	505 (96%)	21 (4%)	0	100	100
73	By	105/132 (80%)	104 (99%)	1 (1%)	0	100	100
74	Bz	121/147 (82%)	111 (92%)	10 (8%)	0	100	100
75	BA	136/149 (91%)	127 (93%)	9 (7%)	0	100	100
76	BB	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
78	BD	105/130 (81%)	100 (95%)	5 (5%)	0	100	100
79	BE	445/464 (96%)	418 (94%)	27 (6%)	0	100	100
81	BG	162/182 (89%)	156 (96%)	6 (4%)	0	100	100
83	BI	1409/1451 (97%)	1337 (95%)	72 (5%)	0	100	100
84	BJ	1513/1539 (98%)	1438 (95%)	75 (5%)	0	100	100
85	BK	265/267 (99%)	253 (96%)	12 (4%)	0	100	100
86	BL	179/310 (58%)	170 (95%)	9 (5%)	0	100	100
87	BM	282/355 (79%)	265 (94%)	17 (6%)	0	100	100
88	BN	272/283 (96%)	257 (94%)	15 (6%)	0	100	100
89	BO	34/142 (24%)	30 (88%)	4 (12%)	0	100	100
90	BP	58/100 (58%)	49 (84%)	9 (16%)	0	100	100
91	BQ	618/1032 (60%)	578 (94%)	40 (6%)	0	100	100
92	BR	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
93	BS	429/1086 (40%)	416 (97%)	13 (3%)	0	100	100
94	BT	4/297 (1%)	4 (100%)	0	0	100	100

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

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	At	46	TRP
22	Av	114	ALA
26	Az	138	ASP
57	Bi	565	VAL
65	Bq	143	LYS
28	AB	184	VAL
22	Av	113	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	
3	Ac	235/235 (100%)	235 (100%)	0	100	100
4	Ad	330/391 (84%)	328 (99%)	2 (1%)	86	93
5	Ae	306/326 (94%)	306 (100%)	0	100	100
6	Af	68/68 (100%)	68 (100%)	0	100	100
7	Ag	170/172 (99%)	170 (100%)	0	100	100
11	Ak	93/93 (100%)	93 (100%)	0	100	100
12	Al	46/203 (23%)	46 (100%)	0	100	100
13	Am	156/156 (100%)	156 (100%)	0	100	100
14	An	138/138 (100%)	138 (100%)	0	100	100
15	Ao	309/345 (90%)	309 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Ap	110/110 (100%)	110 (100%)	0	100	100
17	Aq	239/269 (89%)	239 (100%)	0	100	100
18	Ar	135/135 (100%)	135 (100%)	0	100	100
19	As	208/209 (100%)	208 (100%)	0	100	100
20	At	168/224 (75%)	168 (100%)	0	100	100
21	Au	150/151 (99%)	150 (100%)	0	100	100
22	Av	187/211 (89%)	187 (100%)	0	100	100
23	Aw	309/331 (93%)	309 (100%)	0	100	100
24	Ax	125/130 (96%)	125 (100%)	0	100	100
25	Ay	168/208 (81%)	168 (100%)	0	100	100
26	Az	218/295 (74%)	218 (100%)	0	100	100
27	AA	157/212 (74%)	157 (100%)	0	100	100
28	AB	255/278 (92%)	255 (100%)	0	100	100
29	AC	256/277 (92%)	256 (100%)	0	100	100
31	AE	49/55 (89%)	49 (100%)	0	100	100
32	AF	103/150 (69%)	103 (100%)	0	100	100
33	AG	35/89 (39%)	35 (100%)	0	100	100
34	AH	164/184 (89%)	164 (100%)	0	100	100
35	AI	115/144 (80%)	115 (100%)	0	100	100
36	AJ	164/165 (99%)	164 (100%)	0	100	100
37	AK	226/286 (79%)	226 (100%)	0	100	100
38	AL	132/132 (100%)	132 (100%)	0	100	100
39	AM	113/170 (66%)	113 (100%)	0	100	100
40	AN	91/139 (66%)	91 (100%)	0	100	100
41	AO	109/138 (79%)	109 (100%)	0	100	100
42	AP	339/359 (94%)	339 (100%)	0	100	100
43	AQ	45/98 (46%)	45 (100%)	0	100	100
44	AR	258/324 (80%)	258 (100%)	0	100	100
45	AS	657/691 (95%)	657 (100%)	0	100	100
46	AT	151/273 (55%)	151 (100%)	0	100	100
47	AU	443/461 (96%)	442 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	AV	119/149 (80%)	119 (100%)	0	100	100
51	Bc	158/158 (100%)	158 (100%)	0	100	100
52	Bd	319/319 (100%)	319 (100%)	0	100	100
53	Be	396/396 (100%)	396 (100%)	0	100	100
54	Bf	304/317 (96%)	303 (100%)	1 (0%)	92	96
55	Bg	117/122 (96%)	117 (100%)	0	100	100
56	Bh	249/269 (93%)	249 (100%)	0	100	100
57	Bi	582/683 (85%)	582 (100%)	0	100	100
58	Bj	148/148 (100%)	148 (100%)	0	100	100
59	Bk	216/228 (95%)	216 (100%)	0	100	100
60	Bl	113/116 (97%)	113 (100%)	0	100	100
61	Bm	209/258 (81%)	208 (100%)	1 (0%)	88	94
62	Bn	94/94 (100%)	94 (100%)	0	100	100
63	Bo	161/177 (91%)	161 (100%)	0	100	100
64	Bp	382/406 (94%)	382 (100%)	0	100	100
65	Bq	161/167 (96%)	161 (100%)	0	100	100
66	Br	481/506 (95%)	481 (100%)	0	100	100
67	Bs	82/93 (88%)	82 (100%)	0	100	100
68	Bt	93/93 (100%)	93 (100%)	0	100	100
69	Bu	378/386 (98%)	378 (100%)	0	100	100
70	Bv	433/540 (80%)	433 (100%)	0	100	100
71	Bw	609/647 (94%)	608 (100%)	1 (0%)	93	97
72	Bx	491/660 (74%)	491 (100%)	0	100	100
73	By	96/116 (83%)	96 (100%)	0	100	100
74	Bz	107/126 (85%)	106 (99%)	1 (1%)	78	88
75	BA	130/141 (92%)	130 (100%)	0	100	100
76	BB	101/102 (99%)	101 (100%)	0	100	100
78	BD	98/120 (82%)	98 (100%)	0	100	100
79	BE	404/420 (96%)	403 (100%)	1 (0%)	93	97
81	BG	153/171 (90%)	152 (99%)	1 (1%)	84	91
83	BI	1306/1335 (98%)	1306 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	BJ	1405/1426 (98%)	1405 (100%)	0	100	100
85	BK	235/235 (100%)	235 (100%)	0	100	100
86	BL	168/291 (58%)	168 (100%)	0	100	100
87	BM	256/322 (80%)	256 (100%)	0	100	100
88	BN	249/256 (97%)	249 (100%)	0	100	100
89	BO	35/35 (100%)	35 (100%)	0	100	100
90	BP	57/57 (100%)	57 (100%)	0	100	100
91	BQ	582/958 (61%)	582 (100%)	0	100	100
92	BR	133/133 (100%)	132 (99%)	1 (1%)	81	89
93	BS	399/1002 (40%)	399 (100%)	0	100	100
95	BU	285/403 (71%)	285 (100%)	0	100	100
96	BV	197/197 (100%)	197 (100%)	0	100	100
98	BX	126/142 (89%)	126 (100%)	0	100	100
99	BY	280/280 (100%)	279 (100%)	1 (0%)	91	95
All	All	20827/24225 (86%)	20816 (100%)	11 (0%)	93	98

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Ad	320	ASN
4	Ad	338	ARG
47	AU	189	ASN
54	Bf	337	ASN
61	Bm	184	ASN
71	Bw	545	ASN
74	Bz	60	ASN
79	BE	421	ARG
81	BG	24	ARG
92	BR	96	ARG
99	BY	229	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
3	Ac	221	ASN
7	Ag	41	ASN

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Mol	Chain	Res	Type
15	Ao	215	GLN
17	Aq	61	ASN
18	Ar	11	GLN
24	Ax	133	GLN
25	Ay	56	ASN
26	Az	141	GLN
28	AB	197	GLN
29	AC	259	GLN
29	AC	265	ASN
39	AM	94	GLN
41	AO	83	ASN
42	AP	255	HIS
42	AP	270	ASN
42	AP	310	ASN
43	AQ	63	ASN
45	AS	654	HIS
47	AU	189	ASN
51	Bc	157	ASN
52	Bd	32	ASN
52	Bd	72	ASN
52	Bd	121	ASN
52	Bd	167	ASN
53	Be	210	ASN
56	Bh	55	ASN
57	Bi	117	ASN
57	Bi	303	ASN
60	Bl	44	ASN
62	Bn	95	ASN
63	Bo	112	GLN
64	Bp	180	ASN
66	Br	100	GLN
66	Br	311	GLN
68	Bt	44	ASN
69	Bu	59	GLN
69	Bu	279	ASN
70	Bv	103	HIS
71	Bw	76	GLN
71	Bw	199	ASN
71	Bw	315	ASN
71	Bw	505	ASN
71	Bw	625	ASN
71	Bw	644	HIS

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Mol	Chain	Res	Type
71	Bw	683	HIS
74	Bz	60	ASN
74	Bz	98	ASN
79	BE	190	ASN
83	BI	351	ASN
83	BI	1119	ASN
84	BJ	331	ASN
84	BJ	556	ASN
84	BJ	680	GLN
84	BJ	941	ASN
84	BJ	1044	ASN
84	BJ	1364	GLN
88	BN	160	HIS
88	BN	168	ASN
91	BQ	209	ASN
91	BQ	433	ASN
92	BR	50	GLN
93	BS	663	HIS
93	BS	1043	GLN
96	BV	231	ASN
99	BY	229	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	277/278 (99%)	64 (23%)	0
2	Ab	2234/2314 (96%)	447 (20%)	0
49	Ba	195/196 (99%)	43 (22%)	0
50	Bb	1384/1395 (99%)	256 (18%)	0
All	All	4090/4183 (97%)	810 (19%)	0

All (810) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	6	U
1	Aa	7	G
1	Aa	13	A
1	Aa	35	A
1	Aa	47	U
1	Aa	55	A
1	Aa	57	C

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Mol	Chain	Res	Type
1	Aa	60	A
1	Aa	67	A
1	Aa	68	U
1	Aa	70	U
1	Aa	71	C
1	Aa	74	U
1	Aa	80	A
1	Aa	81	A
1	Aa	87	A
1	Aa	89	A
1	Aa	93	A
1	Aa	94	U
1	Aa	97	G
1	Aa	99	U
1	Aa	101	A
1	Aa	102	U
1	Aa	104	U
1	Aa	109	G
1	Aa	112	A
1	Aa	127	U
1	Aa	128	G
1	Aa	129	G
1	Aa	139	A
1	Aa	141	G
1	Aa	145	A
1	Aa	148	A
1	Aa	155	U
1	Aa	156	A
1	Aa	163	U
1	Aa	169	A
1	Aa	171	U
1	Aa	172	C
1	Aa	175	U
1	Aa	176	U
1	Aa	177	G
1	Aa	187	U
1	Aa	192	G
1	Aa	194	G
1	Aa	196	G
1	Aa	201	U
1	Aa	213	U
1	Aa	215	U

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Mol	Chain	Res	Type
1	Aa	216	U
1	Aa	217	U
1	Aa	218	A
1	Aa	220	A
1	Aa	221	U
1	Aa	222	U
1	Aa	232	A
1	Aa	252	U
1	Aa	253	A
1	Aa	255	A
1	Aa	260	G
1	Aa	261	A
1	Aa	262	A
1	Aa	263	A
1	Aa	264	G
2	Ab	280	A
2	Ab	281	G
2	Ab	282	U
2	Ab	297	U
2	Ab	298	U
2	Ab	299	U
2	Ab	308	A
2	Ab	311	A
2	Ab	312	A
2	Ab	313	U
2	Ab	319	U
2	Ab	327	U
2	Ab	330	A
2	Ab	334	U
2	Ab	335	G
2	Ab	337	A
2	Ab	356	A
2	Ab	358	A
2	Ab	359	C
2	Ab	360	A
2	Ab	361	G
2	Ab	367	C
2	Ab	368	G
2	Ab	370	G
2	Ab	376	G
2	Ab	378	U
2	Ab	384	G

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Mol	Chain	Res	Type
2	Ab	390	A
2	Ab	391	U
2	Ab	392	A
2	Ab	393	A
2	Ab	394	U
2	Ab	402	A
2	Ab	403	A
2	Ab	404	G
2	Ab	408	C
2	Ab	422	U
2	Ab	424	A
2	Ab	428	C
2	Ab	429	A
2	Ab	430	G
2	Ab	439	U
2	Ab	441	A
2	Ab	442	U
2	Ab	443	U
2	Ab	453	U
2	Ab	454	A
2	Ab	456	C
2	Ab	461	G
2	Ab	463	A
2	Ab	464	U
2	Ab	465	A
2	Ab	466	A
2	Ab	494	A
2	Ab	498	A
2	Ab	499	U
2	Ab	500	U
2	Ab	501	U
2	Ab	505	U
2	Ab	506	U
2	Ab	507	U
2	Ab	510	U
2	Ab	520	A
2	Ab	521	A
2	Ab	525	A
2	Ab	531	U
2	Ab	532	A
2	Ab	533	A
2	Ab	534	A

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Mol	Chain	Res	Type
2	Ab	535	U
2	Ab	549	A
2	Ab	550	G
2	Ab	567	U
2	Ab	572	U
2	Ab	589	G
2	Ab	592	U
2	Ab	593	U
2	Ab	594	U
2	Ab	595	A
2	Ab	596	U
2	Ab	597	A
2	Ab	603	G
2	Ab	605	A
2	Ab	622	U
2	Ab	623	G
2	Ab	627	A
2	Ab	628	A
2	Ab	636	A
2	Ab	640	A
2	Ab	650	G
2	Ab	651	G
2	Ab	656	A
2	Ab	657	A
2	Ab	658	A
2	Ab	659	G
2	Ab	667	A
2	Ab	674	G
2	Ab	675	U
2	Ab	677	A
2	Ab	680	G
2	Ab	687	U
2	Ab	691	A
2	Ab	696	A
2	Ab	702	U
2	Ab	703	U
2	Ab	709	G
2	Ab	719	U
2	Ab	720	U
2	Ab	721	U
2	Ab	722	U
2	Ab	734	G

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Mol	Chain	Res	Type
2	Ab	735	U
2	Ab	739	A
2	Ab	740	A
2	Ab	741	U
2	Ab	749	U
2	Ab	750	C
2	Ab	760	U
2	Ab	761	U
2	Ab	762	U
2	Ab	763	G
2	Ab	764	U
2	Ab	768	U
2	Ab	781	A
2	Ab	783	A
2	Ab	785	A
2	Ab	787	U
2	Ab	788	A
2	Ab	800	U
2	Ab	802	A
2	Ab	813	A
2	Ab	814	G
2	Ab	819	U
2	Ab	821	A
2	Ab	826	U
2	Ab	827	A
2	Ab	829	G
2	Ab	841	A
2	Ab	842	G
2	Ab	843	A
2	Ab	857	G
2	Ab	858	A
2	Ab	859	U
2	Ab	863	A
2	Ab	864	C
2	Ab	865	A
2	Ab	873	C
2	Ab	879	A
2	Ab	880	A
2	Ab	884	A
2	Ab	888	A
2	Ab	889	U
2	Ab	907	U

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Mol	Chain	Res	Type
2	Ab	911	U
2	Ab	912	A
2	Ab	913	C
2	Ab	924	U
2	Ab	926	G
2	Ab	932	G
2	Ab	934	A
2	Ab	937	A
2	Ab	948	U
2	Ab	952	A
2	Ab	953	A
2	Ab	954	A
2	Ab	961	A
2	Ab	984	U
2	Ab	985	G
2	Ab	987	U
2	Ab	988	A
2	Ab	990	A
2	Ab	992	A
2	Ab	1006	A
2	Ab	1007	A
2	Ab	1016	A
2	Ab	1021	A
2	Ab	1028	A
2	Ab	1031	A
2	Ab	1032	A
2	Ab	1033	U
2	Ab	1059	A
2	Ab	1062	G
2	Ab	1065	G
2	Ab	1084	U
2	Ab	1086	A
2	Ab	1088	A
2	Ab	1100	U
2	Ab	1102	A
2	Ab	1103	A
2	Ab	1114	U
2	Ab	1120	A
2	Ab	1123	U
2	Ab	1125	G
2	Ab	1127	U
2	Ab	1128	A

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Mol	Chain	Res	Type
2	Ab	1130	U
2	Ab	1131	G
2	Ab	1140	A
2	Ab	1142	U
2	Ab	1149	C
2	Ab	1150	A
2	Ab	1174	G
2	Ab	1175	A
2	Ab	1182	A
2	Ab	1187	U
2	Ab	1195	U
2	Ab	1196	U
2	Ab	1197	G
2	Ab	1198	A
2	Ab	1205	U
2	Ab	1215	A
2	Ab	1218	U
2	Ab	1219	C
2	Ab	1232	A
2	Ab	1234	A
2	Ab	1239	U
2	Ab	1241	U
2	Ab	1243	U
2	Ab	1246	U
2	Ab	1252	A
2	Ab	1253	U
2	Ab	1259	U
2	Ab	1260	A
2	Ab	1272	A
2	Ab	1276	A
2	Ab	1300	A
2	Ab	1301	A
2	Ab	1302	A
2	Ab	1307	U
2	Ab	1308	U
2	Ab	1312	A
2	Ab	1317	A
2	Ab	1327	G
2	Ab	1339	G
2	Ab	1340	G
2	Ab	1341	A
2	Ab	1344	U

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Mol	Chain	Res	Type
2	Ab	1357	U
2	Ab	1358	U
2	Ab	1359	A
2	Ab	1366	A
2	Ab	1370	A
2	Ab	1371	C
2	Ab	1378	A
2	Ab	1379	C
2	Ab	1380	A
2	Ab	1389	A
2	Ab	1408	A
2	Ab	1409	A
2	Ab	1410	G
2	Ab	1411	G
2	Ab	1415	A
2	Ab	1416	A
2	Ab	1436	G
2	Ab	1458	G
2	Ab	1460	A
2	Ab	1469	G
2	Ab	1471	U
2	Ab	1473	U
2	Ab	1474	U
2	Ab	1475	A
2	Ab	1484	A
2	Ab	1485	A
2	Ab	1490	G
2	Ab	1491	A
2	Ab	1500	A
2	Ab	1508	A
2	Ab	1513	A
2	Ab	1527	C
2	Ab	1529	A
2	Ab	1540	U
2	Ab	1543	U
2	Ab	1556	A
2	Ab	1560	C
2	Ab	1597	G
2	Ab	1619	A
2	Ab	1620	A
2	Ab	1625	G
2	Ab	1632	A

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Mol	Chain	Res	Type
2	Ab	1641	G
2	Ab	1648	G
2	Ab	1649	G
2	Ab	1650	U
2	Ab	1656	A
2	Ab	1657	A
2	Ab	1682	U
2	Ab	1686	U
2	Ab	1688	A
2	Ab	1689	A
2	Ab	1690	U
2	Ab	1691	G
2	Ab	1700	A
2	Ab	1701	C
2	Ab	1710	U
2	Ab	1711	G
2	Ab	1712	U
2	Ab	1716	C
2	Ab	1725	C
2	Ab	1730	C
2	Ab	1737	G
2	Ab	1742	U
2	Ab	1749	A
2	Ab	1750	A
2	Ab	1753	U
2	Ab	1758	C
2	Ab	1759	A
2	Ab	1762	A
2	Ab	1764	U
2	Ab	1771	A
2	Ab	1774	C
2	Ab	1779	A
2	Ab	1780	G
2	Ab	1788	G
2	Ab	1799	G
2	Ab	1899	U
2	Ab	1900	A
2	Ab	1901	A
2	Ab	1908	U
2	Ab	1911	U
2	Ab	1912	A
2	Ab	1913	A

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Mol	Chain	Res	Type
2	Ab	1919	U
2	Ab	1921	U
2	Ab	1931	A
2	Ab	1932	G
2	Ab	1933	A
2	Ab	1940	G
2	Ab	1944	G
2	Ab	1960	A
2	Ab	1962	A
2	Ab	1963	A
2	Ab	1969	C
2	Ab	1970	G
2	Ab	1972	A
2	Ab	1974	G
2	Ab	1977	U
2	Ab	1981	A
2	Ab	1982	U
2	Ab	1991	G
2	Ab	1999	U
2	Ab	2000	U
2	Ab	2001	U
2	Ab	2006	U
2	Ab	2013	A
2	Ab	2014	A
2	Ab	2017	U
2	Ab	2019	A
2	Ab	2028	A
2	Ab	2029	U
2	Ab	2038	U
2	Ab	2039	G
2	Ab	2041	U
2	Ab	2052	A
2	Ab	2070	U
2	Ab	2071	A
2	Ab	2072	U
2	Ab	2073	G
2	Ab	2077	G
2	Ab	2079	C
2	Ab	2082	A
2	Ab	2084	U
2	Ab	2086	A
2	Ab	2100	A

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Mol	Chain	Res	Type
2	Ab	2117	U
2	Ab	2119	A
2	Ab	2122	G
2	Ab	2123	A
2	Ab	2124	A
2	Ab	2133	A
2	Ab	2135	G
2	Ab	2142	A
2	Ab	2170	U
2	Ab	2172	A
2	Ab	2185	U
2	Ab	2188	G
2	Ab	2196	G
2	Ab	2197	A
2	Ab	2198	U
2	Ab	2200	U
2	Ab	2207	A
2	Ab	2212	A
2	Ab	2214	C
2	Ab	2224	G
2	Ab	2225	A
2	Ab	2241	C
2	Ab	2256	U
2	Ab	2260	A
2	Ab	2261	G
2	Ab	2263	G
2	Ab	2267	C
2	Ab	2268	G
2	Ab	2271	A
2	Ab	2272	G
2	Ab	2276	G
2	Ab	2279	U
2	Ab	2280	U
2	Ab	2290	U
2	Ab	2293	G
2	Ab	2296	A
2	Ab	2304	C
2	Ab	2307	U
2	Ab	2317	A
2	Ab	2348	A
2	Ab	2349	G
2	Ab	2354	A

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Mol	Chain	Res	Type
2	Ab	2357	G
2	Ab	2396	A
2	Ab	2397	A
2	Ab	2398	U
2	Ab	2399	A
2	Ab	2412	G
2	Ab	2424	A
2	Ab	2430	A
2	Ab	2436	U
2	Ab	2447	U
2	Ab	2455	A
2	Ab	2456	A
2	Ab	2462	A
2	Ab	2463	A
2	Ab	2464	U
2	Ab	2474	A
2	Ab	2475	U
2	Ab	2485	A
2	Ab	2487	A
2	Ab	2502	U
2	Ab	2512	A
2	Ab	2513	A
2	Ab	2516	A
2	Ab	2522	A
2	Ab	2524	U
2	Ab	2527	G
2	Ab	2537	A
2	Ab	2538	A
2	Ab	2539	C
2	Ab	2540	U
2	Ab	2559	A
2	Ab	2561	A
2	Ab	2562	U
2	Ab	2563	G
2	Ab	2566	U
2	Ab	2569	U
2	Ab	2571	A
2	Ab	2572	U
2	Ab	2584	A
2	Ab	2586	U
2	Ab	2587	U
2	Ab	2589	U

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Mol	Chain	Res	Type
49	Ba	16	A
49	Ba	17	A
49	Ba	18	U
49	Ba	20	A
49	Ba	21	A
49	Ba	25	A
49	Ba	26	A
49	Ba	28	A
49	Ba	29	U
49	Ba	30	U
49	Ba	31	U
49	Ba	35	G
49	Ba	41	G
49	Ba	48	G
49	Ba	57	U
49	Ba	64	A
49	Ba	65	A
49	Ba	73	C
49	Ba	74	C
49	Ba	76	A
49	Ba	77	A
49	Ba	81	A
49	Ba	92	A
49	Ba	97	A
49	Ba	98	G
49	Ba	110	U
49	Ba	111	U
49	Ba	113	U
49	Ba	131	C
49	Ba	132	A
49	Ba	142	A
49	Ba	143	U
49	Ba	144	A
49	Ba	149	A
49	Ba	166	C
49	Ba	172	A
49	Ba	185	C
49	Ba	189	A
49	Ba	191	A
49	Ba	199	C
49	Ba	200	A
49	Ba	208	U

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Mol	Chain	Res	Type
49	Ba	209	A
50	Bb	222	U
50	Bb	223	A
50	Bb	233	G
50	Bb	250	U
50	Bb	251	U
50	Bb	252	A
50	Bb	257	A
50	Bb	283	U
50	Bb	294	A
50	Bb	295	A
50	Bb	300	A
50	Bb	301	G
50	Bb	305	A
50	Bb	306	G
50	Bb	314	G
50	Bb	326	G
50	Bb	331	U
50	Bb	344	G
50	Bb	353	A
50	Bb	355	C
50	Bb	356	U
50	Bb	357	A
50	Bb	365	U
50	Bb	366	U
50	Bb	367	U
50	Bb	368	U
50	Bb	372	C
50	Bb	383	A
50	Bb	386	U
50	Bb	389	G
50	Bb	401	A
50	Bb	408	G
50	Bb	409	A
50	Bb	413	A
50	Bb	417	A
50	Bb	418	A
50	Bb	425	G
50	Bb	426	A
50	Bb	432	A
50	Bb	433	G
50	Bb	434	A

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Mol	Chain	Res	Type
50	Bb	441	C
50	Bb	448	G
50	Bb	449	U
50	Bb	457	A
50	Bb	458	G
50	Bb	472	A
50	Bb	473	A
50	Bb	474	A
50	Bb	480	A
50	Bb	481	A
50	Bb	482	A
50	Bb	490	A
50	Bb	491	G
50	Bb	493	A
50	Bb	499	G
50	Bb	503	A
50	Bb	505	U
50	Bb	506	A
50	Bb	507	C
50	Bb	513	C
50	Bb	519	G
50	Bb	522	G
50	Bb	526	U
50	Bb	527	A
50	Bb	529	U
50	Bb	542	A
50	Bb	554	A
50	Bb	555	U
50	Bb	557	G
50	Bb	558	A
50	Bb	559	C
50	Bb	565	G
50	Bb	568	U
50	Bb	569	U
50	Bb	571	A
50	Bb	572	A
50	Bb	583	A
50	Bb	608	A
50	Bb	611	A
50	Bb	612	A
50	Bb	613	A
50	Bb	615	A

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Mol	Chain	Res	Type
50	Bb	617	C
50	Bb	632	U
50	Bb	639	A
50	Bb	640	A
50	Bb	642	G
50	Bb	643	A
50	Bb	655	A
50	Bb	675	A
50	Bb	678	A
50	Bb	692	U
50	Bb	693	U
50	Bb	694	A
50	Bb	708	G
50	Bb	711	A
50	Bb	713	A
50	Bb	715	A
50	Bb	718	A
50	Bb	724	C
50	Bb	742	U
50	Bb	744	G
50	Bb	753	U
50	Bb	766	A
50	Bb	776	A
50	Bb	779	A
50	Bb	780	G
50	Bb	781	U
50	Bb	802	U
50	Bb	803	A
50	Bb	805	A
50	Bb	806	A
50	Bb	831	U
50	Bb	847	G
50	Bb	850	A
50	Bb	863	G
50	Bb	868	G
50	Bb	880	G
50	Bb	891	A
50	Bb	892	A
50	Bb	913	U
50	Bb	914	C
50	Bb	915	G
50	Bb	936	A

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Mol	Chain	Res	Type
50	Bb	938	U
50	Bb	946	U
50	Bb	947	C
50	Bb	950	C
50	Bb	953	A
50	Bb	954	A
50	Bb	956	A
50	Bb	967	G
50	Bb	971	C
50	Bb	972	A
50	Bb	983	G
50	Bb	984	U
50	Bb	989	U
50	Bb	994	A
50	Bb	1001	A
50	Bb	1007	U
50	Bb	1008	A
50	Bb	1019	C
50	Bb	1022	A
50	Bb	1023	A
50	Bb	1026	G
50	Bb	1038	U
50	Bb	1048	C
50	Bb	1051	U
50	Bb	1054	A
50	Bb	1065	A
50	Bb	1066	A
50	Bb	1067	G
50	Bb	1068	U
50	Bb	1072	U
50	Bb	1073	U
50	Bb	1075	U
50	Bb	1076	A
50	Bb	1077	A
50	Bb	1100	U
50	Bb	1117	C
50	Bb	1134	A
50	Bb	1143	A
50	Bb	1144	U
50	Bb	1147	A
50	Bb	1156	A
50	Bb	1165	A

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Mol	Chain	Res	Type
50	Bb	1166	U
50	Bb	1167	C
50	Bb	1168	U
50	Bb	1170	U
50	Bb	1171	U
50	Bb	1191	G
50	Bb	1194	U
50	Bb	1195	A
50	Bb	1198	G
50	Bb	1203	A
50	Bb	1205	G
50	Bb	1208	A
50	Bb	1209	A
50	Bb	1213	C
50	Bb	1224	U
50	Bb	1225	A
50	Bb	1226	U
50	Bb	1237	A
50	Bb	1238	C
50	Bb	1239	A
50	Bb	1250	A
50	Bb	1252	G
50	Bb	1259	U
50	Bb	1262	A
50	Bb	1269	C
50	Bb	1270	G
50	Bb	1272	A
50	Bb	1273	A
50	Bb	1279	U
50	Bb	1280	A
50	Bb	1290	A
50	Bb	1291	A
50	Bb	1292	A
50	Bb	1293	C
50	Bb	1297	U
50	Bb	1309	U
50	Bb	1310	A
50	Bb	1311	G
50	Bb	1312	U
50	Bb	1313	U
50	Bb	1328	A
50	Bb	1331	U

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Mol	Chain	Res	Type
50	Bb	1333	C
50	Bb	1347	U
50	Bb	1348	G
50	Bb	1356	U
50	Bb	1357	A
50	Bb	1358	G
50	Bb	1371	A
50	Bb	1374	A
50	Bb	1381	A
50	Bb	1390	A
50	Bb	1391	U
50	Bb	1405	A
50	Bb	1409	A
50	Bb	1410	C
50	Bb	1412	G
50	Bb	1444	A
50	Bb	1452	A
50	Bb	1459	C
50	Bb	1465	A
50	Bb	1466	A
50	Bb	1467	A
50	Bb	1479	U
50	Bb	1481	U
50	Bb	1492	G
50	Bb	1494	C
50	Bb	1495	A
50	Bb	1497	U
50	Bb	1498	A
50	Bb	1499	U
50	Bb	1503	A
50	Bb	1505	U
50	Bb	1506	U
50	Bb	1507	U
50	Bb	1517	U
50	Bb	1526	A
50	Bb	1527	G
50	Bb	1561	A
50	Bb	1567	C
50	Bb	1570	A
50	Bb	1571	A
50	Bb	1573	G
50	Bb	1574	U

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Mol	Chain	Res	Type
50	Bb	1585	G
50	Bb	1588	C
50	Bb	1593	U
50	Bb	1597	G
50	Bb	1598	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
102	FES	AV	202	48	0,4,4	-	-	-		
103	ATP	Bw	801	100	26,33,33	0.98	2 (7%)	31,52,52	1.72	7 (22%)
102	FES	AV	201	48	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
102	FES	AV	202	48	-	-	0/1/1/1
102	FES	AV	201	48	-	-	0/1/1/1
103	ATP	Bw	801	100	-	5/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
103	Bw	801	ATP	C5-C4	2.15	1.46	1.40
103	Bw	801	ATP	O4'-C1'	2.14	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
103	Bw	801	ATP	N3-C2-N1	-3.68	122.93	128.68
103	Bw	801	ATP	PB-O3B-PG	-3.55	120.65	132.83
103	Bw	801	ATP	C4-C5-N7	-3.04	106.23	109.40
103	Bw	801	ATP	PA-O3A-PB	-2.72	123.49	132.83
103	Bw	801	ATP	O4'-C1'-C2'	-2.63	103.08	106.93
103	Bw	801	ATP	C1'-N9-C4	-2.23	122.72	126.64
103	Bw	801	ATP	C5'-C4'-C3'	-2.17	107.04	115.18

There are no chirality outliers.

All (5) torsion outliers are listed below:

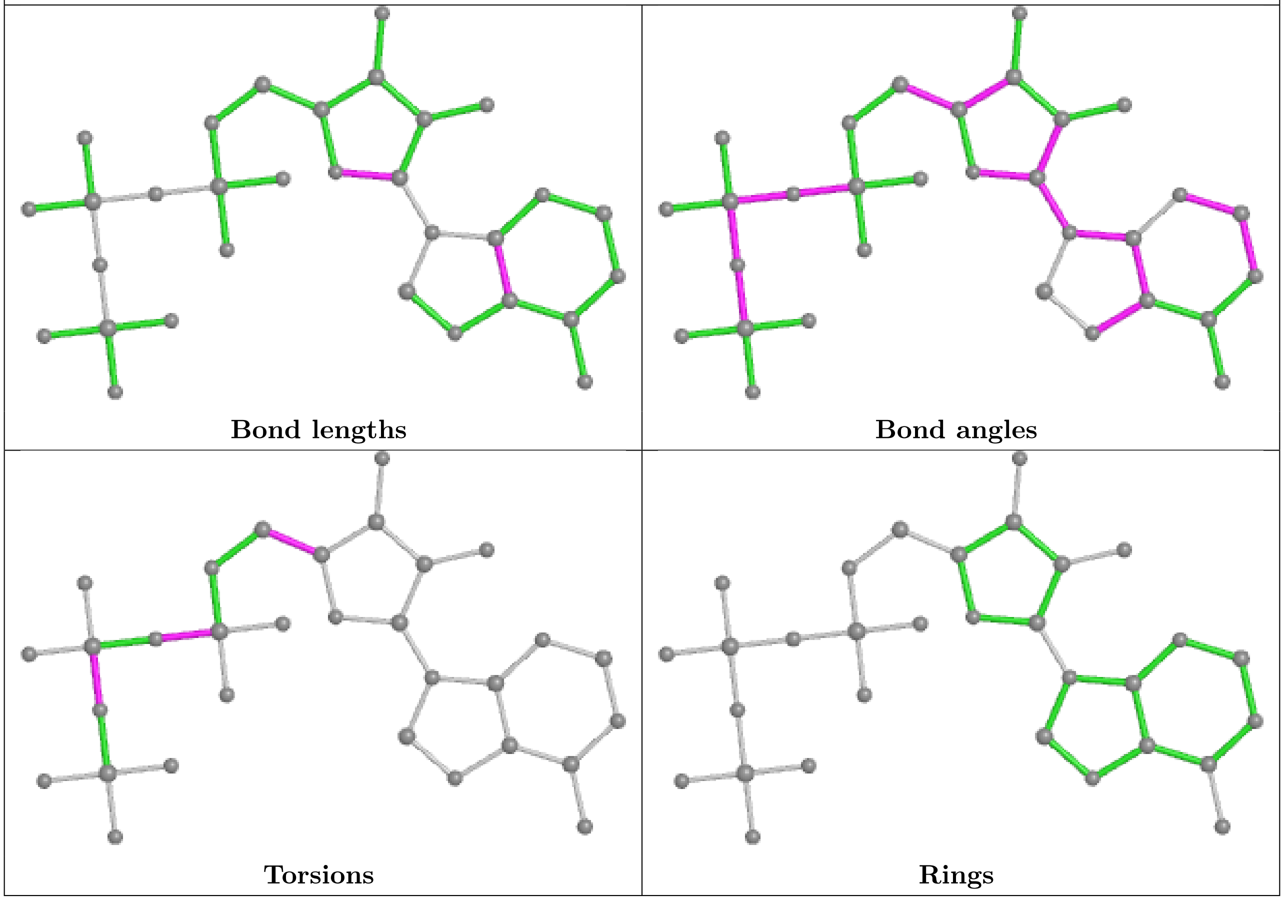
Mol	Chain	Res	Type	Atoms
103	Bw	801	ATP	O4'-C4'-C5'-O5'
103	Bw	801	ATP	C3'-C4'-C5'-O5'
103	Bw	801	ATP	PG-O3B-PB-O1B
103	Bw	801	ATP	PB-O3A-PA-O2A
103	Bw	801	ATP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ATP Bw 801



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
97	BW	18
89	BO	8
99	BY	4
96	BV	4
69	Bu	2

Continued on next page...

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Mol	Chain	Number of breaks
10	Aj	1
8	Ah	1
94	BT	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BO	142:CYS	C	147:UNK	N	25.16
1	BW	47:UNK	C	49:UNK	N	20.28
1	Bu	448:UNK	C	457:GLU	N	19.30
1	BW	201:UNK	C	202:UNK	N	19.15
1	BW	83:UNK	C	84:UNK	N	18.63
1	BO	231:UNK	C	233:UNK	N	17.74
1	BW	72:UNK	C	73:UNK	N	17.39
1	BW	231:UNK	C	232:UNK	N	17.34
1	BY	35:UNK	C	49:UNK	N	17.11
1	BO	191:UNK	C	205:UNK	N	16.91
1	Aj	18:UNK	C	25:UNK	N	16.41
1	BY	80:UNK	C	96:ILE	N	15.46
1	BO	257:UNK	C	259:UNK	N	15.02
1	BW	255:UNK	C	256:UNK	N	14.64
1	BW	125:UNK	C	126:UNK	N	14.49
1	BW	30:UNK	C	31:UNK	N	14.28
1	Bu	288:GLY	C	296:UNK	N	14.15
1	BW	59:UNK	C	60:UNK	N	12.86
1	BO	272:UNK	C	274:UNK	N	12.47
1	BW	166:UNK	C	167:UNK	N	11.86
1	BW	219:UNK	C	220:UNK	N	11.50
1	BY	60:UNK	C	75:UNK	N	10.54
1	BO	164:UNK	C	176:UNK	N	10.12
1	BV	421:UNK	C	422:UNK	N	9.00
1	BW	187:UNK	C	188:UNK	N	8.92
1	BW	243:UNK	C	244:UNK	N	8.85
1	Ah	87:UNK	C	99:UNK	N	8.83
1	BV	332:UNK	C	342:UNK	N	8.49
1	BW	16:UNK	C	17:UNK	N	8.14
1	BV	365:UNK	C	401:UNK	N	8.01
1	BO	243:UNK	C	245:UNK	N	7.55
1	BY	26:UNK	C	29:UNK	N	7.25
1	BW	113:UNK	C	114:UNK	N	7.22
1	BW	100:UNK	C	101:UNK	N	7.15
1	BW	271:UNK	C	272:UNK	N	6.79
1	BV	302:ASN	C	313:UNK	N	6.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BO	214:UNK	C	220:UNK	N	6.02
1	BW	140:UNK	C	141:UNK	N	5.50
1	BT	29:UNK	C	31:UNK	N	3.69

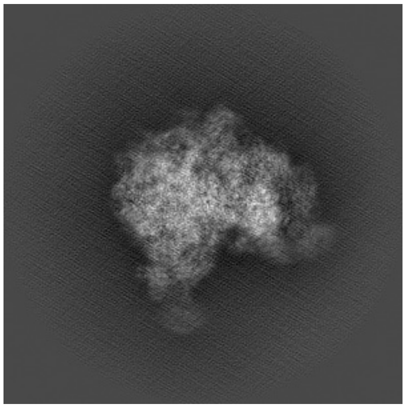
6 Map visualisation ⓘ

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

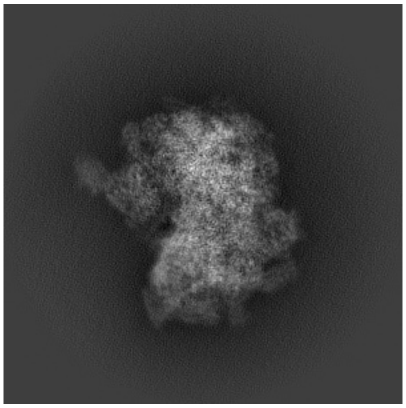
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

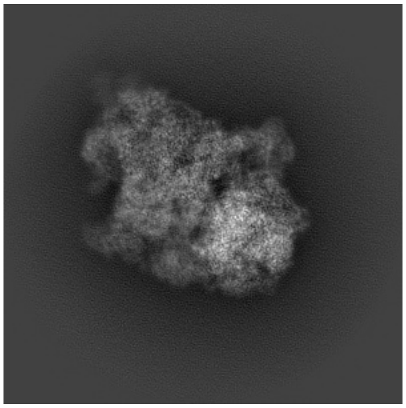
6.1.1 Primary map



X

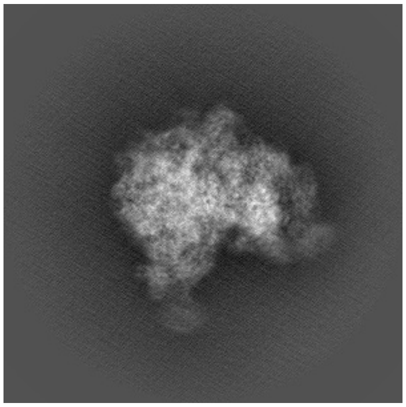


Y

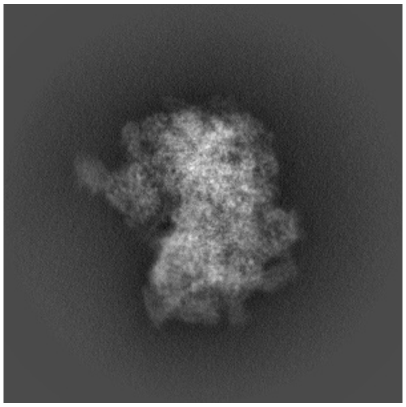


Z

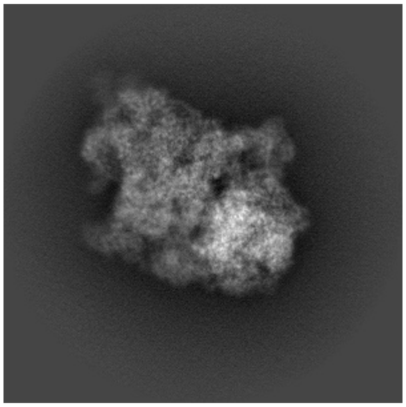
6.1.2 Raw map



X



Y

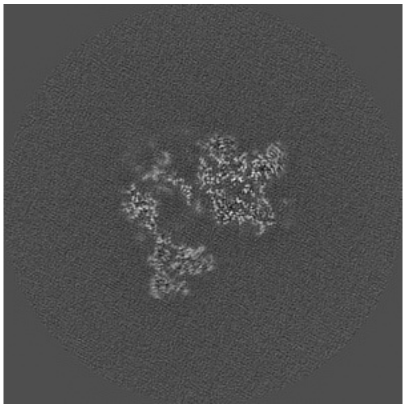


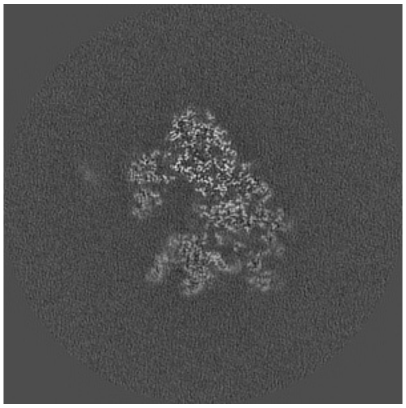
Z

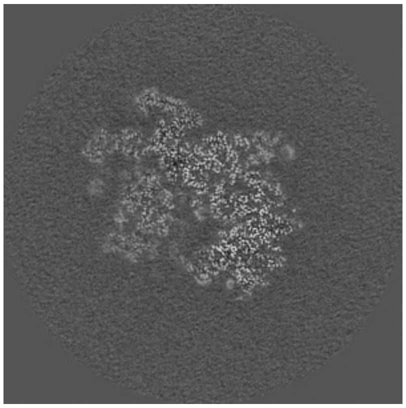
The images above show the map projected in three orthogonal directions.

6.2 Central slices

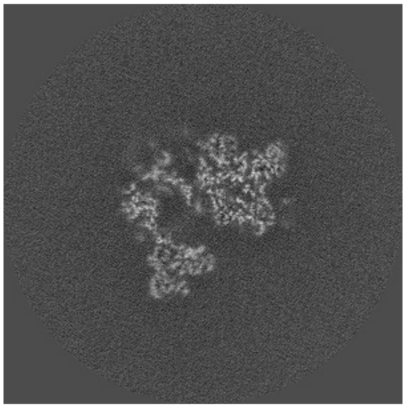
6.2.1 Primary map

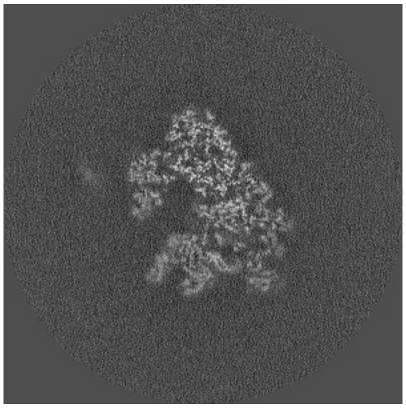

X Index: 275

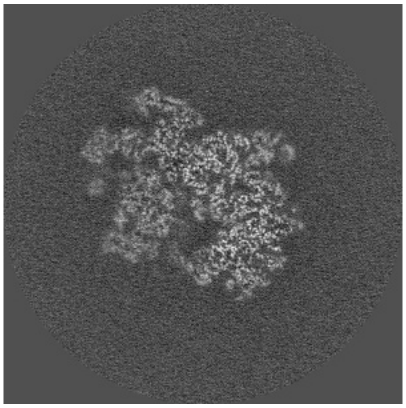

Y Index: 275


Z Index: 275

6.2.2 Raw map


X Index: 275

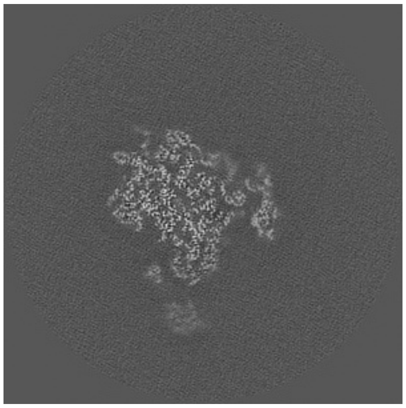

Y Index: 275


Z Index: 275

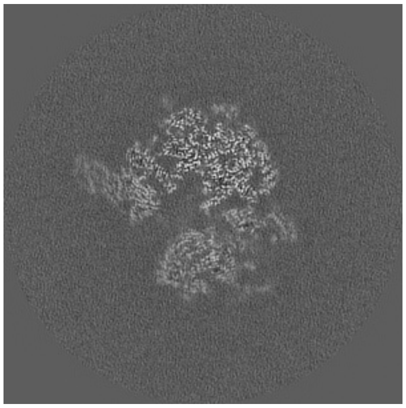
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

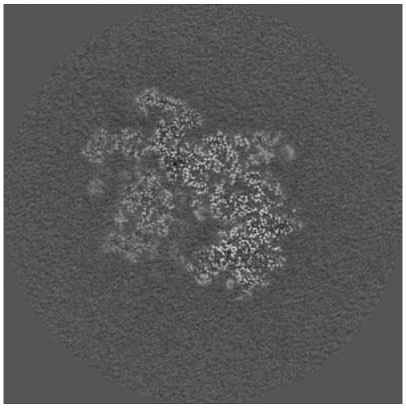
6.3.1 Primary map



X Index: 325

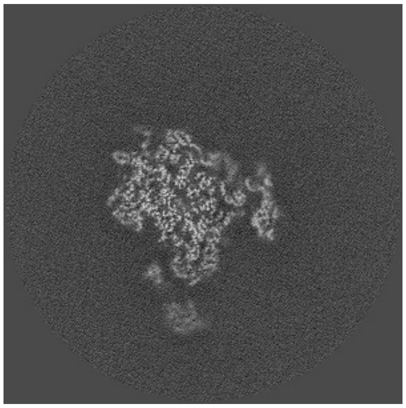


Y Index: 255

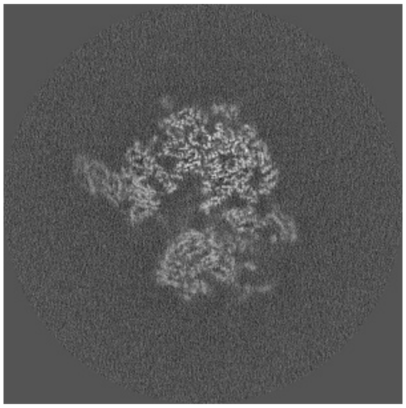


Z Index: 275

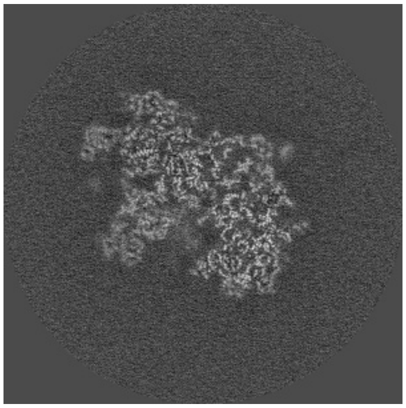
6.3.2 Raw map



X Index: 325



Y Index: 255



Z Index: 285

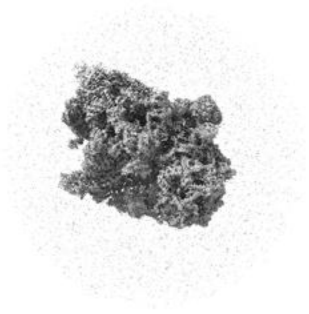
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X

Y



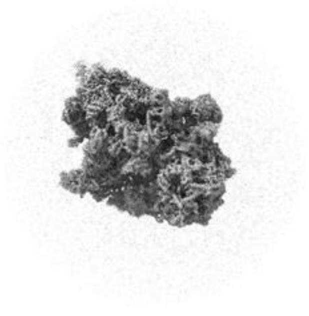
Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X

Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

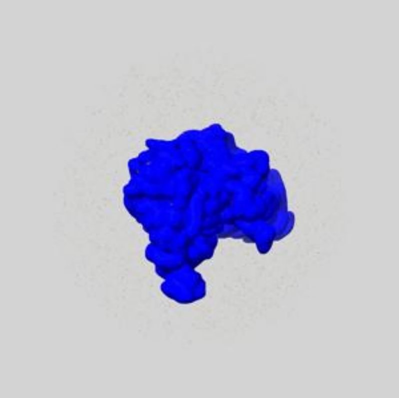
6.5 Mask visualisation

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

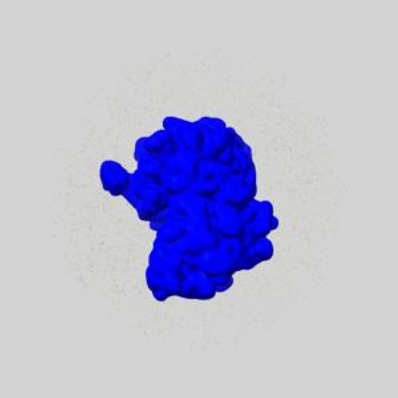
A mask typically either:

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

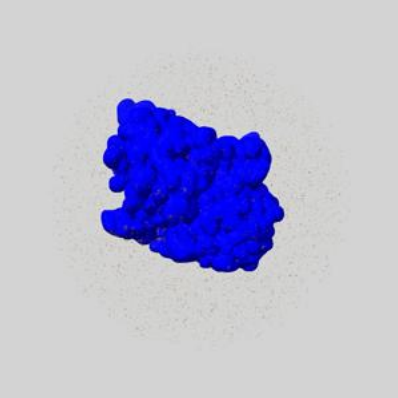
6.5.1 emd_11032_msk_1.map



X



Y

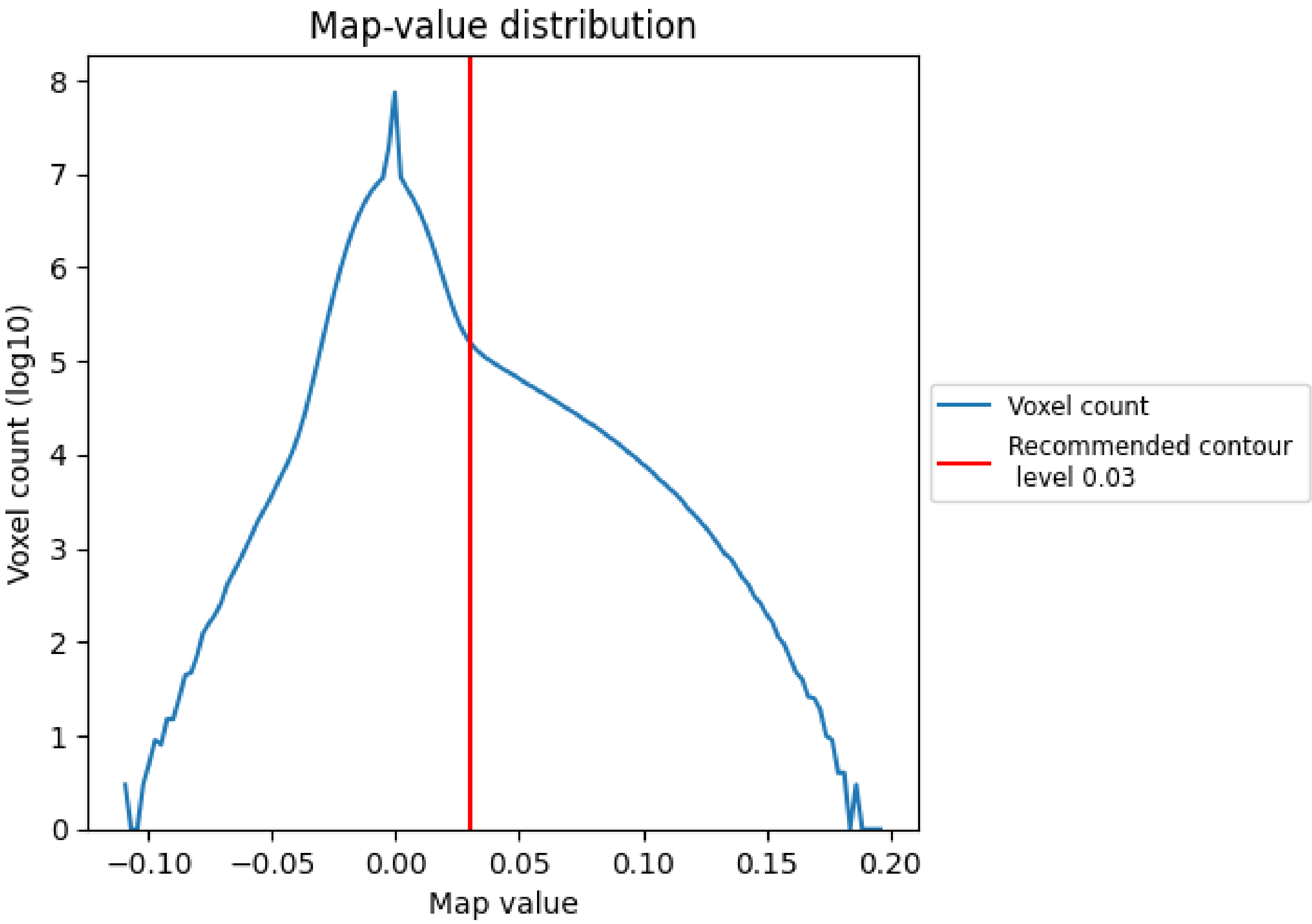


Z

7 Map analysis ⓘ

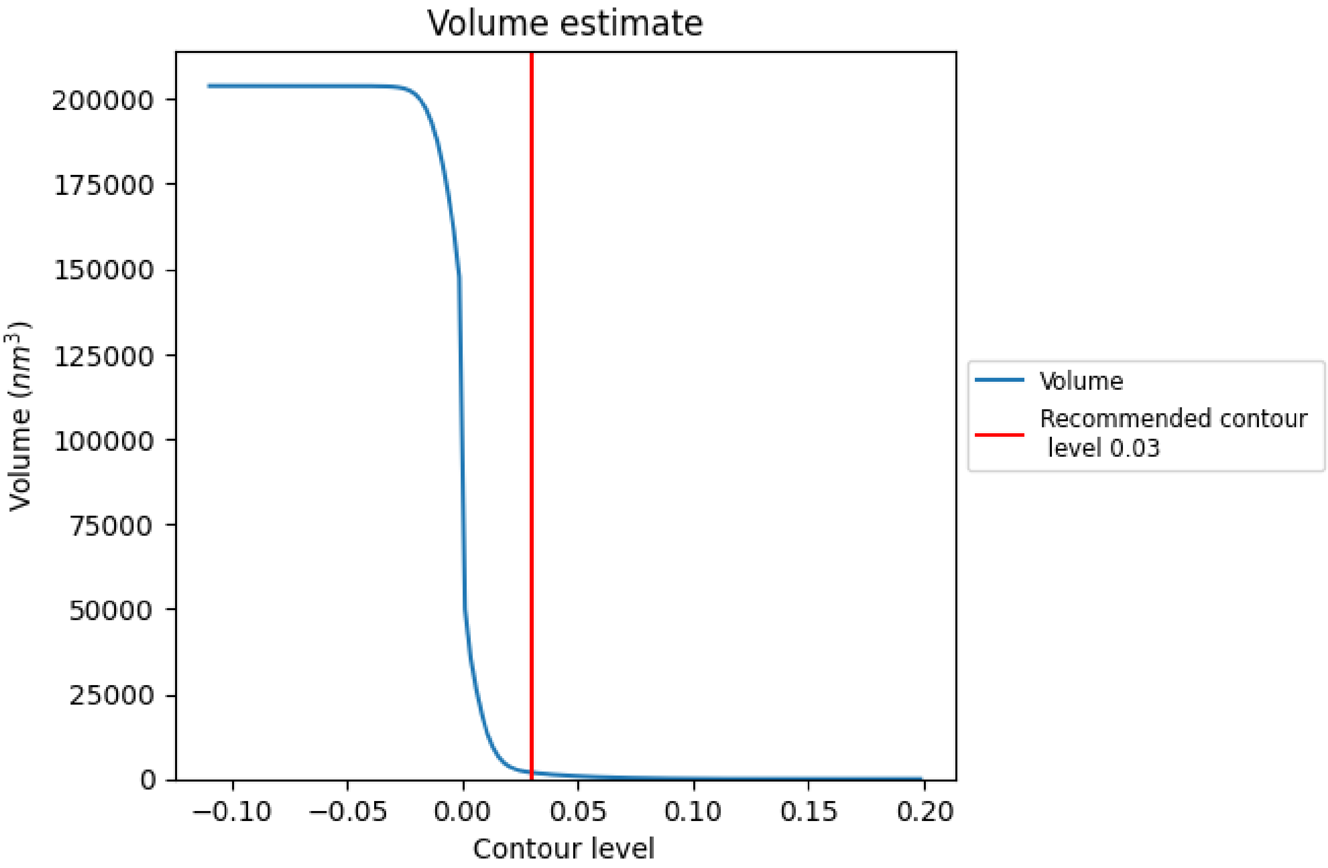
This section contains the results of statistical analysis of the map.

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.

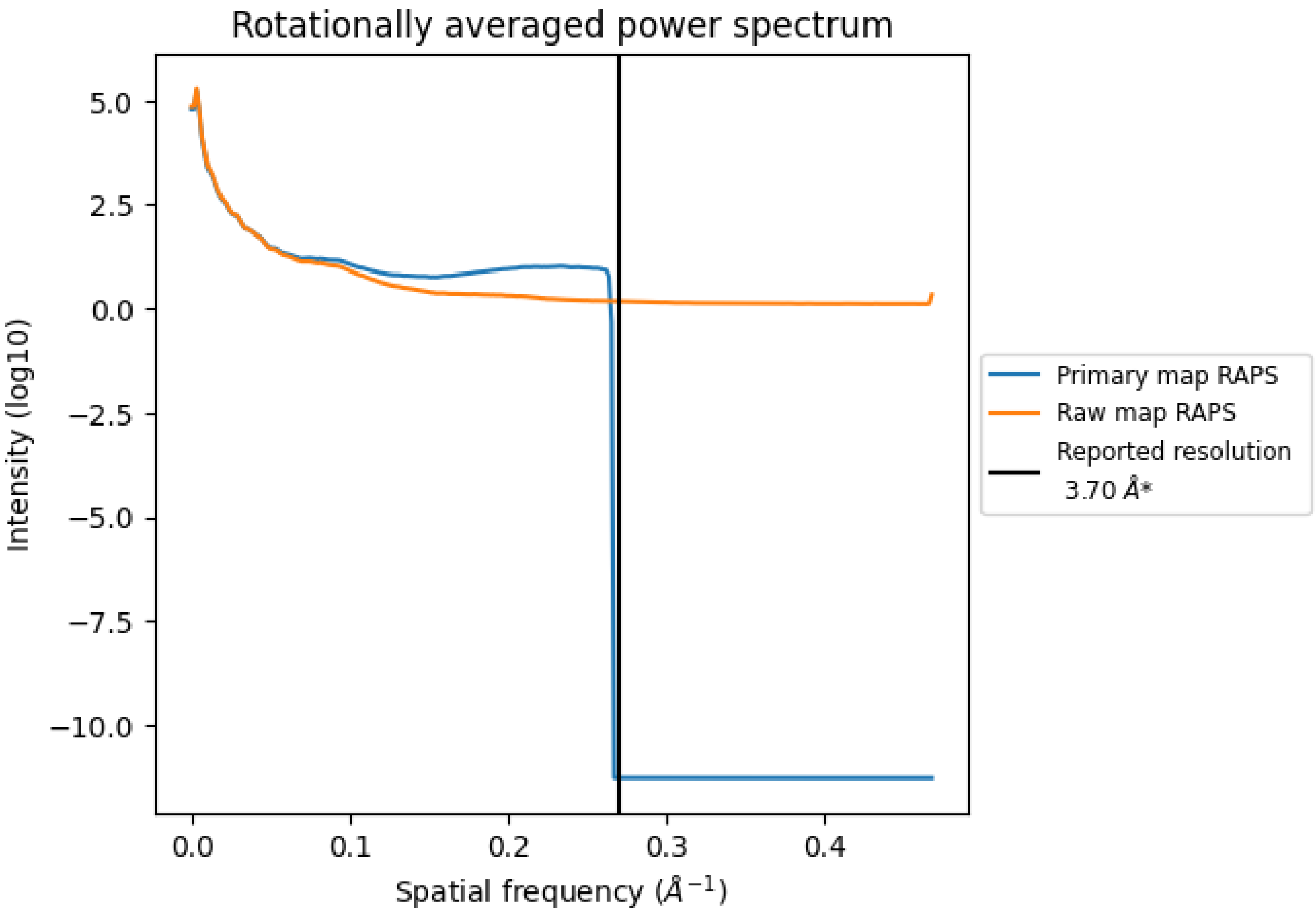
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1885 nm^3; this corresponds to an approximate mass of 1703 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

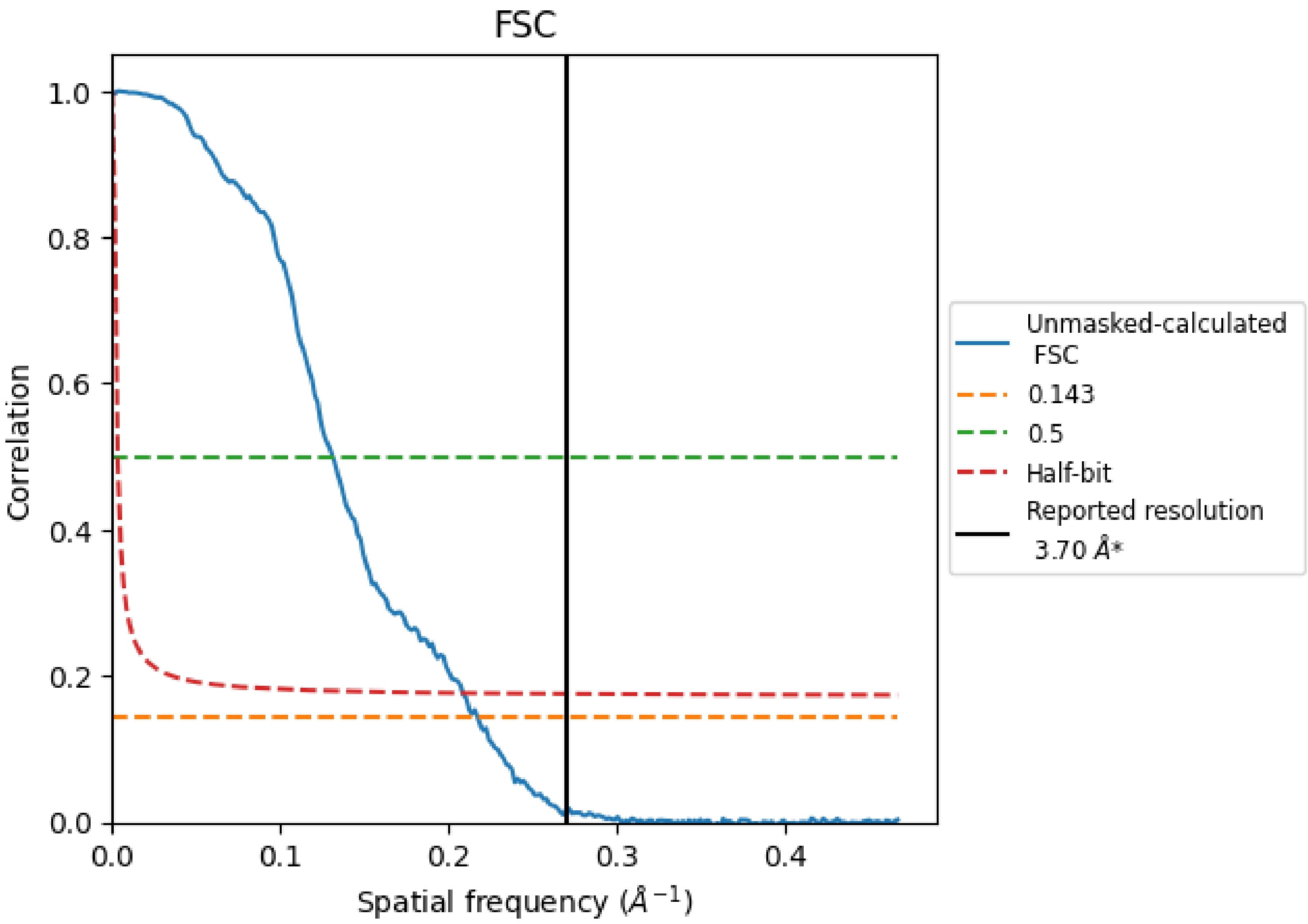


*Reported resolution corresponds to spatial frequency of 0.270 $\AA^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8.2 Resolution estimates ⓘ

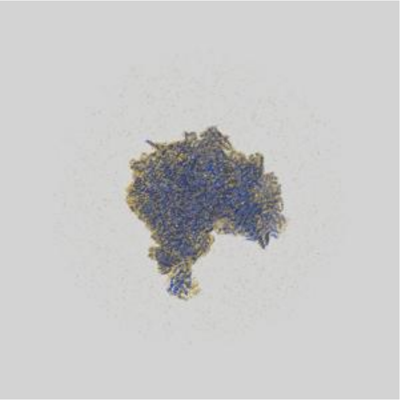
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.60	7.62	4.79

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

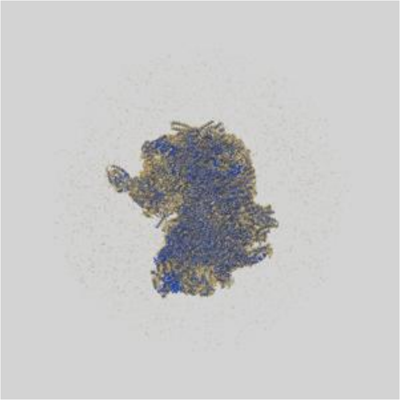
9 Map-model fit

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

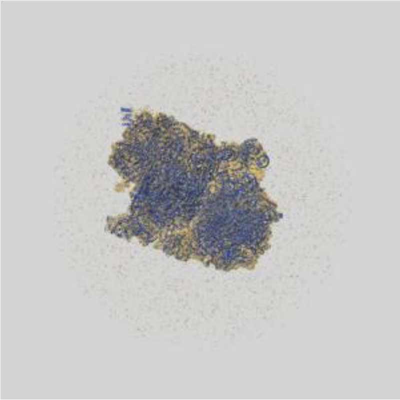
9.1 Map-model overlay



X



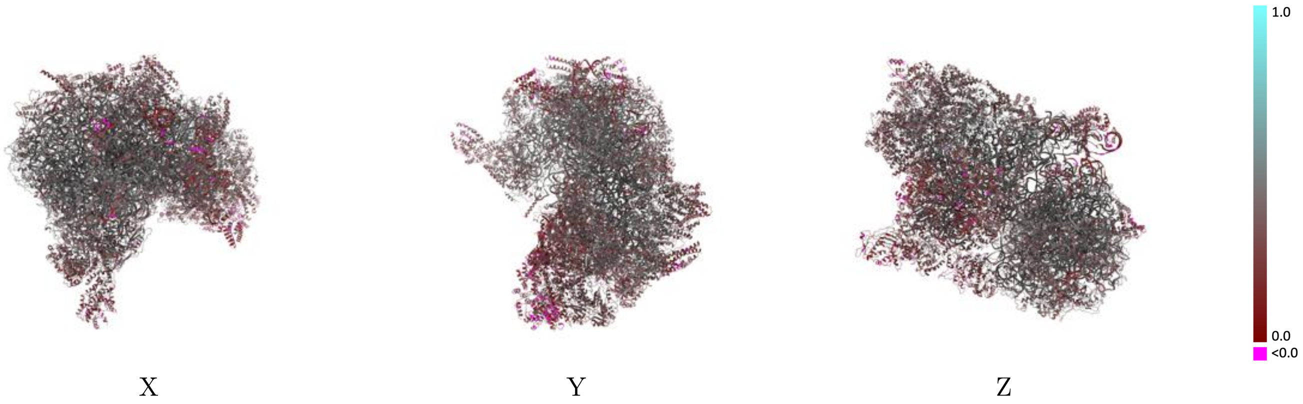
Y



Z

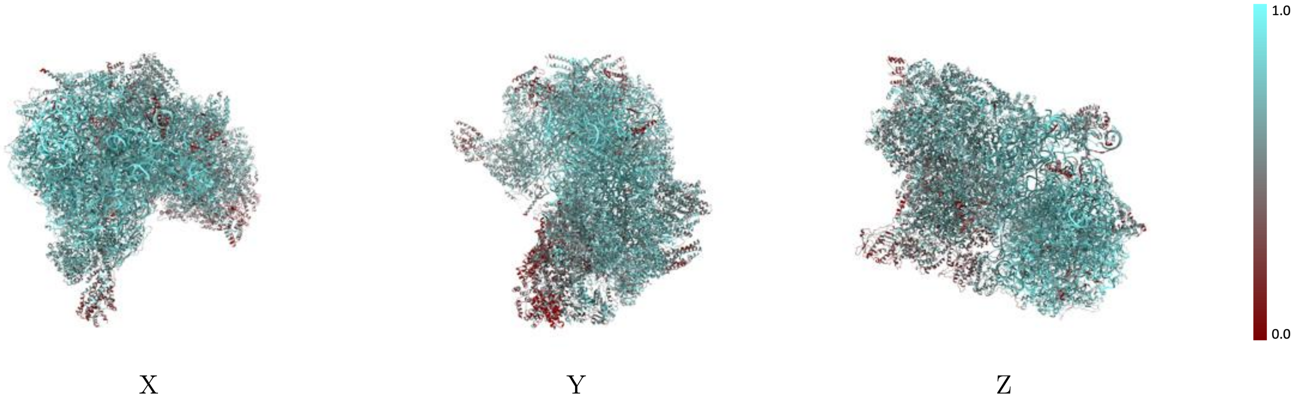
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



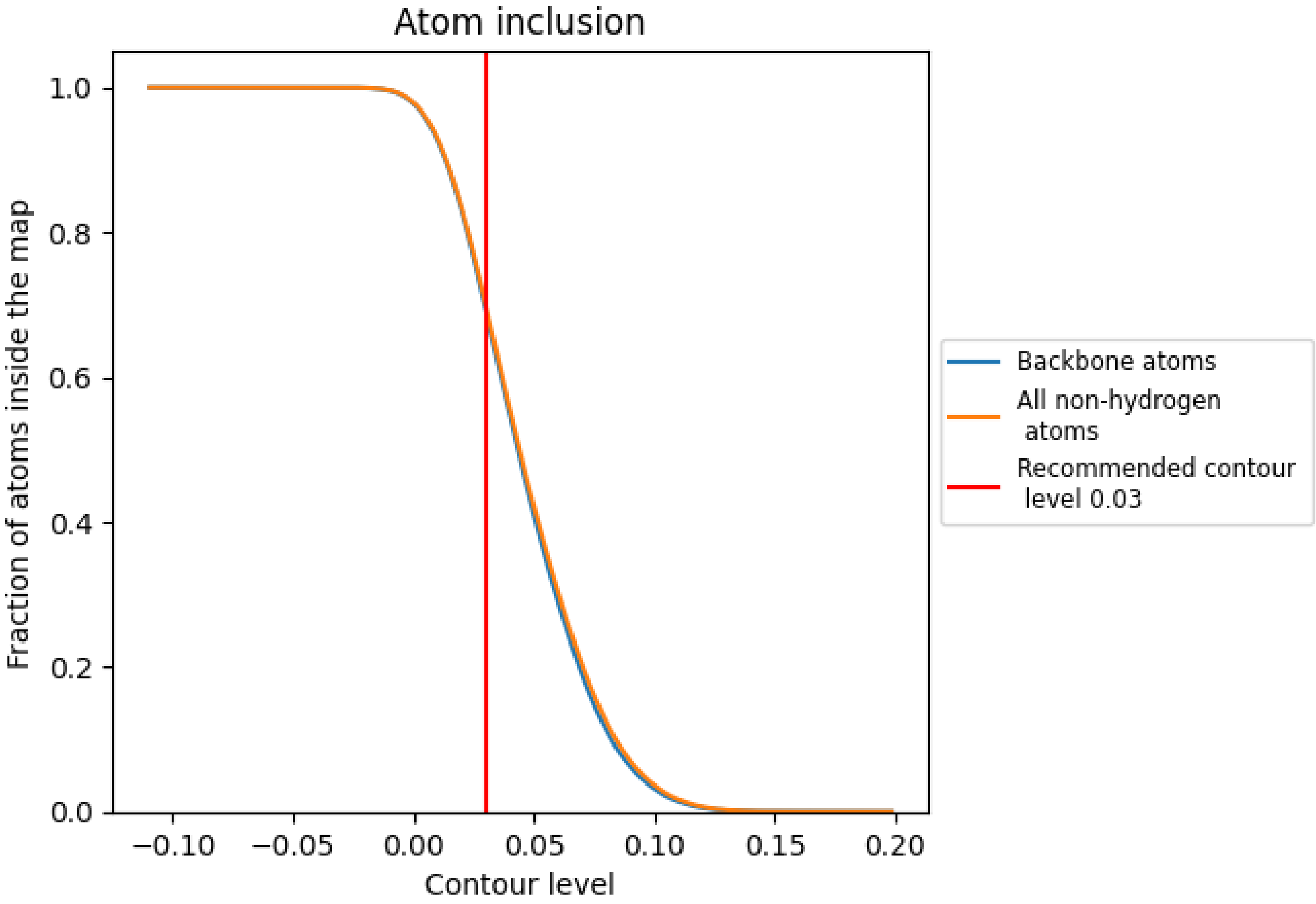
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7010	0.3830
AA	0.7606	0.4440
AB	0.7120	0.4090
AC	0.6715	0.3650
AD	0.9000	0.5190
AE	0.6906	0.4150
AF	0.7748	0.4570
AG	0.7702	0.4630
AH	0.5038	0.2540
AI	0.6988	0.3960
AJ	0.7348	0.4430
AK	0.3641	0.1780
AL	0.7863	0.4570
AM	0.6827	0.3790
AN	0.6474	0.3750
AO	0.7150	0.3930
AP	0.7073	0.3860
AQ	0.7822	0.4570
AR	0.5124	0.2630
AS	0.5915	0.3190
AT	0.5240	0.2980
AU	0.6745	0.3660
AV	0.7623	0.4500
Aa	0.8761	0.4320
Ab	0.8931	0.4460
Ac	0.7561	0.4580
Ad	0.7238	0.4340
Ae	0.7371	0.4290
Af	0.5025	0.2960
Ag	0.7409	0.4160
Ah	0.3774	0.2760
Ai	0.5967	0.2870
Aj	0.3768	0.2440
Ak	0.4289	0.2720
Al	0.6995	0.3830

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Chain	Atom inclusion	Q-score
Am	0.5014	0.3110
An	0.6150	0.3510
Ao	0.7227	0.4260
Ap	0.7455	0.4650
Aq	0.7382	0.4290
Ar	0.7467	0.4510
As	0.6911	0.3850
At	0.7580	0.4460
Au	0.7380	0.4330
Av	0.7536	0.4390
Aw	0.7332	0.4300
Ax	0.6957	0.4060
Ay	0.7381	0.4240
Az	0.6721	0.3820
BA	0.5616	0.3540
BB	0.6231	0.3650
BC	0.8865	0.4930
BD	0.6725	0.3790
BE	0.6721	0.4120
BF	0.7826	0.4430
BG	0.5394	0.3170
BH	0.7143	0.3560
BI	0.6642	0.3950
BJ	0.6599	0.3690
BK	0.7417	0.4310
BL	0.6967	0.4100
BM	0.3524	0.2350
BN	0.7116	0.3860
BO	0.3006	0.2350
BP	0.5723	0.2930
BQ	0.5206	0.2920
BR	0.5924	0.3300
BS	0.3966	0.2270
BT	0.6088	0.3160
BU	0.4715	0.2790
BV	0.5002	0.2710
BW	0.2189	0.2080
BX	0.5665	0.3580
BY	0.5390	0.2720
Ba	0.8742	0.4210
Bb	0.8428	0.4080
Bc	0.6981	0.4420

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Chain	Atom inclusion	Q-score
Bd	0.5334	0.3400
Be	0.6934	0.4220
Bf	0.7072	0.4390
Bg	0.6853	0.4030
Bh	0.4651	0.3010
Bi	0.6010	0.3720
Bj	0.6396	0.3880
Bk	0.5932	0.3520
Bl	0.7120	0.4240
Bm	0.3903	0.2720
Bn	0.6311	0.3780
Bo	0.7266	0.4180
Bp	0.6986	0.4030
Bq	0.5595	0.3700
Br	0.6388	0.3620
Bs	0.5134	0.3060
Bt	0.6913	0.4000
Bu	0.6137	0.3590
Bv	0.5986	0.3290
Bw	0.5103	0.3060
Bx	0.4969	0.3070
By	0.5482	0.3250
Bz	0.6656	0.3690