



## wwPDB EM Validation Summary Report ⓘ

May 14, 2024 – 03:47 am BST

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)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	<b>FAILED</b>
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2



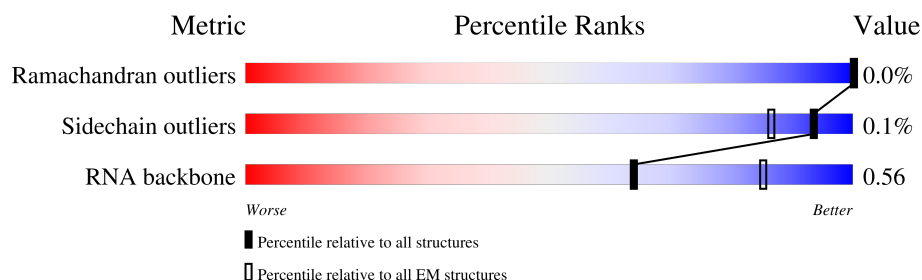
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	Aa	278	76% 23%
2	Ab	2314	77% 19% .
3	Ac	262	100%
4	Ad	439	85% 15%
5	Ae	358	94% 6%
6	Af	68	100%
7	Ag	179	98% .
8	Ah	106	100%
9	Ai	61	100%

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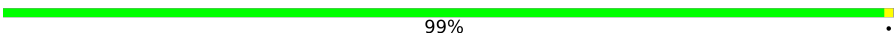

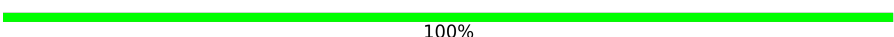






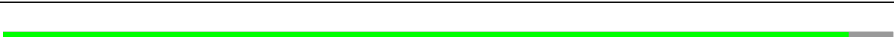


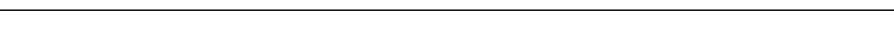
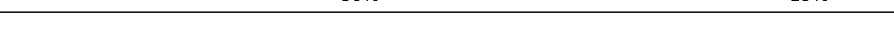
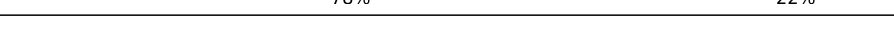

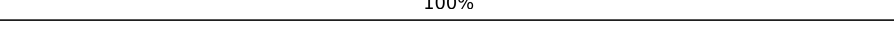
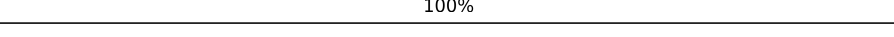
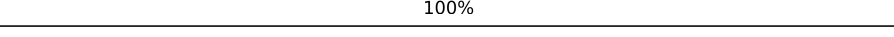
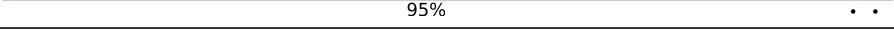
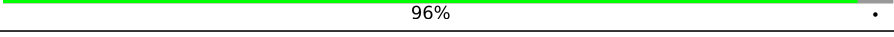
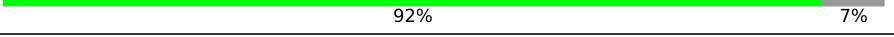

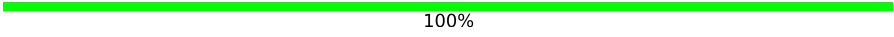
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Mol	Chain	Length	Quality of chain
10	Aj	69	100%
11	Ak	105	100%
12	Al	223	24% 76%
13	Am	166	100%
14	An	158	100%
15	Ao	391	84% 16%
16	Ap	119	99% .
17	Aq	305	90% 10%
18	Ar	143	100%
19	As	237	99%
20	At	242	75% 24%
21	Au	170	99% .
22	Av	235	86% . 12%
23	Aw	364	94% 6%
24	Ax	138	96% .
25	Ay	234	81% 19%
26	Az	321	73% . 26%
27	AA	237	74% 26%
28	AB	289	90% . 9%
29	AC	307	93% 7%
30	AD	36	100%
31	AE	64	89% 11%
32	AF	164	70% 30%
33	AG	93	41% 59%
34	AH	199	89% 11%

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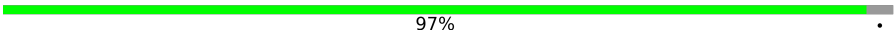

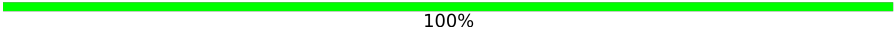

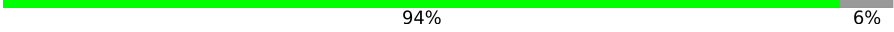
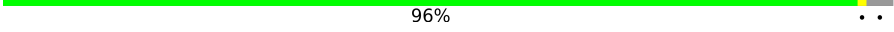
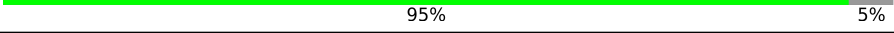

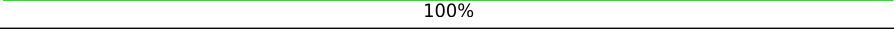
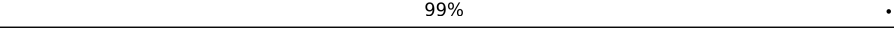
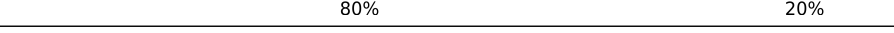
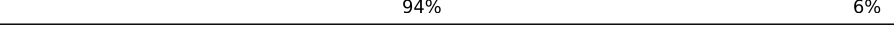
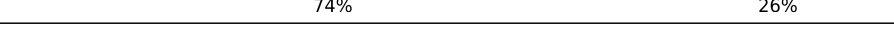


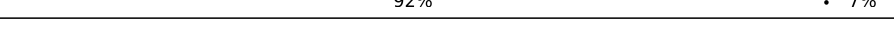
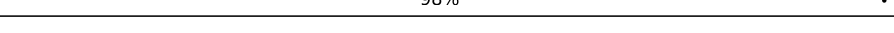
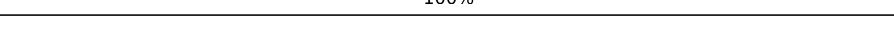







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Mol	Chain	Length	Quality of chain
35	AI	155	
36	AJ	179	
37	AK	309	
38	AL	145	
39	AM	184	
40	AN	158	
41	AO	155	
42	AP	386	
43	AQ	109	
44	AR	348	
45	AS	764	
46	AT	299	
47	AU	499	
48	AV	160	
49	Ba	196	
50	Bb	1395	
51	Bc	159	
52	Bd	330	
53	Be	405	
54	Bf	351	
55	Bg	141	
56	Bh	276	
57	Bi	737	
58	Bj	152	
59	Bk	238	

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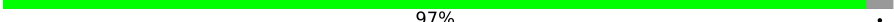

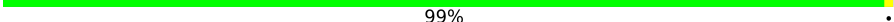

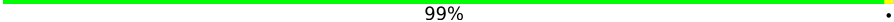

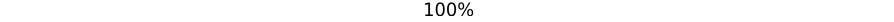

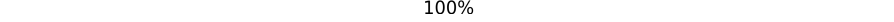
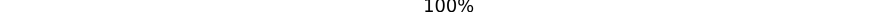

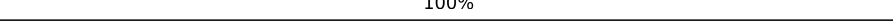
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Mol	Chain	Length	Quality of chain
60	Bl	133	 97%
61	Bm	276	 80% 19%
62	Bn	101	 100%
63	Bo	196	 91% 9%
64	Bp	437	 94% 6%
65	Bq	182	 96% ..
66	Br	549	 95% 5%
67	Bs	98	 89% 11%
68	Bt	102	 100%
69	Bu	567	 99% .
70	Bv	579	 80% 20%
71	Bw	703	 94% 6%
72	Bx	719	 74% 26%
73	By	132	 81% 19%
74	Bz	147	 83% . 16%
75	BA	149	 92% . 7%
76	BB	112	 98% .
77	BC	37	 100%
78	BD	130	 82% 18%
79	BE	464	 96% .
80	BF	23	 100%
81	BG	182	 90% . 10%
82	BH	63	 100%
83	BI	1451	 97% .
84	BJ	1539	 98% .

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Mol	Chain	Length	Quality of chain
85	BK	267	 100%
86	BL	310	 58% 42%
87	BM	355	 80% 20%
88	BN	283	 97% .
89	BO	142	 100%
90	BP	100	 99% .
91	BQ	1032	 60% 40%
92	BR	143	 99% .
93	BS	1086	 40% 60%
94	BT	297	 100%
95	BU	439	 70% 30%
96	BV	310	 100%
97	BW	285	 100%
98	BX	151	 88% 12%
99	BY	327	 100%



## 2 Entry composition

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

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

- Molecule 1 is a RNA chain called LSU rRNA\_1.

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

- Molecule 2 is a RNA chain called LSU rRNA\_2.

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

- Molecule 3 is a protein called Ribosomal protein L2.

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

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

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

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

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

- Molecule 6 is a protein called Ymf69.

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



- Molecule 7 is a protein called Ymf60.

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

- Molecule 8 is a protein called bL7/L12m.

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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



- Molecule 13 is a protein called Ymf74.

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

There are 9 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- Molecule 16 is a protein called Ribosomal protein L14.

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

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

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

- Molecule 18 is a protein called Ribosomal protein L16.



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

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

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

- Molecule 20 is a protein called bL19m.

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

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

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

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

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

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

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

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

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

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



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

- Molecule 26 is a protein called bL25m.

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

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

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

- Molecule 28 is a protein called Ribosomal protein L28.

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

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

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

- Molecule 30 is a protein called bL32m.

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

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

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

- Molecule 32 is a protein called bL35m.



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

- Molecule 33 is a protein called Ribosomal protein.

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

- Molecule 34 is a protein called mL40.

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

- Molecule 35 is a protein called Ribosomal protein L27.

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

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

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

- Molecule 37 is a protein called mL46.

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

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

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

- Molecule 39 is a protein called mL53.



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

- Molecule 40 is a protein called mL54.

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

- Molecule 41 is a protein called mL64.

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

- Molecule 42 is a protein called mL101.

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

- Molecule 43 is a protein called mL102.

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

- Molecule 44 is a protein called mL103.

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

- Molecule 45 is a protein called mL104.

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

There is a discrepancy between the modelled and reference sequences:



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

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

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

- Molecule 47 is a protein called mL106.

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

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

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

- Molecule 49 is a RNA chain called SSU rRNA\_1.

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

There are 11 discrepancies between the modelled and reference sequences:

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

- Molecule 50 is a RNA chain called SSU rRNA\_2.



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

- Molecule 51 is a protein called Ymf73.

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

- Molecule 52 is a protein called Ymf64.

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

- Molecule 53 is a protein called Ymf76.

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

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

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

- Molecule 55 is a protein called Ribosomal protein S6.

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

- Molecule 56 is a protein called Ymf63.

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

- Molecule 57 is a protein called Ribosomal protein S9.



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

- Molecule 58 is a protein called Ymf59.

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

- Molecule 59 is a protein called Ymf61.

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

- Molecule 60 is a protein called Ribosomal protein S12.

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

- Molecule 61 is a protein called Ribosomal protein S13.

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

- Molecule 62 is a protein called Ribosomal protein S14.

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

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

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

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



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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 66 is a protein called Ribosomal protein S18.

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

- Molecule 67 is a protein called Ribosomal protein S19.

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

- Molecule 68 is a protein called bS21m.

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

- Molecule 69 is a protein called mS23.

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

- Molecule 70 is a protein called mS26.



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

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

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

- Molecule 72 is a protein called mS31.

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

- Molecule 73 is a protein called mS33.

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

- Molecule 74 is a protein called mS34.

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

- Molecule 75 is a protein called Ribosomal subunit protein.

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

- Molecule 76 is a protein called mS37.

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

- Molecule 77 is a protein called mS38.



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

- Molecule 78 is a protein called IGR motif protein.

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

- Molecule 79 is a protein called mS45.

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

- Molecule 80 is a protein called mS75.

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

- Molecule 81 is a protein called mS76.

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

- Molecule 82 is a protein called mS77.

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

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

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

- Molecule 84 is a protein called mS78.



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

- Molecule 85 is a protein called mS79.

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

- Molecule 86 is a protein called SelR domain protein.

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

- Molecule 87 is a protein called mS81.

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

- Molecule 88 is a protein called mS82.

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

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

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

- Molecule 90 is a protein called mS84,mS84.

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

- Molecule 91 is a protein called mS85.



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

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

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

- Molecule 93 is a protein called mS87.

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

- Molecule 94 is a protein called mS88.

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

- Molecule 95 is a protein called mS89.

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

- Molecule 96 is a protein called mS90.

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

- Molecule 97 is a protein called mS91.

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

- Molecule 98 is a protein called Ribosomal protein S3.



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

- Molecule 99 is a protein called mS93.

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

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

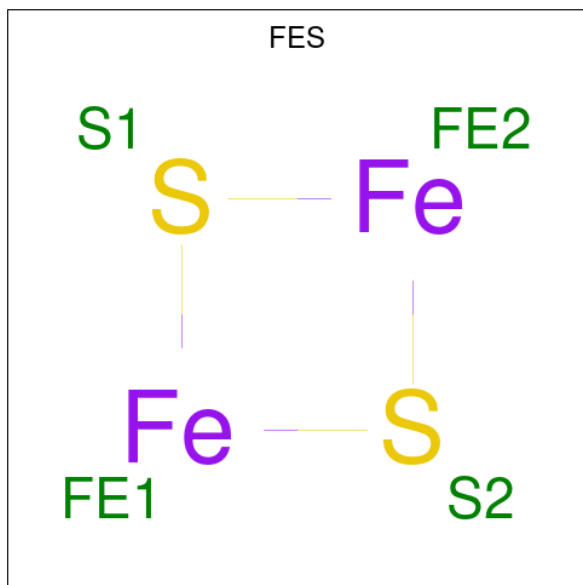
Mol	Chain	Residues	Atoms		AltConf
100	Aa	28	Total	Mg	0
			28	28	
100	Ab	270	Total	Mg	0
			270	270	
100	Ad	1	Total	Mg	0
			1	1	
100	Ae	1	Total	Mg	0
			1	1	
100	Aq	1	Total	Mg	0
			1	1	
100	AB	1	Total	Mg	0
			1	1	
100	AF	1	Total	Mg	0
			1	1	
100	AQ	1	Total	Mg	0
			1	1	
100	Ba	10	Total	Mg	0
			10	10	
100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

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



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

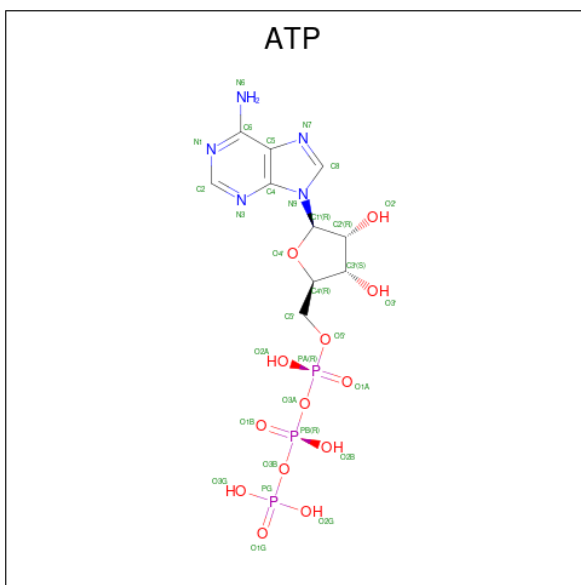
- Molecule 102 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

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





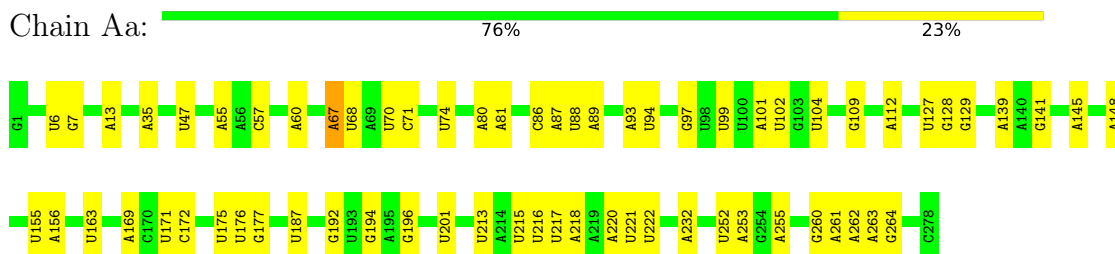
Mol	Chain	Residues	Atoms						AltConf
103	Bw	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	



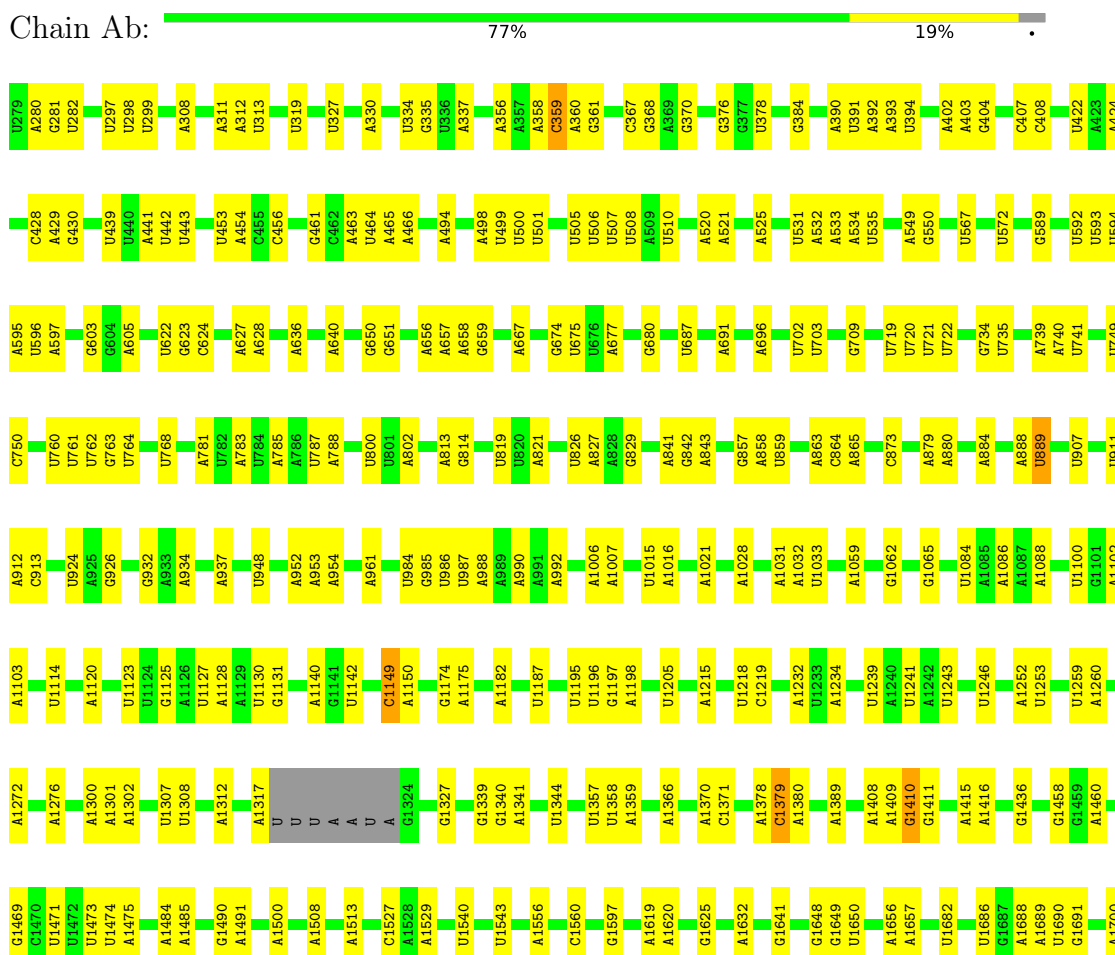
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

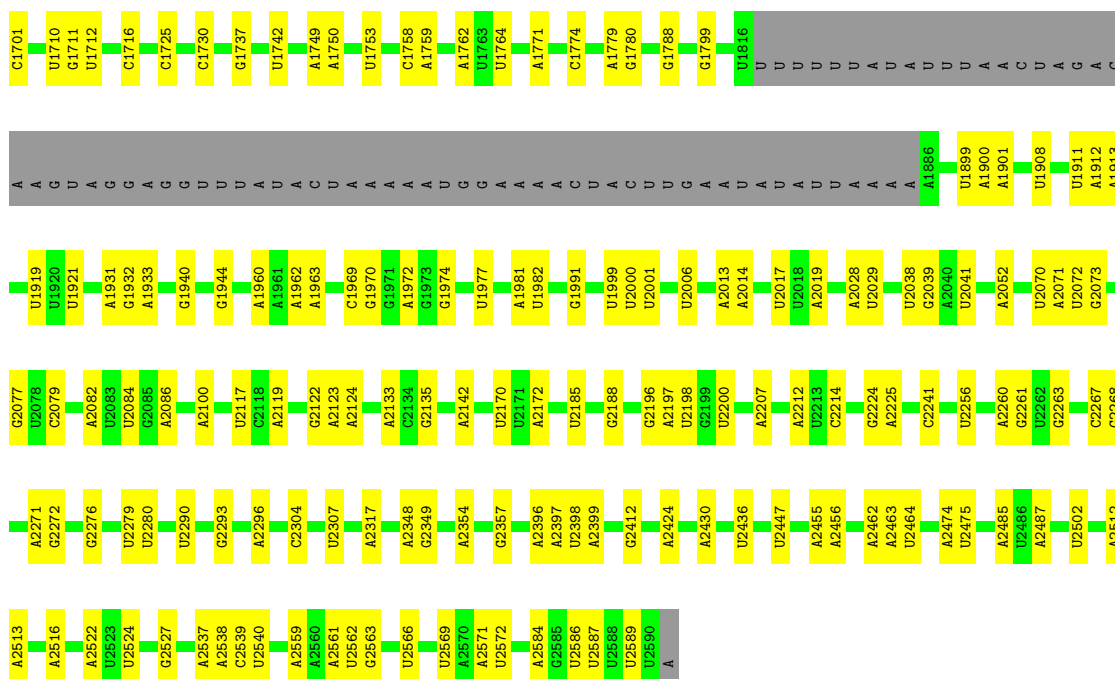
#### • Molecule 1: LSU rRNA\_1



#### • Molecule 2: LSU rRNA\_2







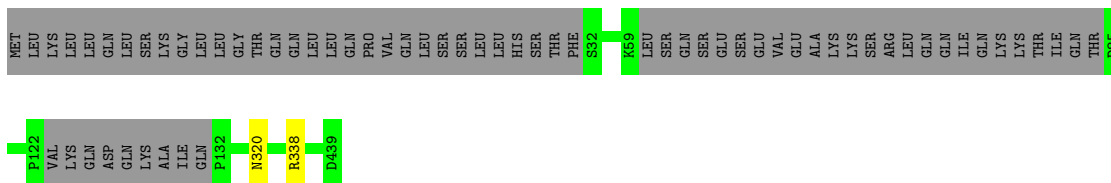
- Molecule 3: Ribosomal protein L2

Chain Ac:  100%



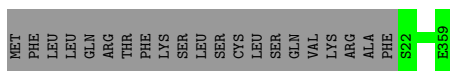
- Molecule 4: 50S ribosomal protein L3

Chain Ad: 



- Molecule 5: 50S ribosomal protein L4

Chain Ae:  94% 6%



- Molecule 6: Ymf69

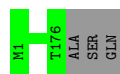
Chain Af:  100%

There are no outlier residues recorded for this chain.



- Molecule 7: Ymf60

Chain Ag:  98%



- Molecule 8: bL7/L12m

Chain Ah:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: bL7/12m

Chain Ai:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: bL7/12m

Chain Aj:  100%

There are no outlier residues recorded for this chain.

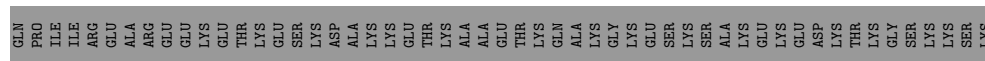
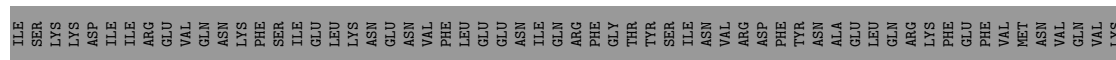
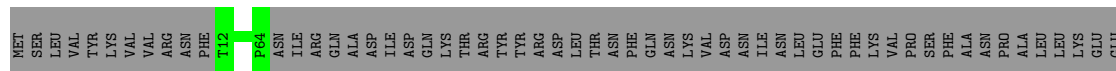
- Molecule 11: Ribosomal protein L7/L12 carboxy-terminal domain protein

Chain Ak:  100%

There are no outlier residues recorded for this chain.

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

Chain Al:  24%  76%



- Molecule 13: Ymf74

Chain Am:  100%

There are no outlier residues recorded for this chain.


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

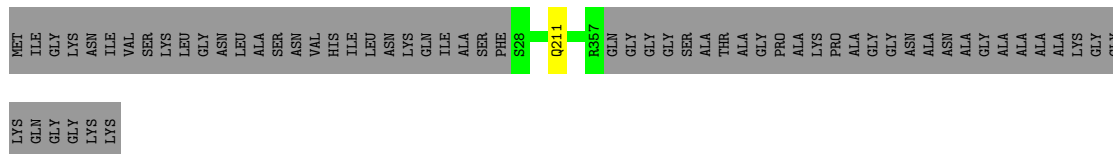
Chain An:  100%



There are no outlier residues recorded for this chain.

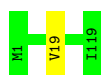
- Molecule 15: 50S ribosomal protein L13

Chain Ao:  84% 16%



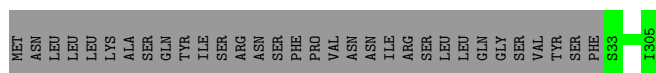
- Molecule 16: Ribosomal protein L14

Chain Ap:  99%



- Molecule 17: Ribosomal protein L15, putative

Chain Aq:  90% 10%



- Molecule 18: Ribosomal protein L16

Chain Ar:  100%

There are no outlier residues recorded for this chain.

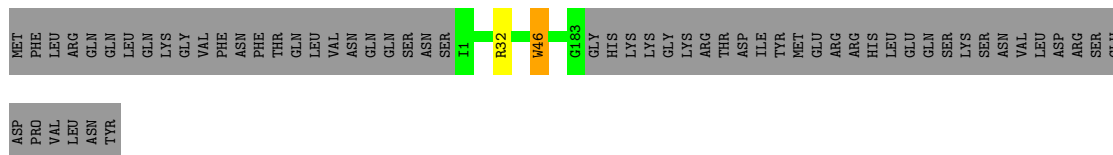
- Molecule 19: 50S ribosomal protein L17

Chain As:  99%



- Molecule 20: bL19m

Chain At:  75% 24%



- Molecule 21: 50S ribosomal protein L20

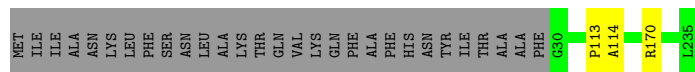


Chain Au:  99%



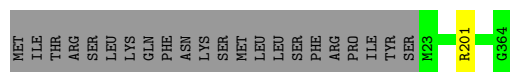
- Molecule 22: 50S ribosomal protein L21

Chain Av:  86% 12%



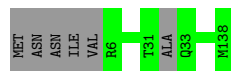
- Molecule 23: Ribosomal protein L22/L17e

Chain Aw:  94% 6%




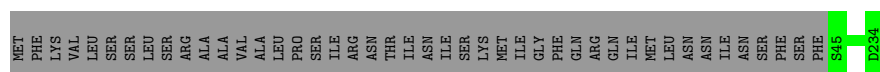
- Molecule 24: Ribosomal protein L23, putative

Chain Ax:  96%



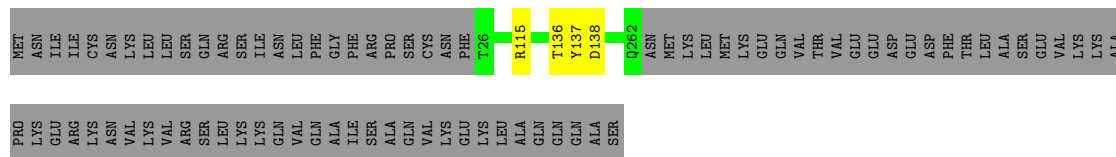
- Molecule 25: 50S ribosomal protein L24

Chain Ay:  81% 19%




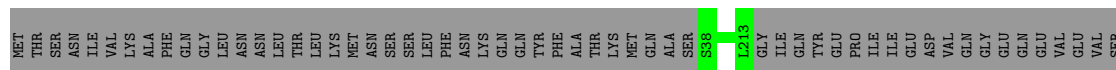
- Molecule 26: bL25m

Chain Az:  73% 26%



- Molecule 27: 50S ribosomal protein L27

Chain AA:  74% 26%





GLN  
GLN  
SER  
LYS

- Molecule 28: Ribosomal protein L28

Chain AB:  90% 9%

MET PHE SER LEU ILE LYS VAL ALA PRO VAL LEU GLY ASN PHE ILE GLN ARG ASN PHE S23 P182 I183 V184 Q286 ASN VAL LYS

- Molecule 29: 39-S ribosomal protein L47

Chain AC:  93% 7%

MET ASN PHE LEU PHE ARG GLN THR PHE ASN SER ILE LYS THR SER PHE GLN ALA THR ARG S21 T304 GLY LYS ILE

- Molecule 30: bL32m

Chain AD:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L33

Chain AE:  89% 11%

MET ALA K6 N62 ARG GLN SER LYS

- Molecule 32: bL35m

Chain AF:  70% 30%

MET PHE LEU LEU LYS VAL GLY VAL ALA LEU CYS ASN THR ILE ASN VAL VAL LYS GLN PRO LEU GLN GLN SER VAL MET GLN LYS MET ILE GLN SER SER PHE ASP PHE ASN SER LEU ILE PHE MET PRO TYR GLN THR PHE A50 H164

- Molecule 33: Ribosomal protein

Chain AG:  41% 59%

MH G38 PHE CYS SER THR GLN GLU MET GLN GLY GLU GLN GLN ILE ILE ILE GLN ASN ASN GLU CYS LEU ASN GLN MET VAL MET MET ASP GLN ILE TYR ILE ILE MET SER LYS ILE GLN ASN ASP CYS MET MET THR TYR SER ILE SER ASP LEU TYR ASN ILE ILE GLN


- Molecule 34: mL40

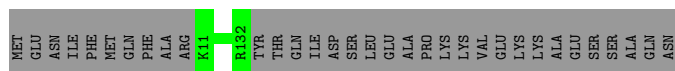
Chain AH:  89% 11%

MET SER GLN PHE LEU ALA LYS VAL ARG ASP SER LEU THR GLN LEU CYS SER GLN THR ARG V23 D198



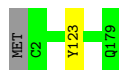
- Molecule 35: Ribosomal protein L27

Chain AI:  79% 21%




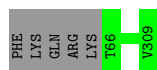
- Molecule 36: Ribosomal protein L51/S25/CI-B8 domain protein

Chain AJ:  99% ..



- Molecule 37: mL46

Chain AK:  79% 21%



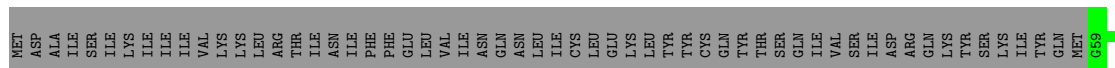
- Molecule 38: Large subunit ribosomal protein

Chain AL:  100%

There are no outlier residues recorded for this chain.

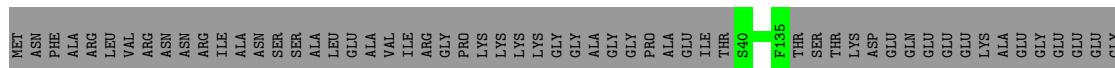
- Molecule 39: mL53

Chain AM:  68% 32%




- Molecule 40: mL54


Chain AN:  61% 39%



- Molecule 41: mL64

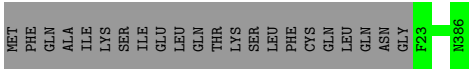


Chain AO:  77% 23%

 MET PHE GLN ALA ILE ARG THR LYS GLU ILE ALA ARG GLU GLU LYS THR GLY LYS SER GLN SER GLN SER VAL VAL SER LEU GLN ASP LYS LYS ARG GLY PHE GLY ALA LYS VAL LYS LYS

- Molecule 42: mL101

Chain AP:  94% 6%

 MET PHE GLN ALA ILE SER ILE THR GLN PHE LEU THR PHE SER ILE PHE CYS GLN LEU GLN ASN GLY F23 N366


- Molecule 43: mL102

Chain AQ:  46% 54%

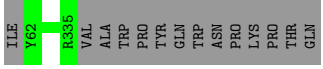
 MET ASN ALA LEU ILE PHE ARG ASN THR PHE LEU PHE ASN TRP ILE SER GLN SER SER SER MET PHE GLN LEU GLN GLU ASP THR GLN LYS LYS LEU ASN GLU LEU GLN GLY ALA PHE ASP PHE T90

 L109

- Molecule 44: mL103

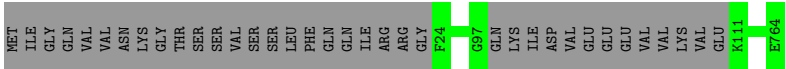
Chain AR:  79% 21%

 MET LEU LEU SER GLN SER ILE GLN LYS VAL ALA ASN ALA PHE LYS GLN ILE SER ARG GLN TYR LYS ALA ILE SER CYS PHE ILE SER SER SER ASP LYS ASN ASP ASP GLY SER ASN ASN GLN ALA GLU GLY ASP SER SER LYS LYS ASN ASN GLU LYS LYS GLN THR THR ASN ASP PHE ASP

 ILE Y62 R335 VAL TRP PRO TYR GLN TRP ASN PRO LYS PRO THR GLN

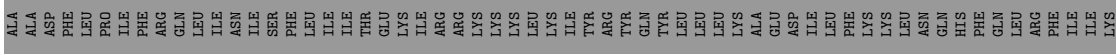
- Molecule 45: mL104

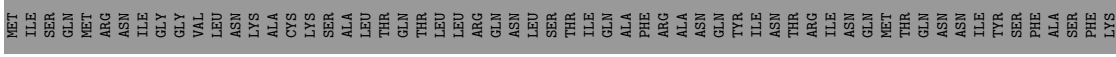
Chain AS:  95% 5%

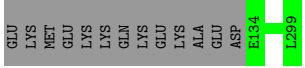
 MET ILE GLY GLN VAL VAL ASN LYS THR SER SER VAL SER SER PHE GLN ILE ARG GLU ILE GLN ARG GLY F24 G97 GLN LYS LYS ILE ASP VAL GLU GLU VAL VAL VAL LYS VAL GLU K111 E764

- Molecule 46: Signal peptide-binding domain protein

Chain AT:  56% 44%

 ALA ALA ASP PHE LEU PRO ILE PHE ARG GLN LEU ILE ASN ILE SER PHE LEU ILE ILE THR GLU THR LYS ILE ARG LYS LYS LYS LYS ILE TYR ARG TYR GLN VAL VAL VAL LEU LEU LYS LEU LEU ASP ASP ILE LEU PHE LYS LYS LYS THR MET MET GLN ASN ASN HIS PHE ILE TYR SER PHE ARG PHE ILE ILE LYS

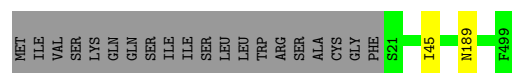
 MET ILE SER GLN MET ARG ASN ILE GLY GLY VAL LEU ASN LYS ALA CYS LYS SER ILE ALA LEU THR THR LEU ARG LYS ASN GLN ARG TYR PHE ALA ARG ALA ASN TYR ILE ASN THR ARG ILE ASN GLN MET THR GLN ASN ASN ASN TYR SER PHE ALA SER PHE ILE LYS

 GLU LYS MET GLU LYS LYS GLN LYS GLU ALA ASP E134 L299




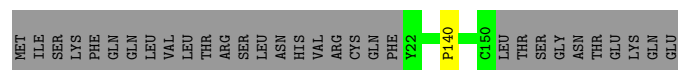
- Molecule 47: mL106

Chain AU:  96%




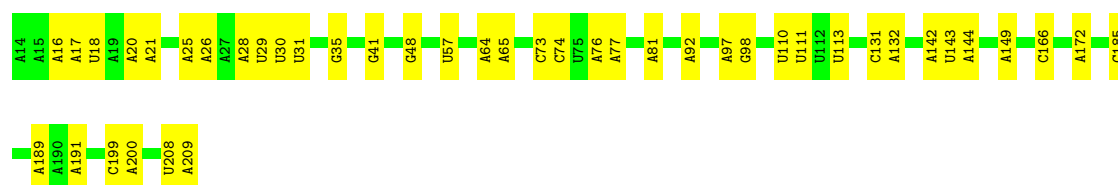
- Molecule 48: Iron-binding zinc finger CDGSH type protein

Chain AV:  80%




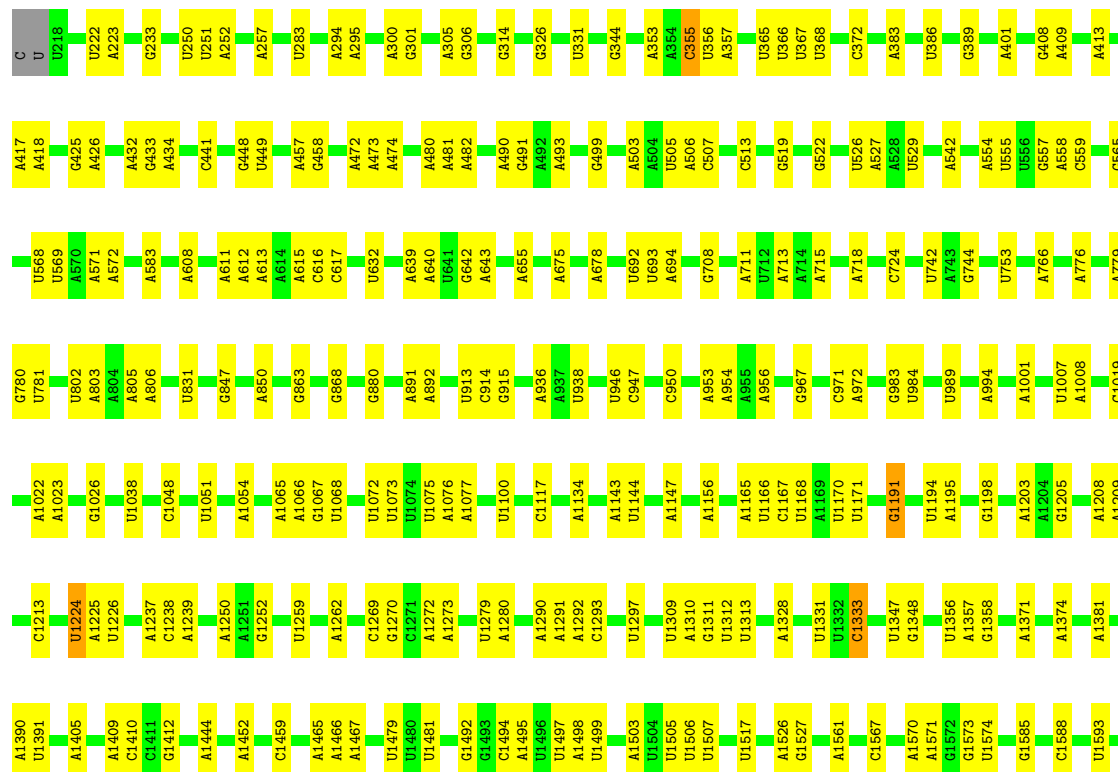
- Molecule 49: SSU rRNA\_1

Chain Ba:  78%



- Molecule 50: SSU rRNA\_2

Chain Bb:  81%







• Molecule 51: Ymf73

Chain Bc:  100%

There are no outlier residues recorded for this chain.

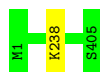
• Molecule 52: Ymf64

Chain Bd:  100%

There are no outlier residues recorded for this chain.

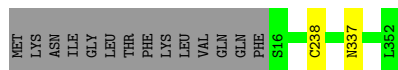
• Molecule 53: Ymf76

Chain Be:  100%



• Molecule 54: 30S ribosomal protein S5

Chain Bf:  95%



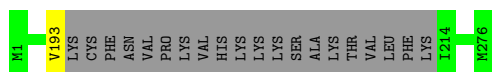
• Molecule 55: Ribosomal protein S6

Chain Bg:  96%




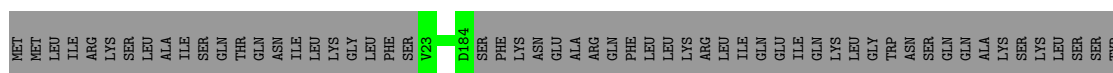
• Molecule 56: Ymf63

Chain Bh:  92% 7%

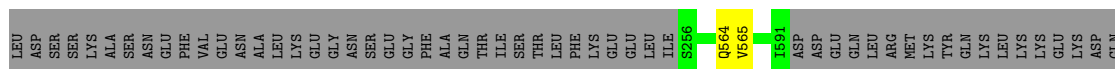


• Molecule 57: Ribosomal protein S9

Chain Bi:  85% 15%







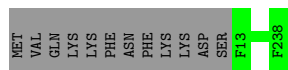
- Molecule 58: Ymf59

Chain Bj: 100%

There are no outlier residues recorded for this chain.

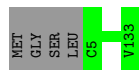
- Molecule 59: Ymf61

Chain Bk: 95% 5%



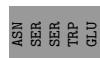
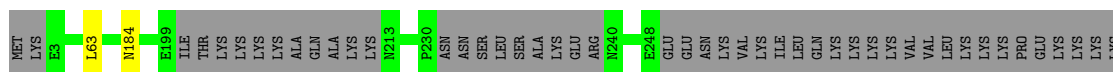
- Molecule 60: Ribosomal protein S12

Chain Bl: 97% 0%



- Molecule 61: Ribosomal protein S13

Chain Bm: 80% 19%



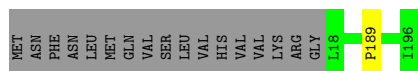
- Molecule 62: Ribosomal protein S14

Chain Bn: 100%

There are no outlier residues recorded for this chain.

- Molecule 63: 30S ribosomal protein S15

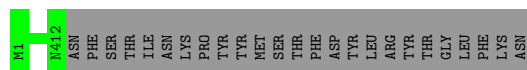
Chain Bo: 91% 9%



- Molecule 64: 30S ribosomal protein S16

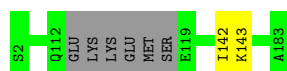


Chain Bp:  94% 6%



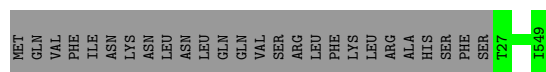
- Molecule 65: 30S ribosomal protein S17

Chain Bq:  96% ..




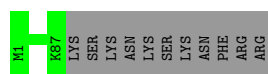
- Molecule 66: Ribosomal protein S18

Chain Br:  95% 5%



- Molecule 67: Ribosomal protein S19

Chain Bs:  89% 11%



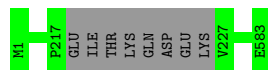
- Molecule 68: bS21m

Chain Bt:  100%


There are no outlier residues recorded for this chain.

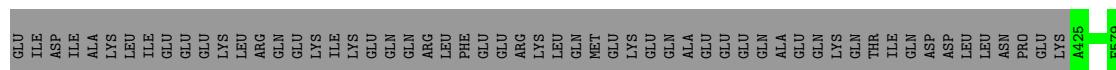
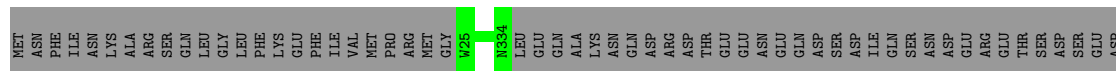
- Molecule 69: mS23

Chain Bu:  99% .



- Molecule 70: mS26

Chain Bv:  80% 20%



- Molecule 71: Ribosomal death-associated protein



MET	LYS	ILE	GLY	PHE	ILE	GLU	THR	ILE	LYS	ARG	VAL	GLY	LYS	ASN	LEU	GLY	ALA	THR	LYS	GLU	E22	I38	ASP	ASP	ASP	SER	SER	THR	HIS	LYS	ARG	M49	I110	ASP	ASP	TYR	LYS	LYS	GLN	GLU	ASP	SER	MET	ARG	H121	I366	N545	M703
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MET	LYS	ILE	LYS	ILE	VAL	TYR	GLY	ASN	LEU	PHE	ARG	VAL	ILE	ASN	GLU	GLN	LEU	LYS	SER	LYS	LYS	ARG	VAL	LYS	LYS	GLU	GLU	LEU	ILE	TYR	ILE	SER	SER	LYS	CYS	CYS	ASP	MET	ILE	LYS	ALA	LEU	LYS	SER	VAL	GLN	ARG	GLN	VAL	VAL	PHE	VAL	GLN	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	LYS	PHE	CYS	SER	VAL	PRO	ASN	GLN	ASN	GLN	GLY	GLY	SER	THR	ASN	GLU	GLN	GLN	GLN	ALA	ALA	ALA	ALA	ALA	ALA	THR	THR	THR	THR	ALA	ALA	ALA	GLN	GLN	GLN	PRO	ALA	ALA	LEU	ASN	ASN	ASN	LYS	ASP	GLN	LYS	LYS	LYS	THR	GLN	ASN
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HIS	GLU	GLN	LYS	ASP	GLN	LYS	GLN	HIS	ASN	GLN	SER	SER	ILE	TYR	GLY	GLY	ASN	SER	GLU	GLU	ILE	LYS	LYS	SER	VAL	VAL	ASN	ASP	PHE	SER	SER	THR	TYR	LYS	LEU	LEU	SER	ASP	LYS	LYS	ILE	LYS	ALA	GLY	ASN	LYS	GLN	THR	PHE
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ALA	K182	D387	GLN	GLU	LYS	GLU	ASP	ASP	GLN	GLU	E396	H719
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MET	P2	K108	ILE	GLY	LYS	LYS	LYS	GLY	GLY	GLY	LYS	VAL	THR	LEU	MET	ASP	VAL	PHE	GLU	THR	LYS	ALA	ASP	GLU	ASP	PHE
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MET	ALA	GLN	LYS	GLU	LYS	ALA	ALA	A10	N60	X132	HIS	VAL	GLN	LYS	SER	GLY	GLN	GLU	SER	GLU	ASN	GLU	ALA	GLU
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MET ILE SER THR ASN ILE SER LYS PHE PHE PHE S12 K74 P149


MET  
ALA  
P3  
Q112

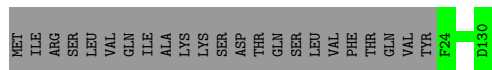
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



There are no outlier residues recorded for this chain.

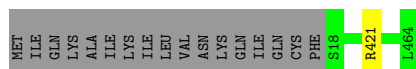
- Molecule 78: IGR motif protein

Chain BD:  82% 18%



- Molecule 79: mS45

Chain BE:  96%



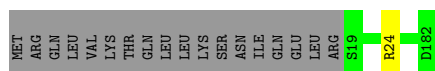
- Molecule 80: mS75

Chain BF:  100%

There are no outlier residues recorded for this chain.

- Molecule 81: mS76

Chain BG:  90% 10%



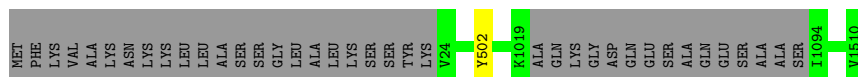
- Molecule 82: mS77

Chain BH:  100%

There are no outlier residues recorded for this chain.

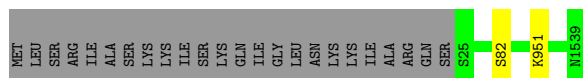
- Molecule 83: Enoyl-CoA hydratase/isomerase

Chain BI:  97%



- Molecule 84: mS78

Chain BJ:  98%



- Molecule 85: mS79



There are no outlier residues recorded for this chain.

- Chain BL:  58% 42%



- Molecule 88: mS82

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

There are no outlier residues recorded for this chain.

- Molecule 90: mS84,mS84

- Molecule 91: mS85

Chain BQ: 



[illegible]

- Molecule 92: Iron donor protein CyaY

Chain BR:  99%

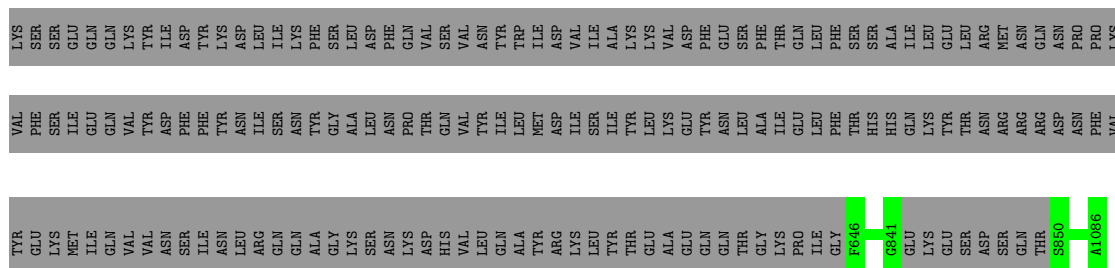
Diagram showing three vertical bars labeled M1, R96, and V143. M1 and V143 are green, and R96 is yellow.

- Molecule 93: mS87

Chain BS:  40% 60%

ASN	PHE	ASN	LEU	ARG	SER	GLN	MET
LYS	LEU	VAL	MET	PRO	ASP	GLN	ILE
Gly	SER	SER	LYS	GLN	GLN	GLN	ARG
PHE	GLU	PHE	ILE	ARG	GLN	PRO	SER
ASN	VAL	ASN	LYS	GLN	GLN	LEU	ILE
GLN	ASN	Tyr	SER	ARG	GLY	ASN	LEU
LEU	MET	TYR	TYR	GLU	GLY	ASN	LYS
GLY	PHE	LYS	GLU	ASN	PHE	GLY	VAL
LYS	THR	ASN	GLN	GLN	ARG	LYS	LYS
ASN	ASN	SER	ASN	ASN	ASN	ASN	GLY
THR	SER	SER	GLY	ASP	SER	GLN	ASN
GLU	GLN	SER	ASN	GLN	SER	LYS	LEU
PHE	ASP	LYS	PRO	ALA	SER	GLN	THR
ASN	ALA	PHE	SER	SER	ASN	PHE	LYS
LYS	ASN	ASN	GLU	GLU	GLN	ASP	GLY
VAL	SER	ASP	GLN	GLN	GLN	GLN	ASN
GLN	LEU	VAL	GLU	SER	ASN	LYS	SER
PHE	VAL	ASN	MET	GLU	SER	ARG	PHE
GLU	THR	GLU	ARG	GLY	THR	ASN	ASN
ILE	SER	PHE	MET	GLN	GLY	PHE	ALA
ILE	SER	PHE	ILE	TYR	THR	ASN	LYS
ASN	PHE	LEU	ILE	GLN	THR	ASN	LEU
THR	ASN	ILE	GLU	GLN	SER	ASN	GLN
LYS	ASN	HIS	CYS	LYS	SER	GLN	ASN
LYS	ILE	PHE	TYR	SER	SER	GLN	ILE
ILE	ASP	ALA	ASN	SER	ASN	GLY	PRO
PHE	LEU	GLN	SER	THR	GLN	ALA	VAL
ASN	SER	THR	CYS	SER	ARG	ASN	ARG
ASN	SER	LYS	GLY	SER	ASN	ALA	CYS
LEU	LEU	GLN	LEU	TYR	GLN	ASP	PHE
LEU	LEU	LEU	TYR	GLY	PRO	ARG	SER
ASN	SER	LYS	ASP	LYS	ASN	ASN	SER
LEU	LEU	ILE	LYS	GLU	LYS	ALA	SER
LYS	PHE	ILE	THR	GLY	GLU	ASP	THR
GLN	GLY	TYR	ILE	MET	VAL	LYS	GLY
TYR	ASN	LYS	ALA	PHE	LEU	GLN	GLU
GLU	ALA	ASP	THR	LEU	SER	LYS	GLY
ILE	ASP	ASP	PHE	ASN	PHE	LYS	ASN
CYS	THR	ILE	GLN	GLN	ASN	ASN	GLU
ARG	GLN	GLN	THR	LEU	LEU	PHE	GLY
GLU	GLN	ASN	TYR	PHE	LYS	THR	ASP
ILE	TYR	ASN	LYS	TYR	LYS	ALA	ALA
VAL	ILE	ILE	ASP	SER	PHE	PHE	PRO
GLU	GLN	SER	ASN	GLU	GLU	LYS	LYS
ALA	ALA	ARG	PHE	ASN	ASP	GLN	ASN
LEU	SER	VAL	VAL	ASN	GLN	GLN	GLN
SER	LYS	CYS	LYS	LYS	SER	SER	GLN
ARG	THR	ILE	GLY	THR	ASN	ASN	GLU
GLY	LEU	ASP	LYS	GLU	ARG	ASN	GLN
ASN	ALA	PRO	LYS	LYS	ASP	GLN	GLN
LEU	THR	TYR	GLY	GLN	SER	GLN	GLN
LEU	LEU	LEU	VAL	GLN	SER	TYR	GLN
HIS	MET	ASN	SER	GLY	ASN	ARG	LYS
ASN	ASN	LEU	LEU	ALA	GLN	LYS	ASP
HIS	LEU	SER	ASN	ASN	GLN	ARG	GLN
SER	THR	SER	GLN	ASN	ASP	GLU	GLN
PHE	ILE	ARG	THR	HIS	ASN	ASP	PRO
THR	HIS	ILE	ILE	GLN	LYS	GLY	GLN
THR	HIS	THR	THR	GLN	GLN	GLN	GLN





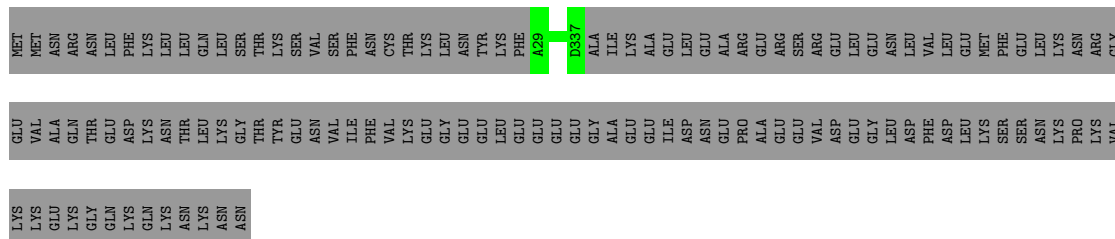
- Molecule 94: mS88

Chain BT:  100%

There are no outlier residues recorded for this chain.

- Molecule 95: mS89

Chain BU: 



- Molecule 96: mS90

Chain BV:  100%

There are no outlier residues recorded for this chain.

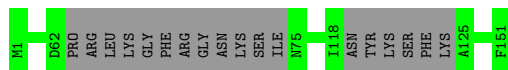
- Molecule 97: mS91

Chain BW:  100%

There are no outlier residues recorded for this chain.

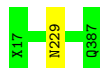
- Molecule 98: Ribosomal protein S3

Chain BX: 



- Molecule 99: mS93

Chain BY:  100%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	99300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	92000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

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

## 5.2 Too-close contacts

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	22381/27039 (83%)	21256 (95%)	1118 (5%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ac	235/235 (100%)	235 (100%)	0	100	100
4	Ad	330/391 (84%)	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
79	BE	421	ARG
81	BG	24	ARG
99	BY	229	ASN
92	BR	96	ARG
61	Bm	184	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
88	BN	168	ASN
91	BQ	433	ASN
53	Be	210	ASN
52	Bd	167	ASN
92	BR	50	GLN

### 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



5 of 810 RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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	$\# Z  > 2$
103	ATP	Bw	801	100	26,33,33	0.98	2 (7%)	31,52,52	1.72	7 (22%)
102	FES	AV	202	48	0,4,4	-	-	-		
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
103	ATP	Bw	801	100	-	5/18/38/38	0/3/3/3
102	FES	AV	201	48	-	-	0/1/1/1

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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

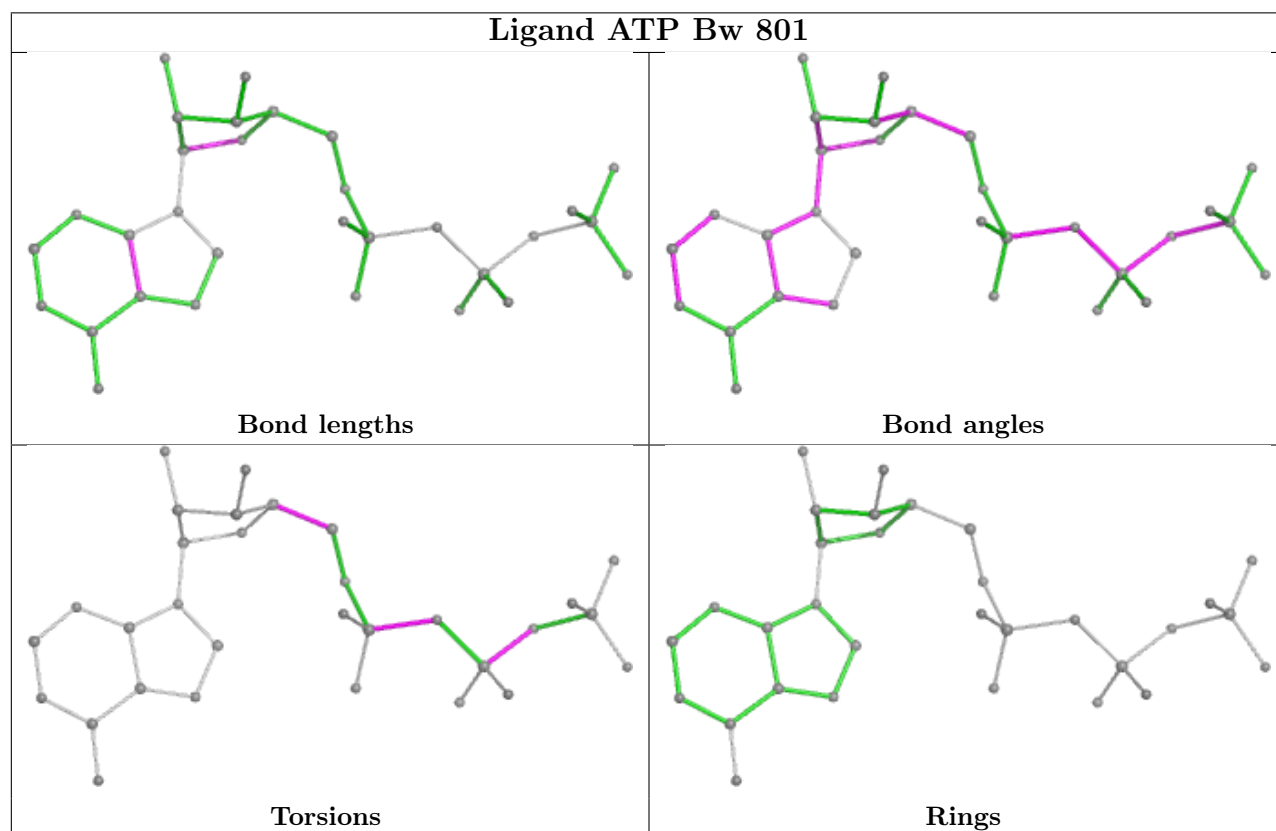
There are no ring outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.



The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
97	BW	18
89	BO	8
99	BY	4
96	BV	4
69	Bu	2
10	Aj	1
8	Ah	1
94	BT	1

The worst 5 of 39 chain breaks are listed below:



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



## 6 Map visualisation

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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

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

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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



## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



## 8 Fourier-Shell correlation

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



## 9 Map-model fit

This section was not generated.