Full wwPDB EM Validation Report (i)

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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

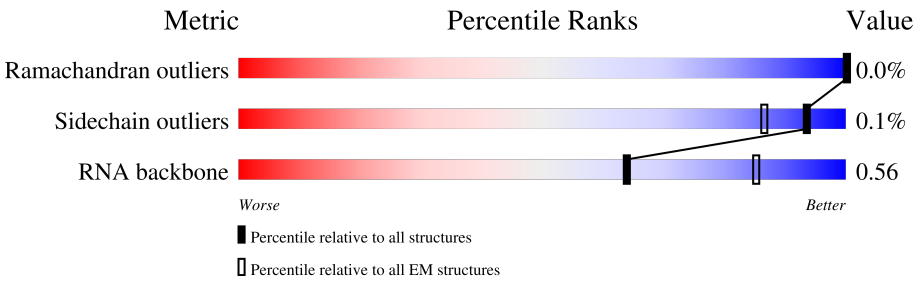
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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%

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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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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Mol	Chain	Length	Quality of chain
35	AI	155	79% 21%
36	AJ	179	99%
37	AK	309	79% 21%
38	AL	145	100%
39	AM	184	68% 32%
40	AN	158	61% 39%
41	AO	155	77% 23%
42	AP	386	94% 6%
43	AQ	109	46% 54%
44	AR	348	79% 21%
45	AS	764	95% 5%
46	AT	299	56% 44%
47	AU	499	96%
48	AV	160	80% 19%
49	Ba	196	78% 22%
50	Bb	1395	81% 18%
51	Bc	159	100%
52	Bd	330	100%
53	Be	405	100%
54	Bf	351	95%
55	Bg	141	96%
56	Bh	276	92% 7%
57	Bi	737	85% 15%
58	Bj	152	100%
59	Bk	238	95% 5%

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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 (i)

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
			Total	C	H	N	O	S		
7	Ag	176	3072	997	1555	265	253	2	0	0

- Molecule 8 is a protein called bL7/L12m.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	Ak	105	1705	564	831	151	158	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
			Total	C	H	N	O	S		
12	Al	53	869	278	439	79	72	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
			Total	C	H	N	O	S		
39	AM	126	2085	673	1026	185	198	3	0	0

- Molecule 40 is a protein called mL54.

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

- Molecule 41 is a protein called mL64.

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

- Molecule 42 is a protein called mL101.

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

- Molecule 43 is a protein called mL102.

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

- Molecule 44 is a protein called mL103.

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

- Molecule 45 is a protein called mL104.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	AS	728	12114	3916	6045	1028	1105	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
			Total	C	H	N	O		
77	BC	37	226	111	41	37	37	0	0

- Molecule 78 is a protein called IGR motif protein.

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

- Molecule 79 is a protein called mS45.

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

- Molecule 80 is a protein called mS75.

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

- Molecule 81 is a protein called mS76.

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

- Molecule 82 is a protein called mS77.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
83	BI	1413	23519	7509	11719	1995	2263	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
			Total	C	H	N	O	S		
91	BQ	622	10266	3281	5095	853	1025	12	0	0

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

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

- Molecule 93 is a protein called mS87.

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

- Molecule 94 is a protein called mS88.

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

- Molecule 95 is a protein called mS89.

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

- Molecule 96 is a protein called mS90.

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

- Molecule 97 is a protein called mS91.

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

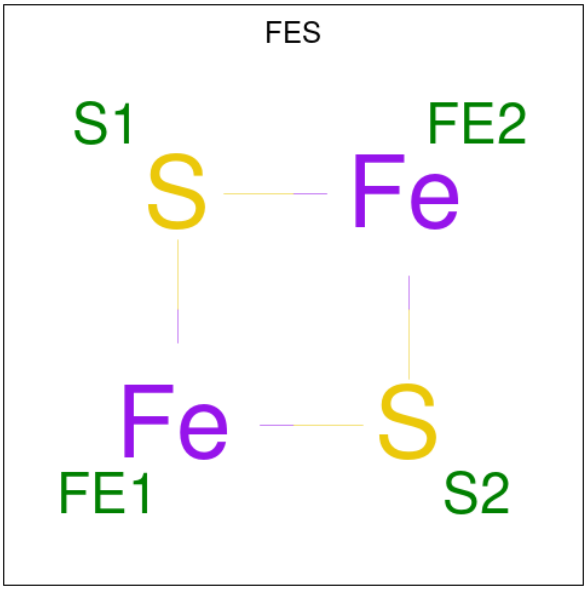
- Molecule 100 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

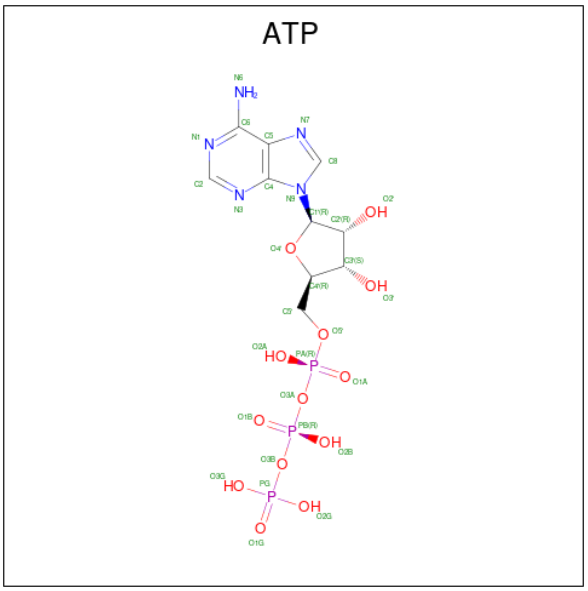
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
101	AG	1	1	1	0
			Total	Zn	
101	BL	1	1	1	0

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



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

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



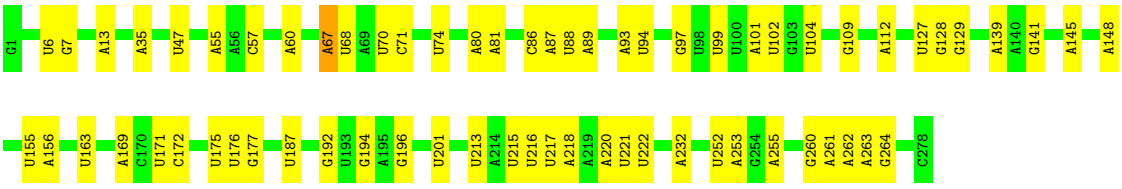
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
103	Bw	1	35	10	4	5	13	3	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

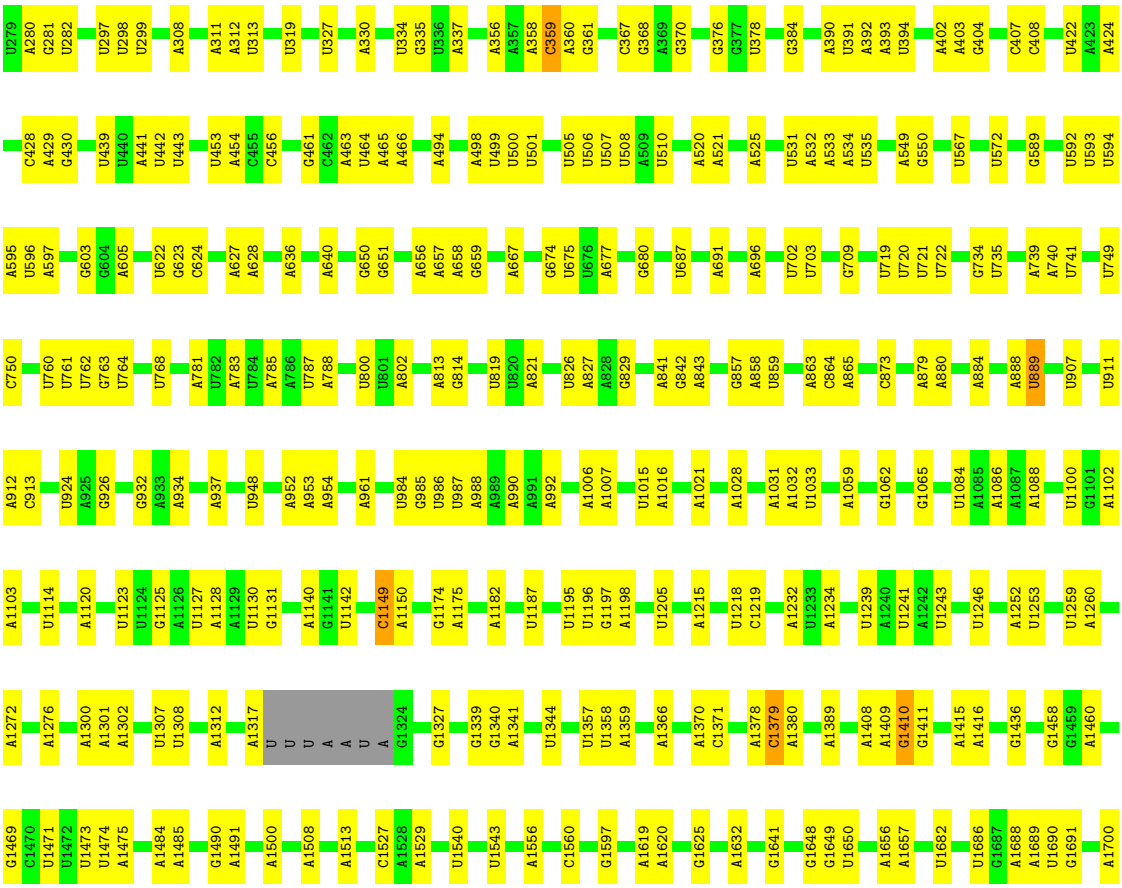
- Molecule 1: LSU rRNA_1

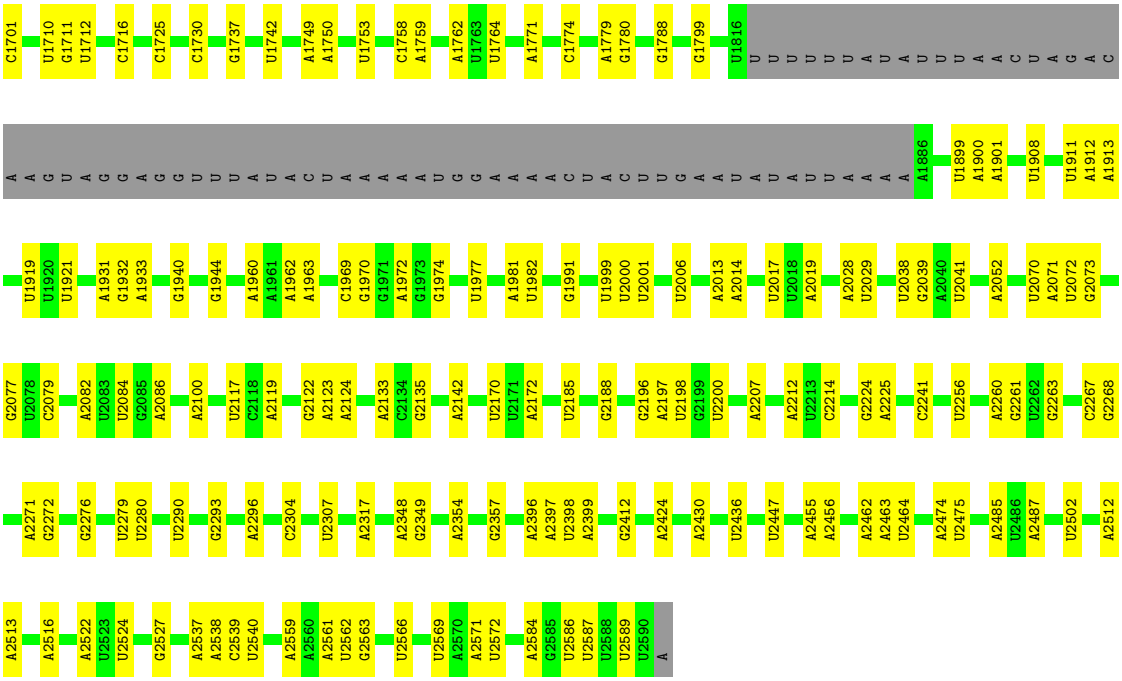
Chain Aa: 76% 23%



- Molecule 2: LSU rRNA_2

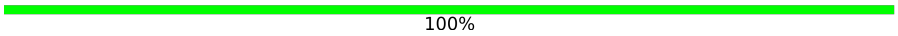
Chain Ab: 77% 19%





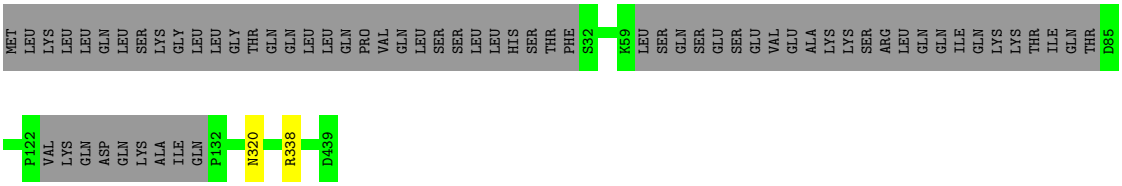
- Molecule 3: Ribosomal protein L2

Chain Ac:



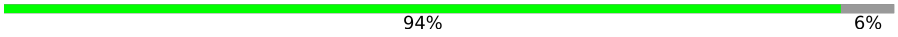
- Molecule 4: 50S ribosomal protein L3

Chain Ad:



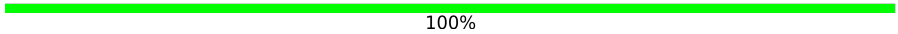
- Molecule 5: 50S ribosomal protein L4

Chain Ae:



- Molecule 6: Ymf69

Chain Af:



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.

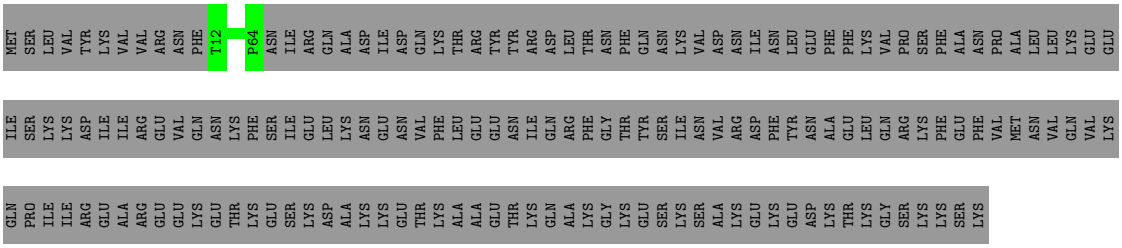
• Molecule 11: Ribosomal protein L7/L12 carboxy-terminal domain protein

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%

MET ILE GLY LYS ASN ILE VAL SER LYS LEU GLY ASN LEU ALA SER ASN VAL HIS ILE LEU ASN LYS GLN ILE ALA SER PHE S28 Q211 R357 GLN GLY GLY GLY SER ALA THR ALA GLY PRO ALA LYS PRO ALA GLY GLY ASN ALA ASN ALA GLY ALA ALA ALA LYS GLY GLY

LYS GLN GLY GLY LYS LYS

• Molecule 16: Ribosomal protein L14

Chain Ap: 99%

M1 V19 I119

• Molecule 17: Ribosomal protein L15, putative

Chain Aq: 90% 10%

MET ASN LEU LEU LEU LYS ALA SER GLN TYR ILE SER ARG ASN SER PHE PRO VAL ASN ASN ILE ARG SER LEU LEU GLN GLY SER VAL TYR SER PHE S33 I305

• 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%

MET G2 I124 Y237

• Molecule 20: bL19m

Chain At: 75% 24%

MET PHE LEU ARG GLN GLN LEU GLN LYS GLY VAL PHE ASN PHE THR GLN LEU VAL ASN GLN GLN SER ASN SER I1 R32 W46 G183 GLY HIS LYS LYS GLY LYS ARG THR ASP ILE TYR MET GLU ARG ARG HIS LEU GLU GLN SER LYS SER ASN VAL LEU ASP ARG SER GLU

ASP PRO VAL LEU ASN TYR

• Molecule 21: 50S ribosomal protein L20

Chain Au: 99%

MET T2 N170

• Molecule 22: 50S ribosomal protein L21

Chain Av: 86% 12%

MET ILE ILE ALA ASN LYS LEU PHE SER ASN LEU ALA LYS THR GLN VAL LYS GLN PHE ALA PHE HIS ASN TYR ILE THR ALA ALA PHE G30 P113 A114 R170 L235

• Molecule 23: Ribosomal protein L22/L17e

Chain Aw: 94% 6%

MET ILE THR ARG SER LEU LYS GLN PHE ASN LYS SER MET LEU LEU SER PHE ARG PRO ILE TYR SER M23 R201 G364

• Molecule 24: Ribosomal protein L23, putative

Chain Ax: 96%

MET ASN ASN ILE VAL R6 T31 ALA Q33 M138

• Molecule 25: 50S ribosomal protein L24

Chain Ay: 81% 19%

MET PHE LYS VAL LEU SER SER LEU SER ARG ALA ALA VAL ALA LEU PRO SER ILE ARG ASN THR ILE ASN ILE SER LYS MET ILE GLY PHE GLN ARG GLN ILE MET LEU ASN ASN ILE ASN SER PHE SER PHE S45 D234

• Molecule 26: bL25m

Chain Az: 73% 26%

MET ASN ILE ILE CYS ASN LYS LEU LEU SER GLN ARG SER ILE ASN LEU PHE GLY PHE ARG PRO SER CYS ASN PHE T26 R115 T136 Y137 D138 Q262 ASN MET LYS LEU MET LYS GLU GLN VAL THR VAL GLU GLU ASP GLU ASP PHE THR LEU ALA SER GLU VAL LYS LYS ALA

PRO LYS GLU ARG LYS ASN VAL LYS VAL ARG SER LEU LYS LYS GLN VAL GLN ALA ILE SER ALA GLN VAL LYS GLU LYS LEU ALA GLN GLN GLN ALA SER

• Molecule 27: 50S ribosomal protein L27

Chain AA: 74% 26%

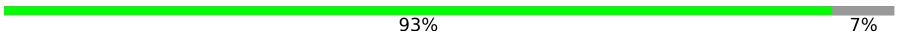
MET THR SER ASN ILE VAL LYS ALA PHE GLN GLY LEU ASN ASN LEU THR LEU LYS MET ASN SER SER LEU PHE ASN LYS GLN GLN TYR PHE ALA THR LYS MET GLN ALA SER S38 L213 GLY ILE GLN TYR GLU PRO ILE ILE GLU ASP VAL GLN GLY GLU GLN GLU VAL GLU VAL SER

• Molecule 28: Ribosomal protein L28

Chain AB:

• Molecule 29: 39-S ribosomal protein L47

Chain AC:



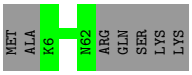
• Molecule 30: bL32m

Chain AD:

There are no outlier residues recorded for this chain.

• Molecule 31: 50S ribosomal protein L33

Chain AE:



• Molecule 32: bL35m

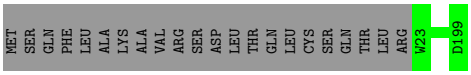
Chain AF:

• Molecule 33: Ribosomal protein

Chain AG:

• Molecule 34: mL40

Chain AH:

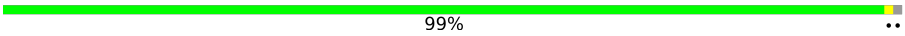


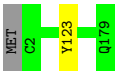
• Molecule 35: Ribosomal protein L27

Chain AI:

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

Chain AJ:



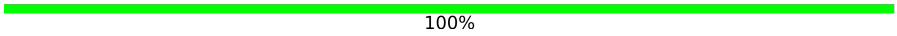


• Molecule 37: mL46

Chain AK:

• Molecule 38: Large subunit ribosomal protein

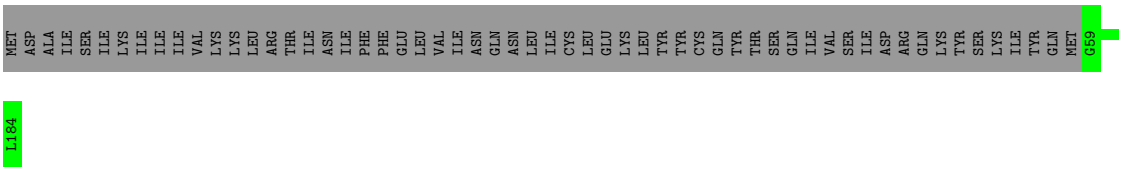
Chain AL:



There are no outlier residues recorded for this chain.

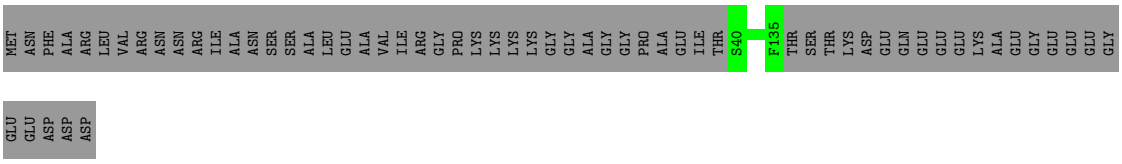
• Molecule 39: mL53

Chain AM:



• Molecule 40: mL54

Chain AN:

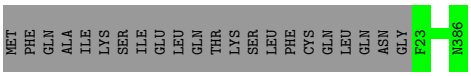


• Molecule 41: mL64

Chain AO: 77% 23%

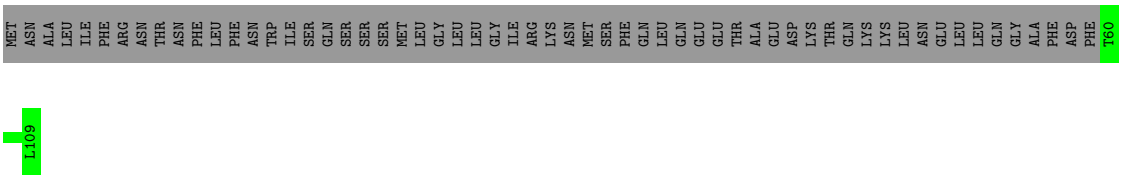
- Molecule 42: mL101

Chain AP: 94% 6%



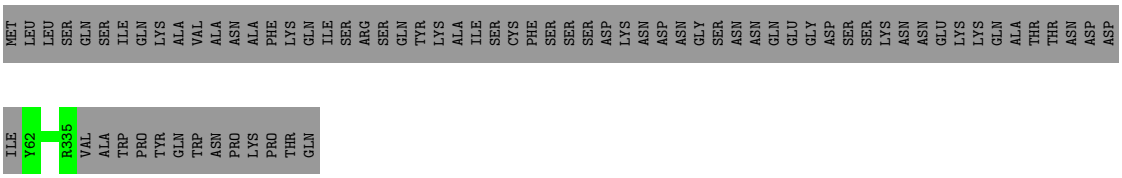
- Molecule 43: mL102

Chain AQ: 46% 54%



- Molecule 44: mL103

Chain AR: 79% 21%

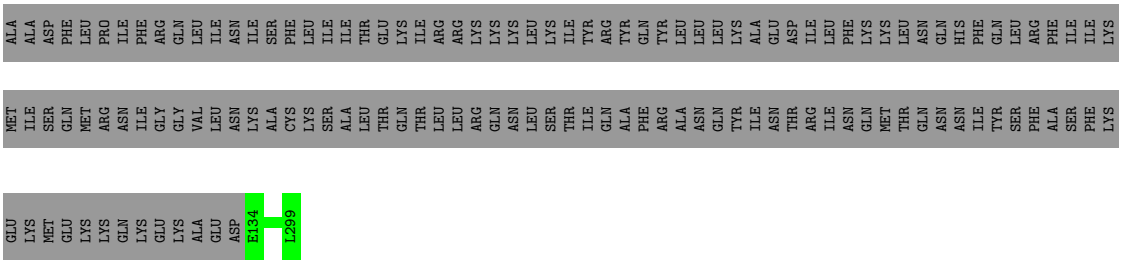


- Molecule 45: mL104

Chain AS: 95% 5%

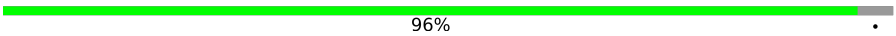
- Molecule 46: Signal peptide-binding domain protein

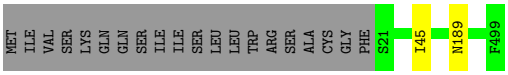
Chain AT: 56% 44%



• Molecule 47: mL106

Chain AU:





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

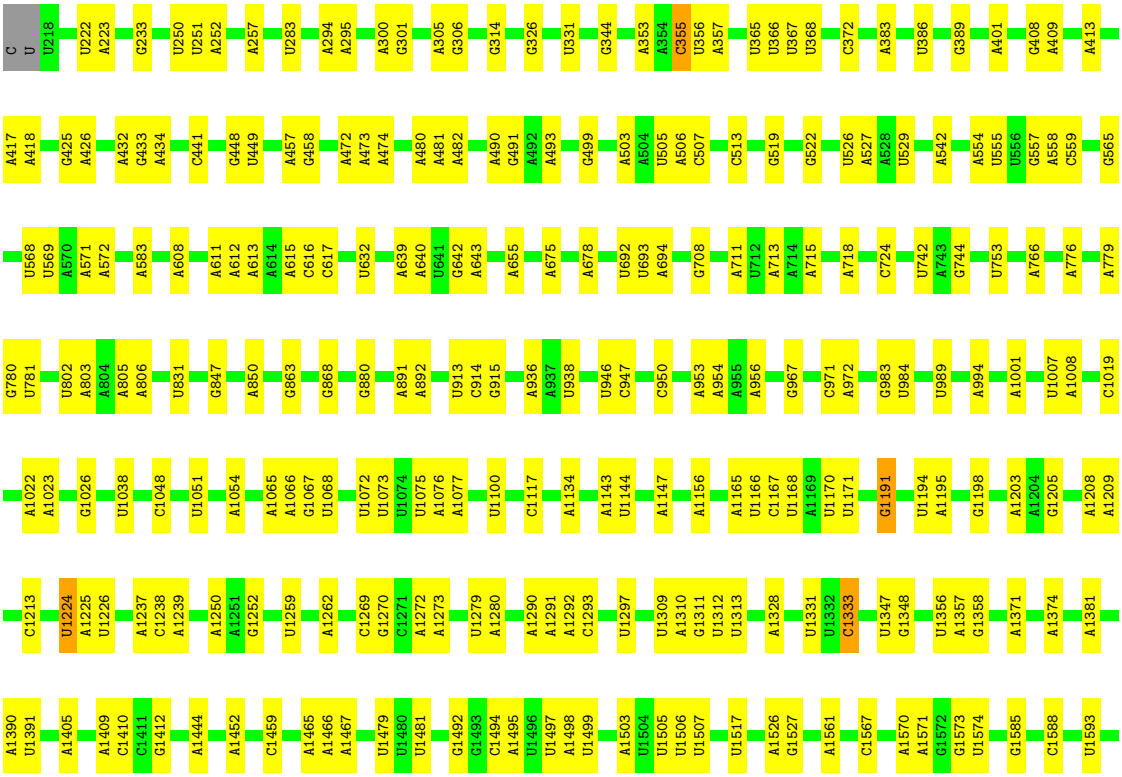
Chain AV:

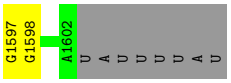
• Molecule 49: SSU rRNA_1

Chain Ba:

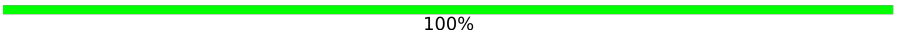
• Molecule 50: SSU rRNA_2

Chain Bb:



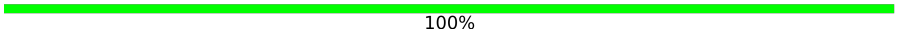


• Molecule 51: Ymf73

Chain Bc: 

There are no outlier residues recorded for this chain.

• Molecule 52: Ymf64

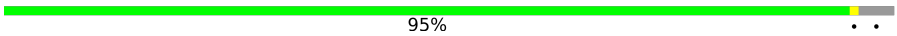
Chain Bd: 

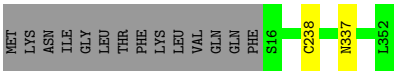
There are no outlier residues recorded for this chain.

• Molecule 53: Ymf76

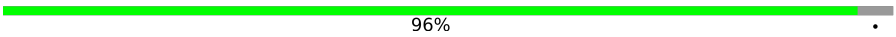
Chain Be:

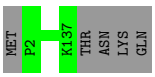
• Molecule 54: 30S ribosomal protein S5

Chain Bf: 

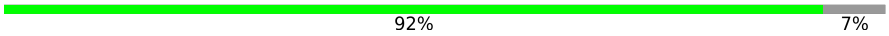


• Molecule 55: Ribosomal protein S6

Chain Bg: 



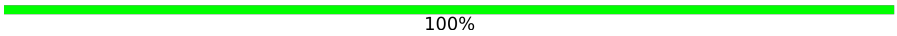
• Molecule 56: Ymf63

Chain Bh: 

• Molecule 57: Ribosomal protein S9

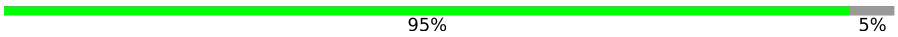
Chain Bi:

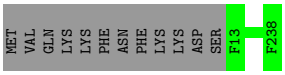
- Molecule 58: Ymf59

Chain Bj: 

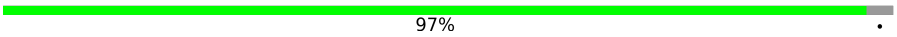
There are no outlier residues recorded for this chain.

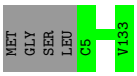
- Molecule 59: Ymf61

Chain Bk: 



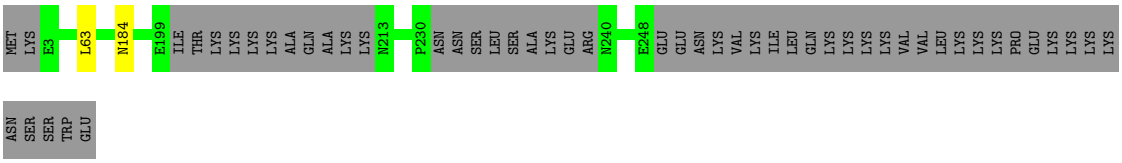
- Molecule 60: Ribosomal protein S12

Chain Bl: 

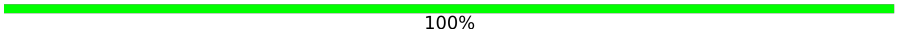


- Molecule 61: Ribosomal protein S13

Chain Bm:



- Molecule 62: Ribosomal protein S14

Chain Bn: 

There are no outlier residues recorded for this chain.

- Molecule 63: 30S ribosomal protein S15

Chain Bo:

- Molecule 64: 30S ribosomal protein S16

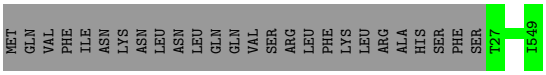
Chain Bp: 94% 6%

• 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%

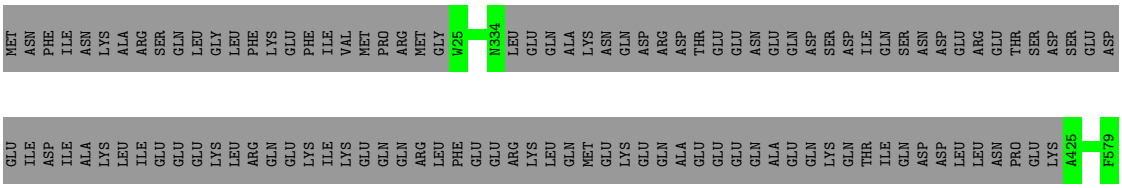
There are no outlier residues recorded for this chain.

• Molecule 69: mS23

Chain Bu: 99%

• Molecule 70: mS26

Chain Bv: 80% 20%

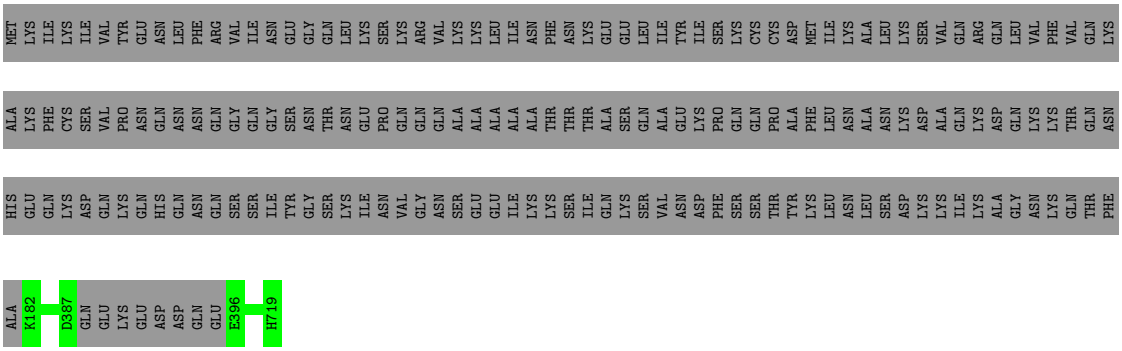


• Molecule 71: Ribosomal death-associated protein

Chain Bw: 94% 6%

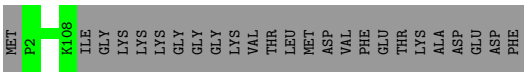
• Molecule 72: mS31

Chain Bx: 74% 26%



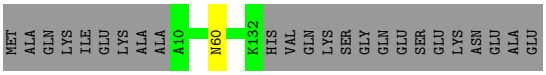
• Molecule 73: mS33

Chain By: 81% 19%



• Molecule 74: mS34

Chain Bz: 83% • 16%



• Molecule 75: Ribosomal subunit protein

Chain BA: 92% • 7%

• Molecule 76: mS37

Chain BB: 98% •

• Molecule 77: mS38

Chain BC: 100%

There are no outlier residues recorded for this chain.

- Molecule 78: IGR motif protein

Chain BD: 82% 18%

- Molecule 79: mS45

Chain BE: 96%

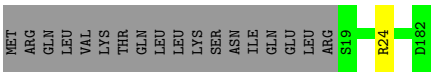
- Molecule 80: mS75

Chain BF: 100%

There are no outlier residues recorded for this chain.

- Molecule 81: mS76

Chain BG: 90% 10%



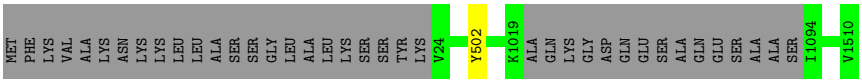
- Molecule 82: mS77

Chain BH: 100%

There are no outlier residues recorded for this chain.

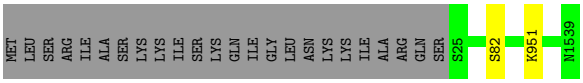
- Molecule 83: Enoyl-CoA hydratase/isomerase

Chain BI: 97%



- Molecule 84: mS78

Chain BJ: 98%



- Molecule 85: mS79

Chain BK: 100%

There are no outlier residues recorded for this chain.

• Molecule 86: SelR domain protein

Chain BL: 58% 42%

MET ARG LYS ASP ILE LYS GLN LYS LEU LEU ARG ILE LYS LYS LYS LYS LYS LYS ASP LYS LYS GLN SER GLN ILE LYS ASN ILE LYS PHE LEU LEU ILE LEU THR GLN TYR GLN GLN GLY LEU GLN SER GLN SER LYS ASP GLN LYS TYR LYS SER ILE ILE LYS TYR ASN ARG ILE LYS

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

GLN LYS E123 S303 SER SER SER GLN THR GLN ASN

• Molecule 87: mS81

Chain BM: 80% 20%

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

LYS ARG GLU GLY GLU GLU GLN TYR ARG PRO ARG K72 N355

• Molecule 88: mS82

Chain BN: 97%

MET ALA ALA SER GLN LYS VAL VAL ASN G10 L283

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

Chain BO: 100%

There are no outlier residues recorded for this chain.

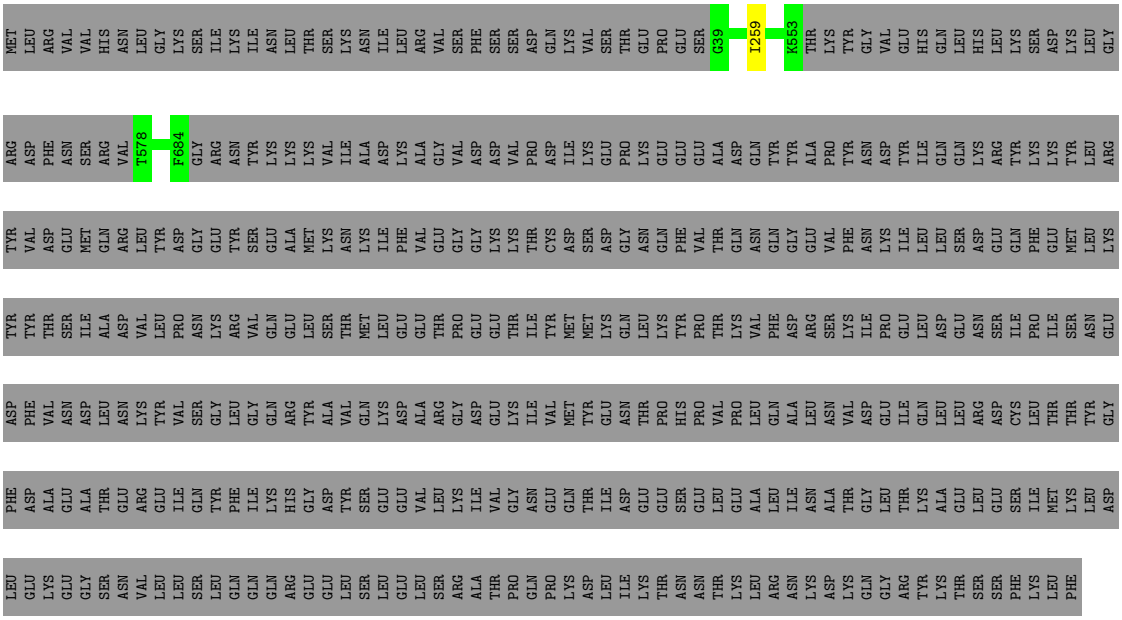
• Molecule 90: mS84,mS84

Chain BP: 99%

X1 D84 K100

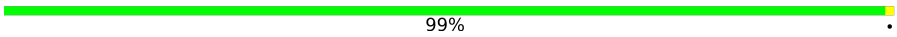
• Molecule 91: mS85

Chain BQ: 60% 40%



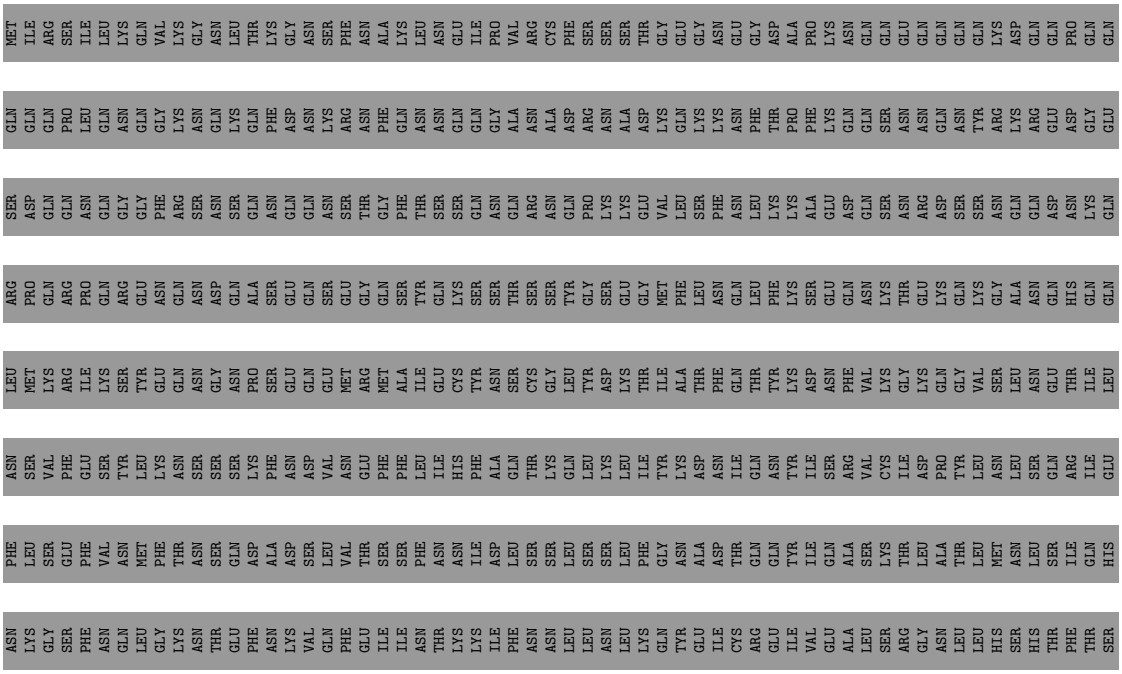
• Molecule 92: Iron donor protein CyaY

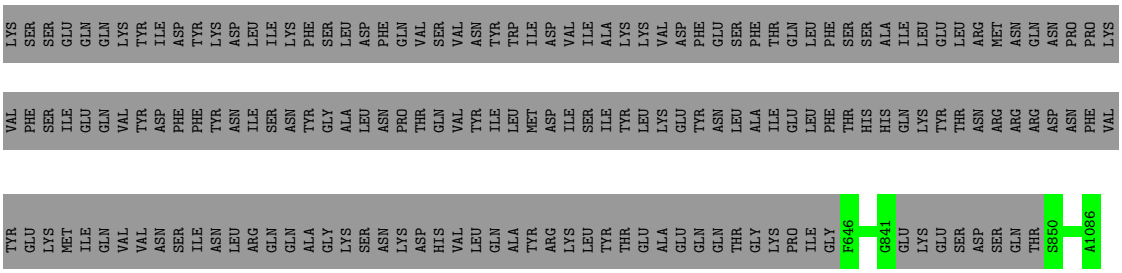
Chain BR:



• Molecule 93: mS87

Chain BS:





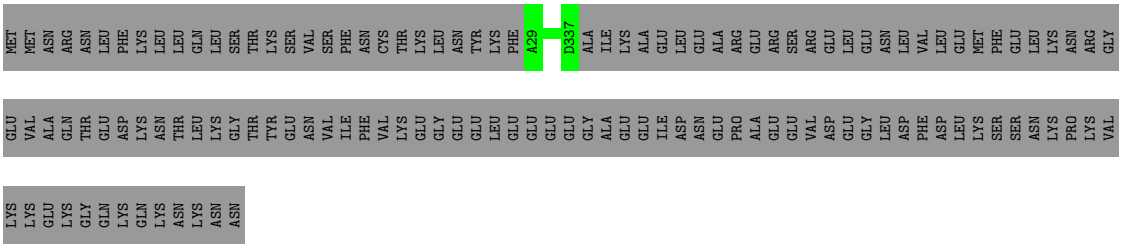
- Molecule 94: mS88

Chain BT: 100%

There are no outlier residues recorded for this chain.

- Molecule 95: mS89

Chain BU: 70% 30%



- Molecule 96: mS90

Chain BV: 100%

There are no outlier residues recorded for this chain.

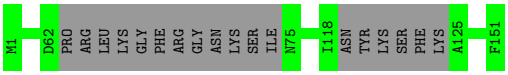
- Molecule 97: mS91

Chain BW: 100%

There are no outlier residues recorded for this chain.

- Molecule 98: Ribosomal protein S3

Chain BX: 88% 12%



- Molecule 99: mS93

Chain BY: 100%

4 Experimental information (i)

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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	92000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: 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

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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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 (i)

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	$\#\|Z\| > 2$
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

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

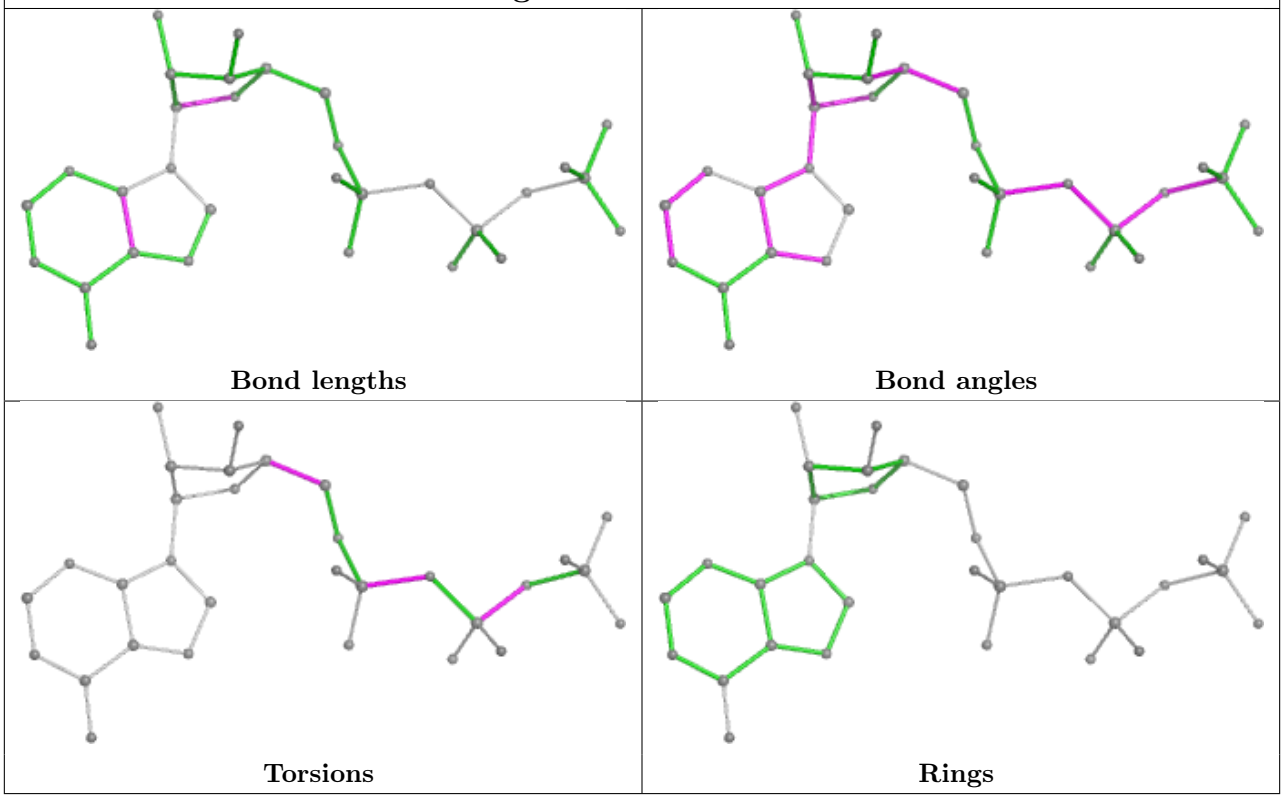
There are no ring outliers.

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 (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

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
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 (i)

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

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

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

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

7 Map analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.