



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 06:33 am BST

PDB ID : 8ANY
EMDB ID : EMD-15544
Title : Human mitochondrial ribosome in complex with LRPPRC, SLIRP, A-site, P-site, E-site tRNAs and mRNA
Authors : Singh, V.; Itoh, Y.; Amunts, A.
Deposited on : 2022-08-06
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

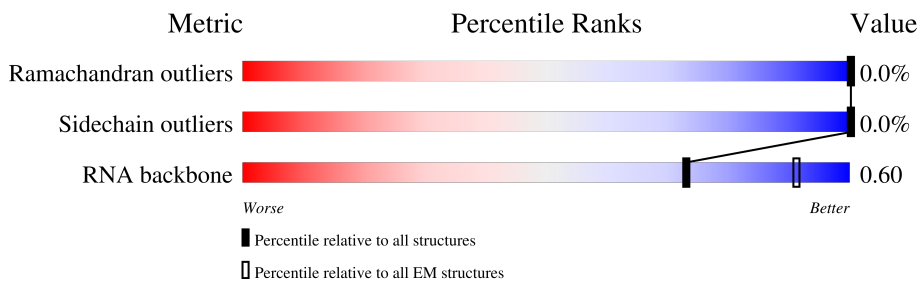
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AA	954	86% (Green), 14% (Yellow)
2	AB	296	76% (Green), 24% (Grey)
3	AC	167	79% (Green), 21% (Grey)
4	AD	430	80% (Green), 20% (Grey)
5	AE	125	98% (Green), . (Grey)
6	AF	242	86% (Green), 14% (Grey)
7	AG	396	83% (Green), 17% (Grey)
8	AH	201	69% (Green), 30% (Grey)
9	AI	194	70% (Green), . (Yellow), 29% (Grey)

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Mol	Chain	Length	Quality of chain	
10	AJ	138	78%	22%
11	AK	128	79%	21%
12	AL	257	68%	32%
13	AM	137	87%	13%
14	AN	130	85%	15%
15	AO	258	75%	25%
16	AP	142	68%	32%
17	AQ	87	99%	.
18	AR	360	82%	18%
19	AS	190	71%	29%
20	AT	173	97%	.
21	AU	205	86%	14%
22	AV	414	87%	13%
23	AW	187	53%	47%
24	AX	398	88%	12%
25	AZ	106	94%	6%
26	A0	217	99%	.
27	A1	323	86%	14%
28	A2	118	99%	.
29	A3	199	35%	65%
30	Aw	68	72%	28%
31	Ax	70	81%	19%
32	Ay	70	80%	20%
33	A	1561	85%	15%
34	B	72	78%	22%

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Mol	Chain	Length	Quality of chain	
35	D	305	78%	22%
36	E	348	87%	12%
37	F	311	81%	19%
38	I	261	81%	19%
39	J	192	91%	9%
40	K	178	99%	.
41	L	145	79%	21%
42	M	296	98%	.
43	N	251	88%	12%
44	O	175	88%	12%
45	P	180	80%	20%
46	Q	292	82%	18%
47	R	149	94%	6%
48	S	205	79%	21%
49	T	206	81%	19%
50	U	153	99%	.
51	V	216	95%	5%
52	W	148	78%	22%
53	X	256	95%	5%
54	Y	250	72%	28%
55	Z	161	76%	24%
56	0	188	59%	41%
57	1	65	86%	14%
58	2	92	50%	50%
59	3	188	51%	49%

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Mol	Chain	Length	Quality of chain	
60	4	103	37%	63%
61	5	423	93%	7%
62	6	380	93%	7%
63	7	338	87%	13%
64	8	206	76%	24%
65	9	137	91%	9%
66	a	142	70%	30%
67	b	215	70%	30%
68	c	332	86%	14%
69	d	306	79%	21%
70	e	279	85%	15%
71	f	212	74%	26%
72	g	166	81%	19%
73	h	158	70%	30%
74	i	128	76%	24%
75	j	123	76%	24%
76	k	112	90%	10%
77	l	138	59%	41%
78	m	128	72%	28%
79	o	102	92%	8%
80	p	206	71%	29%
81	q	222	74%	26%
82	r	196	83%	17%
83	s	439	88%	12%
84	t	198	23%	77%

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Mol	Chain	Length	Quality of chain	
84	u	198	16%	84%
84	v	198	16%	84%
84	w	198	16%	84%
84	x	198	16%	84%
84	y	198	16%	84%
85	H	267	76%	24%
86	z	325	77%	22%
87	AY	395	56%	44%
88	A5	1394	42%	58%
89	A4	689	86%	14%
90	A6	109	68%	32%
91	Az	42	50%	50%

2 Entry composition [i](#)

There are 103 unique types of molecules in this entry. The entry contains 355123 atoms, of which 160326 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 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	AA	954	30565	9088	10305	3647	6571	954	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	AB	225	3654	1164	1826	331	323	10	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	AC	132	2179	699	1096	195	185	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	AD	343	5545	1713	2814	518	487	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	AE	122	1976	614	1004	177	177	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	AF	208	3503	1104	1778	312	298	11	0	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	AG	327	5385	1710	2697	477	487	14	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	AH	140	2343	745	1191	194	210	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	AI	137	2086	642	1066	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	AJ	108	1731	521	892	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	AK	101	1751	537	889	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	AL	174	2998	925	1545	270	251	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	AM	119	1914	594	972	185	157	6	0	0

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	AN	110	1801	562	933	156	147	3	0	0

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	AO	193	3162	1014	1570	294	277	7	0	0

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	AP	97	1590	501	809	134	138	8	0	0

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	AQ	86	1504	460	760	150	126	8	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	AR	295	4845	1533	2436	413	455	8	0	0

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	AS	135	2228	716	1117	198	196	1	0	0

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	AT	168	2767	877	1396	239	244	11	0	0

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	AU	176	2993	916	1505	301	267	4	0	0

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	AV	362	5941	1904	2972	495	558	12	0	0

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	AW	100	1595	498	806	141	146	4	0	0

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	AX	352	5708	1822	2859	499	517	11	0	0

- Molecule 25 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	AZ	100	1701	534	862	153	148	4	0	0

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	A0	215	3589	1130	1802	339	313	5	0	0

- Molecule 27 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	A1	277	4526	1424	2281	382	428	11	0	0

- Molecule 28 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	A2	117	1906	579	971	182	166	8	0	0

- Molecule 29 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	A3	70	1327	401	702	134	89	1	0	0

- Molecule 30 is a RNA chain called A/A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
30	Aw	68	2159	646	725	248	472	68	0	0

- Molecule 31 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
31	Ax	70	2232	665	750	260	487	70	0	0

- Molecule 32 is a RNA chain called E/E-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
32	Ay	70	2235	665	752	261	487	70	0	0

- Molecule 33 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
33	A	1558	49872	14843	16802	5963	10706	1558	0	0

- Molecule 34 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
34	B	72	2303	685	779	269	498	72	0	0

- Molecule 35 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	D	238	3787	1157	1928	376	317	9	0	0

- Molecule 36 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	E	305	4830	1545	2424	418	432	11	0	0

- Molecule 37 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	F	252	4106	1305	2075	370	350	6	0	0

- Molecule 38 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	I	212	3489	1088	1794	304	292	11	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	J	175	2739	847	1409	237	244	2	0	0

- Molecule 40 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
40	K	177	2915	936	1460	259	253	7	0	0

- Molecule 41 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
41	L	115	1835	559	945	171	155	5	0	0

- Molecule 42 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
42	M	289	4701	1476	2387	427	405	6	0	0

- Molecule 43 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
43	N	222	3610	1143	1824	326	307	10	0	0

- Molecule 44 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
44	O	154	2557	792	1298	241	219	7	0	0

- Molecule 45 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
45	P	144	2344	733	1171	224	211	5	0	0

- Molecule 46 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
46	Q	238	4004	1268	2025	352	350	9	0	0

- Molecule 47 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
47	R	140	2374	732	1220	231	187	4	0	0

- Molecule 48 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
48	S	161	2662	835	1369	227	227	4	0	0

- Molecule 49 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
49	T	166	2786	875	1417	254	233	7	0	0

- Molecule 50 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
50	U	152	2486	788	1235	234	226	3	0	0

- Molecule 51 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
51	V	205	3367	1068	1691	298	302	8	0	0

- Molecule 52 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
52	W	116	1847	577	943	171	153	3	0	0

- Molecule 53 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
53	X	244	4109	1322	2065	352	365	5	0	0

- Molecule 54 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
54	Y	181	Total	C	H	N	O	S	0	0
			3159	995	1603	298	259	4		

- Molecule 55 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
55	Z	122	Total	C	H	N	O	S	0	0
			2048	636	1052	186	171	3		

- Molecule 56 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
56	0	110	Total	C	H	N	O	S	0	0
			1817	554	919	176	162	6		

- Molecule 57 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
57	1	56	Total	C	H	N	O	S	0	0
			977	296	513	89	77	2		

- Molecule 58 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
58	2	46	Total	C	H	N	O	S	0	0
			786	233	409	83	60	1		

- Molecule 59 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
59	3	95	Total	C	H	N	O	S	0	0
			1718	539	886	162	128	3		

- Molecule 60 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
60	4	38	Total	C	H	N	O	S	0	0
			705	217	363	72	49	4		

- Molecule 61 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
61	5	394	6432	2073	3222	560	566	11	0	0

- Molecule 62 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
62	6	354	5802	1881	2854	525	533	9	0	0

- Molecule 63 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
63	7	294	4796	1529	2406	405	438	18	0	0

- Molecule 64 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
64	8	157	2698	844	1371	235	246	2	0	0

- Molecule 65 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
65	9	124	1985	644	988	170	181	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
66	a	100	1659	529	819	152	154	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
67	b	150	2395	744	1199	231	218	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
68	c	286	4624	1470	2325	397	423	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
69	d	241	3971	1273	1986	340	359	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
70	e	238	3853	1222	1922	339	364	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
71	f	157	2529	799	1277	207	242	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
72	g	134	2214	719	1101	193	199	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
73	h	110	1780	568	885	156	168	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
74	i	97	1690	532	862	165	127	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
75	j	94	Total	C	H	N	O	S	0	0
			1492	463	747	144	136	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
76	k	101	Total	C	H	N	O	S	0	0
			1562	479	788	148	142	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
77	l	82	Total	C	H	N	O	S	0	0
			1364	437	676	120	128	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
78	m	92	Total	C	H	N	O	S	0	0
			1554	488	763	159	142	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
79	o	94	Total	C	H	N	O	S	0	0
			1608	501	810	165	129	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
80	p	147	Total	C	H	N	O	S	0	0
			2433	748	1228	228	225	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
81	q	165	Total	C	H	N	O	S	0	0
			2766	865	1377	270	249	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
82	r	162	2677	839	1355	252	223	8	0	0

- Molecule 83 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
83	s	386	6306	2023	3151	559	559	14	0	0

- Molecule 84 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
84	t	46	732	228	378	56	70	0	0
84	u	32	541	168	284	40	49	0	0
84	v	32	541	168	284	40	49	0	0
84	w	31	520	159	275	39	47	0	0
84	x	31	520	159	275	39	47	0	0
84	y	31	520	159	275	39	47	0	0

- Molecule 85 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
85	H	202	3398	1067	1737	304	286	4	0	0

- Molecule 86 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
86	z	252	4107	1304	2080	336	381	6	0	0

- Molecule 87 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
87	AY	221	3622	1159	1787	319	352	5	0	0

- Molecule 88 is a protein called Leucine-rich PPR motif-containing protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
88	A5	581	9336	2959	4690	790	871	26	0	0

- Molecule 89 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
89	A4	595	9643	3080	4828	815	892	28	0	0

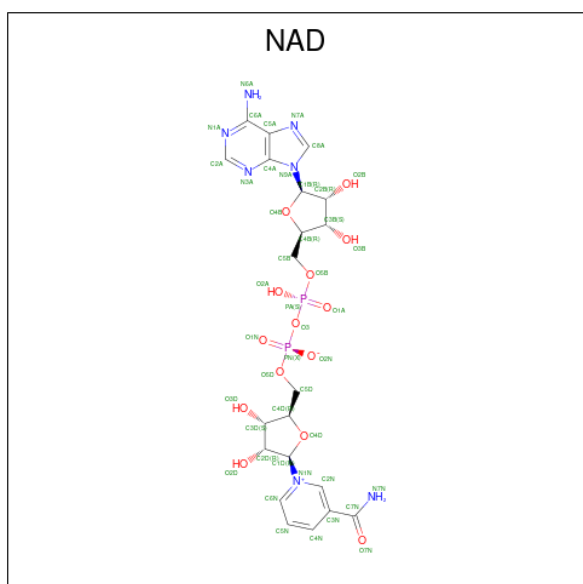
- Molecule 90 is a protein called SRA stem-loop-interacting RNA-binding protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
90	A6	74	1197	384	594	115	103	1	0	0

- Molecule 91 is a RNA chain called mRNA.

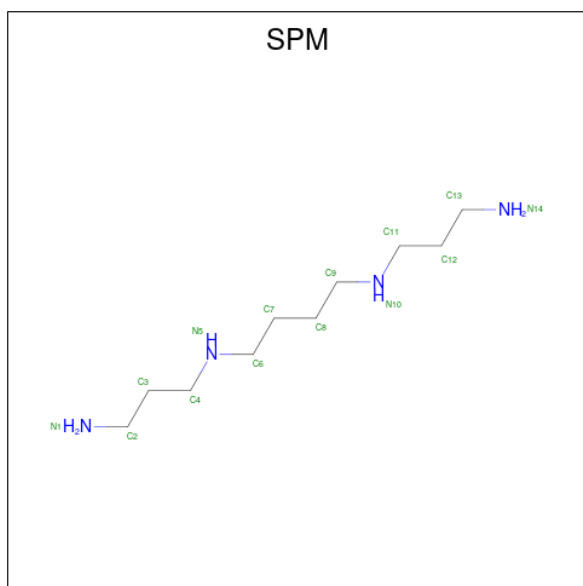
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
91	Az	42	1325	396	445	144	298	42	0	0

- Molecule 92 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



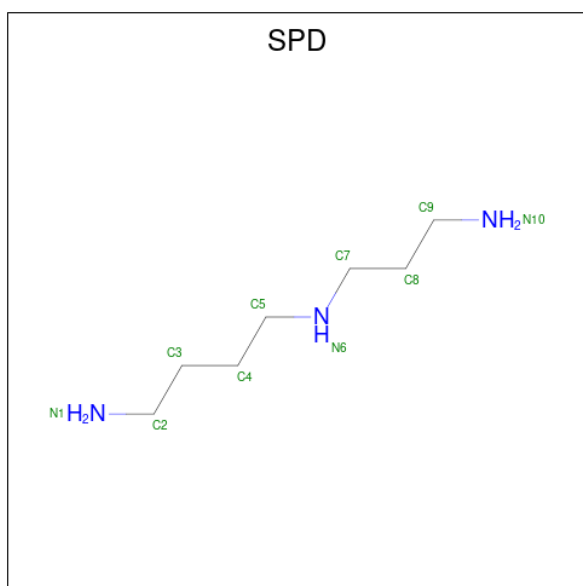
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
92	AA	1	70	21	26	7	14	2	0

- Molecule 93 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
93	AA	1	44	10	30	4	0

- Molecule 94 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms				AltConf
94	AA	1	Total	C	H	N	0
			32	7	22	3	
94	A	1	Total	C	H	N	0
			32	7	22	3	
94	A	1	Total	C	H	N	0
			32	7	22	3	
94	A	1	Total	C	H	N	0
			32	7	22	3	

- Molecule 95 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
95	AA	62	Total	Mg	0
			62	62	
95	AB	1	Total	Mg	0
			1	1	
95	AX	1	Total	Mg	0
			1	1	
95	A3	1	Total	Mg	0
			1	1	
95	Aw	1	Total	Mg	0
			1	1	
95	A	136	Total	Mg	0
			136	136	
95	D	2	Total	Mg	0
			2	2	
95	E	1	Total	Mg	0
			1	1	
95	g	1	Total	Mg	0
			1	1	

- Molecule 96 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
96	AA	16	Total	K	0
			16	16	
96	A	28	Total	K	0
			28	28	
96	D	1	Total	K	0
			1	1	
96	M	1	Total	K	0
			1	1	
96	P	1	Total	K	0
			1	1	

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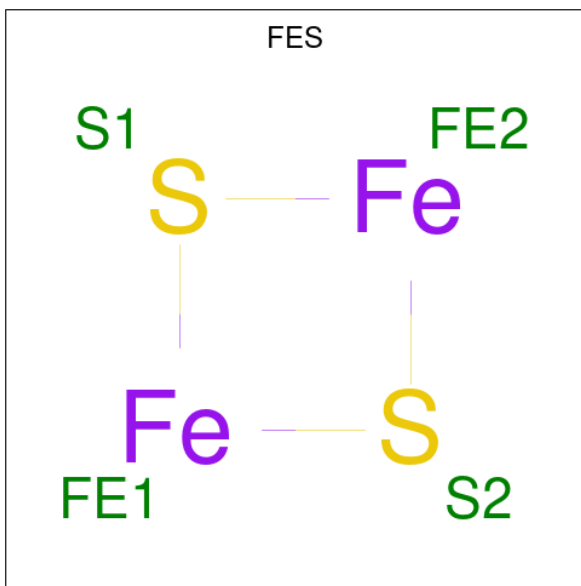
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Mol	Chain	Residues	Atoms	AltConf
96	i	1	Total K 1 1	0
96	o	1	Total K 1 1	0

- Molecule 97 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
97	AO	1	Total Zn 1 1	0
97	0	1	Total Zn 1 1	0
97	4	1	Total Zn 1 1	0

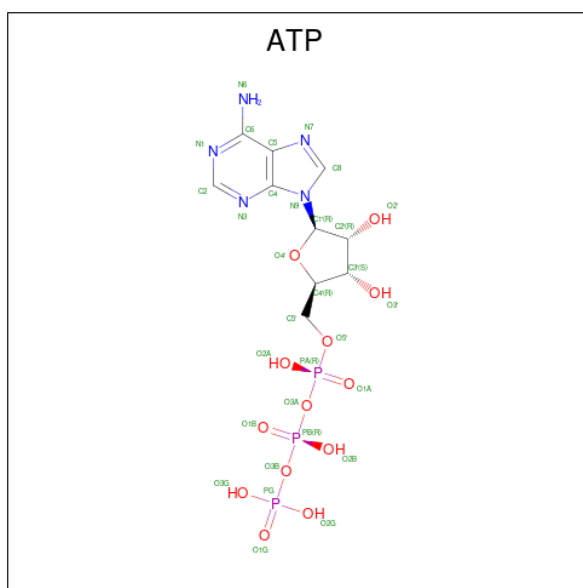
- Molecule 98 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms	AltConf
98	AP	1	Total Fe S 4 2 2	0
98	AT	1	Total Fe S 4 2 2	0
98	r	1	Total Fe S 4 2 2	0

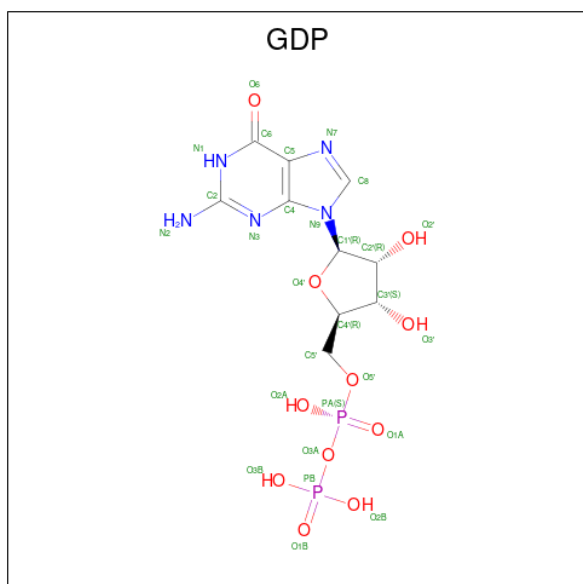
- Molecule 99 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$).



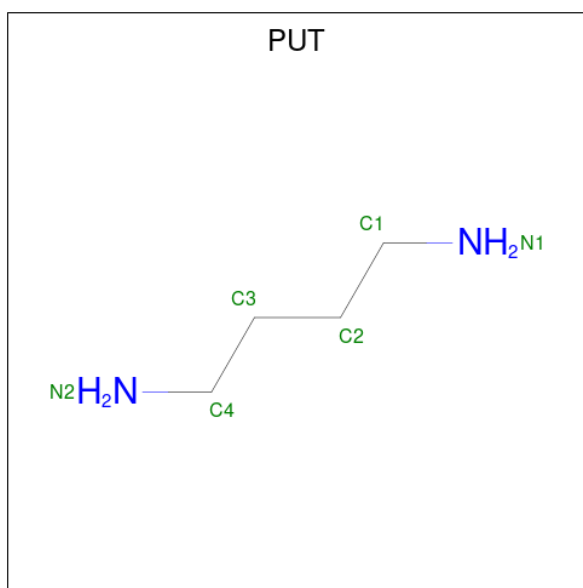
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
99	AX	1	43	10	12	5	13	3	0

- Molecule 100 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



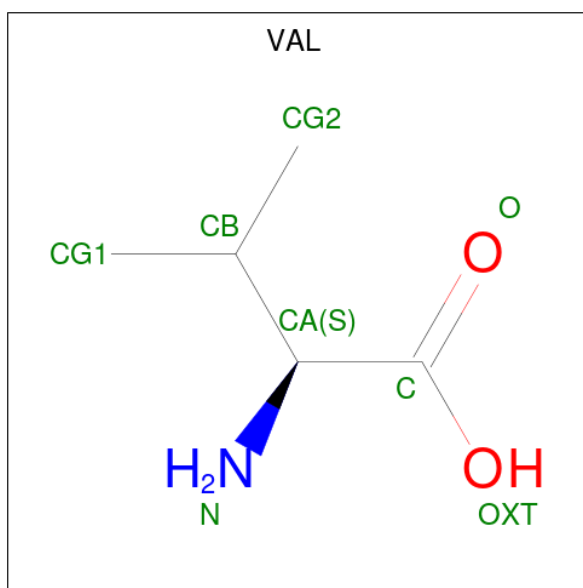
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
100	AX	1	40	10	12	5	11	2	0

- Molecule 101 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
101	A	1	20	4	14	2	0

- Molecule 102 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
102	B	1	18	5	11	1	1	0

- Molecule 103 is water.

Mol	Chain	Residues	Atoms		AltConf
103	AA	1747	Total 1747	O 1747	0
103	AB	60	Total 60	O 60	0
103	AC	48	Total 48	O 48	0
103	AD	66	Total 66	O 66	0
103	AE	20	Total 20	O 20	0
103	AF	29	Total 29	O 29	0
103	AG	53	Total 53	O 53	0
103	AH	46	Total 46	O 46	0
103	AI	30	Total 30	O 30	0
103	AJ	14	Total 14	O 14	0
103	AK	49	Total 49	O 49	0
103	AL	42	Total 42	O 42	0
103	AM	13	Total 13	O 13	0
103	AN	29	Total 29	O 29	0
103	AO	33	Total 33	O 33	0
103	AP	23	Total 23	O 23	0
103	AQ	52	Total 52	O 52	0
103	AR	9	Total 9	O 9	0
103	AS	18	Total 18	O 18	0
103	AT	26	Total 26	O 26	0
103	AU	4	Total 4	O 4	0
103	AW	9	Total 9	O 9	0

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Mol	Chain	Residues	Atoms		AltConf
103	AX	44	Total 44	O 44	0
103	AZ	24	Total 24	O 24	0
103	A0	2	Total 2	O 2	0
103	A1	36	Total 36	O 36	0
103	A2	26	Total 26	O 26	0
103	A3	43	Total 43	O 43	0
103	Aw	4	Total 4	O 4	0
103	Ax	8	Total 8	O 8	0
103	Ay	1	Total 1	O 1	0
103	A	2847	Total 2847	O 2847	0
103	B	55	Total 55	O 55	0
103	D	68	Total 68	O 68	0
103	E	57	Total 57	O 57	0
103	F	74	Total 74	O 74	0
103	I	21	Total 21	O 21	0
103	K	68	Total 68	O 68	0
103	L	27	Total 27	O 27	0
103	M	46	Total 46	O 46	0
103	N	50	Total 50	O 50	0
103	O	34	Total 34	O 34	0
103	P	69	Total 69	O 69	0

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Mol	Chain	Residues	Atoms		AltConf
103	Q	26	Total 26	O 26	0
103	R	59	Total 59	O 59	0
103	S	43	Total 43	O 43	0
103	T	47	Total 47	O 47	0
103	U	25	Total 25	O 25	0
103	V	6	Total 6	O 6	0
103	W	49	Total 49	O 49	0
103	X	11	Total 11	O 11	0
103	Y	23	Total 23	O 23	0
103	Z	35	Total 35	O 35	0
103	0	27	Total 27	O 27	0
103	1	2	Total 2	O 2	0
103	2	33	Total 33	O 33	0
103	3	43	Total 43	O 43	0
103	4	11	Total 11	O 11	0
103	5	15	Total 15	O 15	0
103	6	69	Total 69	O 69	0
103	7	11	Total 11	O 11	0
103	8	14	Total 14	O 14	0
103	9	16	Total 16	O 16	0
103	a	9	Total 9	O 9	0

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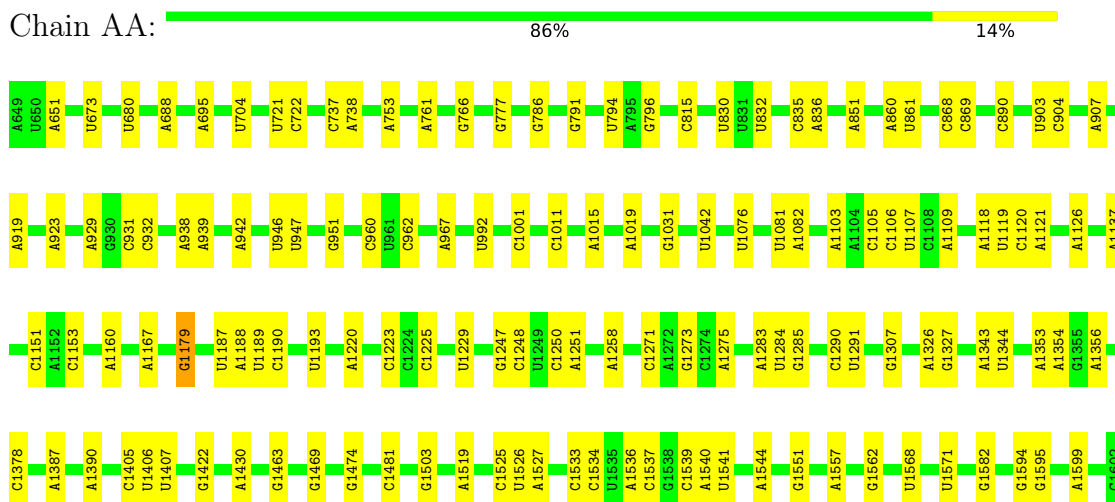
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Mol	Chain	Residues	Atoms		AltConf
103	b	32	Total 32	O 32	0
103	c	16	Total 16	O 16	0
103	d	6	Total 6	O 6	0
103	e	8	Total 8	O 8	0
103	f	18	Total 18	O 18	0
103	g	10	Total 10	O 10	0
103	i	50	Total 50	O 50	0
103	j	21	Total 21	O 21	0
103	l	1	Total 1	O 1	0
103	m	8	Total 8	O 8	0
103	o	33	Total 33	O 33	0
103	p	4	Total 4	O 4	0
103	r	35	Total 35	O 35	0
103	s	40	Total 40	O 40	0
103	H	7	Total 7	O 7	0
103	AY	20	Total 20	O 20	0
103	A4	7	Total 7	O 7	0
103	Az	12	Total 12	O 12	0

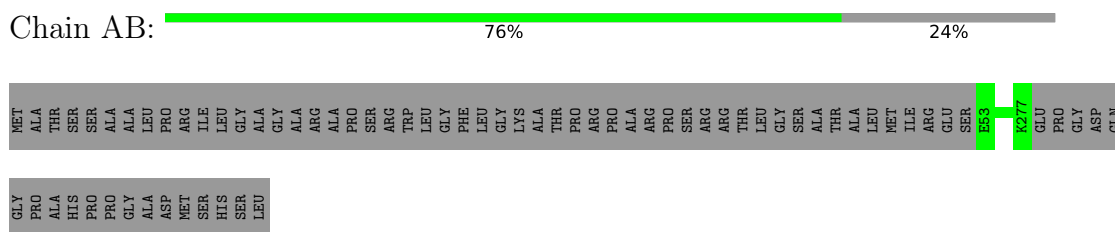
3 Residue-property plots

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

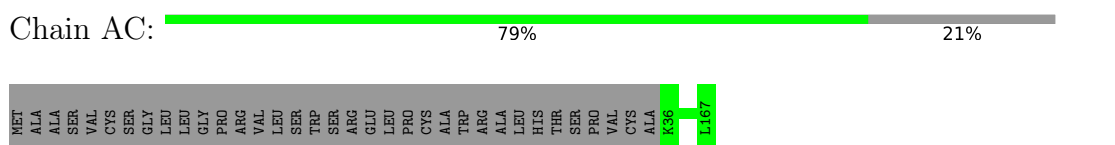
- Molecule 1: 12S mitochondrial rRNA



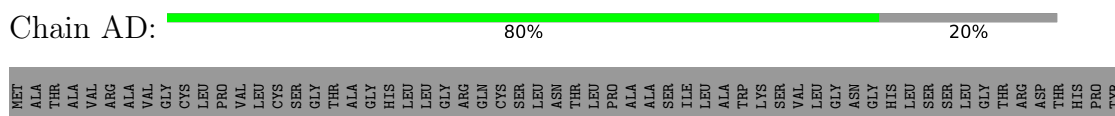
- Molecule 2: 28S ribosomal protein S2, mitochondrial

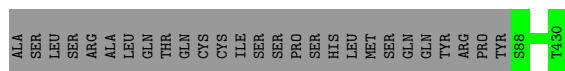


- Molecule 3: 28S ribosomal protein S24, mitochondrial



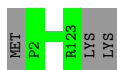
- Molecule 4: 28S ribosomal protein S5, mitochondrial





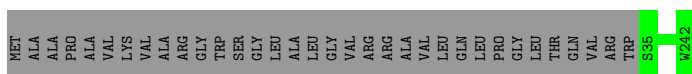
- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain AE: 98%



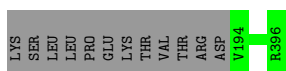
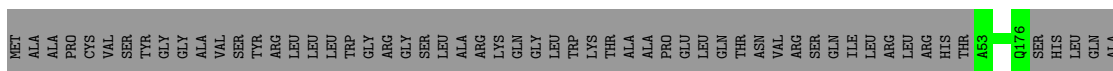
- Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain AF: 86% 14%



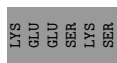
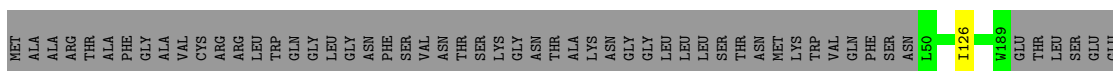
- Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain AG: 83% 17%



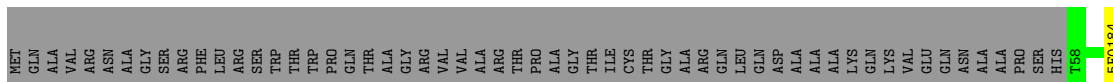
- Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain AH: 69% 30%




- Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain AI: 70% 29%




- Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain AJ:  78% 22%

MET SER TRP SER PHE MET MET LEU LEU HIS GLY LEU LEU ASN THR SER LEU THR CYS GLY PRO PRO ALA LEU VAL PRO ARG ARG LEU TRP ALA THR CYS MET A31 K138

- Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain AK:  79% 21%

MET ALA PHE MET MET GLY SER LEU LEU LEU ARG ARG THR THR PHE LYS GLN MET VAL PRO SER SER ALA ALA SER GLY GLN VAL ARG SER H28 M28

- Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain AL:  68% 32%

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


SER ARG L63 Q236 ALA LYS ARG CYS ASN PRO ASP THR PRO ALA ASP ALA THR ILE LEU LYS ASP GLN

- Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain AM:  87% 13%


MET VAL HIS LEU THR LEU CYS K10 E128 ALA THR ASP THR ALA GLU THR ALA THR

- Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain AN:  85% 15%

MET SER VAL V4 E113 THR THR GLN LEU SER LYS ASN LEU GLU LEU LEU ASN ILE SER SER ALA GLN

- Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain AO:  75% 25%

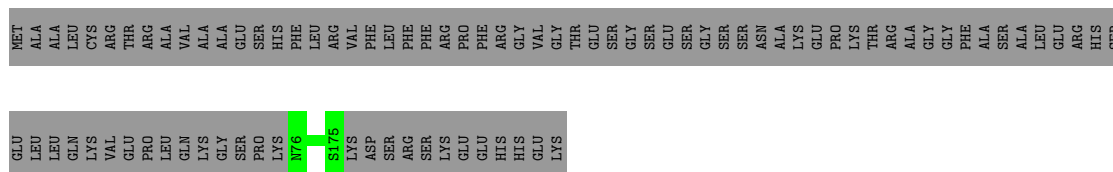
MET ALA ALA SER VAL LEU ASN THR VAL LEU ARG ARG LEU PRO MET SER LEU PHE ARG GLY HIS ARG VAL GLN VAL PRO LEU GLN THR LEU CYS THR LYS ALA PRO SER SER GLU ASP SER LEU SER SER VAL P47 P239 PRO ARG THR PRO ALA GLU ALA SER SER THR THR GLY

GLN THR GLY PRO GLN SER ALA LEU


- Molecule 16: 28S ribosomal protein S18c, mitochondrial

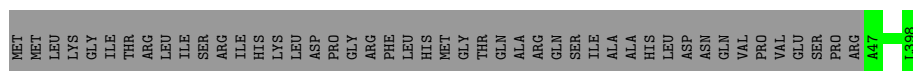
Chain AP:  68% 32%

Chain AW:  53% 47%



- Molecule 24: 28S ribosomal protein S29, mitochondrial

Chain AX:  88% 12%



- Molecule 25: 28S ribosomal protein S33, mitochondrial

Chain AZ:  94% 6%




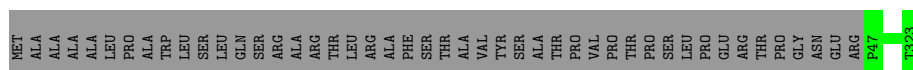
- Molecule 26: 28S ribosomal protein S34, mitochondrial

Chain A0:  99%



- Molecule 27: 28S ribosomal protein S35, mitochondrial

Chain A1:  86% 14%



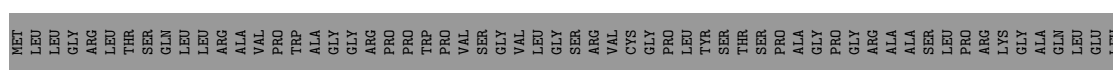
- Molecule 28: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2:  99%



- Molecule 29: Aurora kinase A-interacting protein

Chain A3:  35% 65%



GLU GLU MET MET LEU VAL PRO ARG LYS MET SER SER SER PRO LEU GLU TRP THR THR THR VAL ALA PRO PRO GLN TYR TYR GLN CYS PRO PRO SER SER ILE ILE GLY GLU GLY ASP GLU VAL ALA

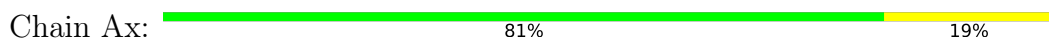
ASP ALA PRO GLN ILE GLN CYS K128 R197 GLY LYS

• Molecule 30: A/A-tRNA



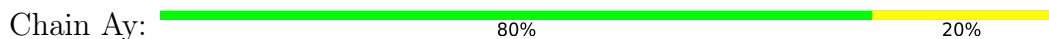
U1 G2 G3 A7 U8 A9 A16 C20 A21 A22 G50 A46 U48 U49 A50 A55 A56 U61 A65 U68 C71 U73 C74 C75 A76

• Molecule 31: P/P-tRNA



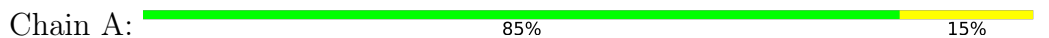
U1 A2 G3 U8 A9 C25 A44 G45 A46 U48 G49 U59 A76

• Molecule 32: E/E-tRNA



U1 A2 G3 C28 U29 G50 A37 A44 G45 U48 A46 U59 C75 A76

• Molecule 33: 16S mitochondrial rRNA



G1671 G1681 C1689 A1692 U1694 C1699 U1700 U1704 A1708 C1711 A1724 A1727 U1728 G1748 C1765 A1805 U1807 A1808 U1809 A1810 A1821 C1827 A1828 A1829 A1832 A1836 A1844 U1854 A1855 A1856 A1869 A1882 G1886 A1887 A1893

C1901 C1902 C1903 G1918 A1937 A1940 G1958 G1985 C1992 A1993 A1994 A2003 G2015 G2022 U2030 A2031 C2036 U2037 U2038 A2039 U2054 A2060 U2069 C2070 U2071 C2079 U2099 A2112 G2113 C2125 U2126 G2147 U2159 A2160 A2163 U2168 A2181

A2192 A2198 A2199 A2200 A2214 C2219 A2220 C2221 U2222 C2225 U2226 A2227 A2228 A2229 A2230 A2237 A2238 A2239 C2240 A2241 A2242 A2243 U2244 A2245 A2246 C2262 C2263 C2284 U2285 A2297 G2300 C2322 C2331 C2332 G2345 G2349 A2350 A2353 C2357 A2361 U2362 A2362

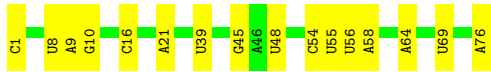
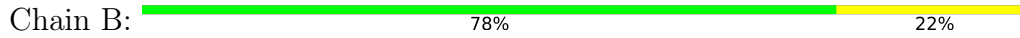
A2363 U2372 G2373 A2374 A2380 A2389 C2400 A2401 U2404 U2407 C2415 C2444 U2445 A2446 A2451 G2478 C2484 U2485 C2493 C2502 C2520 A2521 A2527 A2558 C2570 G2587 G2582 G2593 U2599 A2600 A2601 U2602 U2603 A2617 U2618 G2627 U2628 U2630

A2633 A2634 G2635 U2654 G2655 U2656 C2663 G2666 A2684 A2685 A2696 A2706 C2718 G2719 A2723 G2724 A2725 G2732 A2745 C2761 C2762 A2765 A2766 A2767 A2768 A2775 U2781 A2782 U2786 A2787 C2788 A2791 G2810 G2815 A2832 A2833 C2847 U2864 C2865

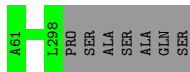
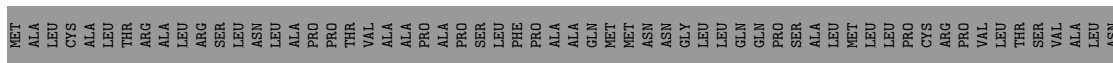
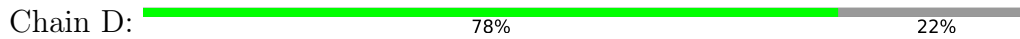
U2862 A2883 C2884 U2885 U2886 U2887 A2888 C2889 A2893 A2910 C2911 C2912 A2913 G2917 A2922 C2928 G2932 A2935 A2956 G2969 A2990 U2991 G2992 A3005 U3006 C3007 G3016 G3040 U3041 A3053 G3054 C3060 U3067 G3090 U3100 A3101 U3102 U3108 U3109 C3110 A3111



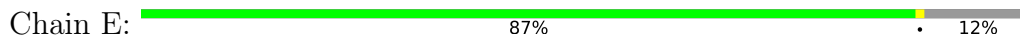
- Molecule 34: mitochondrial tRNA^{Val}



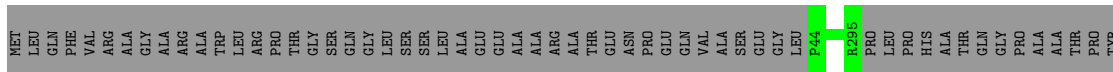
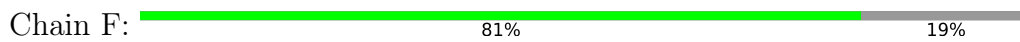
- Molecule 35: 39S ribosomal protein L2, mitochondrial



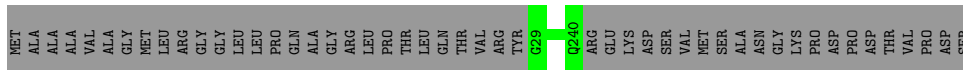
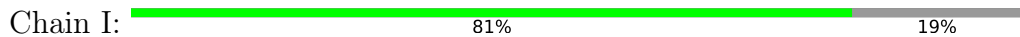
- Molecule 36: 39S ribosomal protein L3, mitochondrial



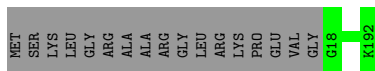
- Molecule 37: 39S ribosomal protein L4, mitochondrial

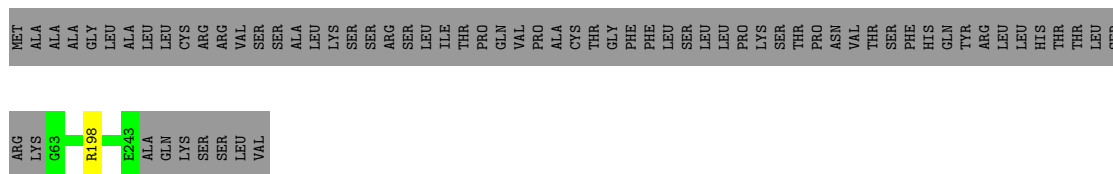


- Molecule 38: 39S ribosomal protein L10, mitochondrial

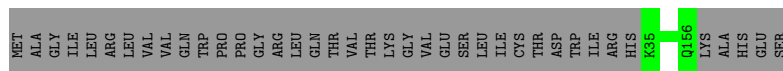
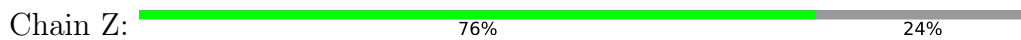


- Molecule 39: 39S ribosomal protein L11, mitochondrial

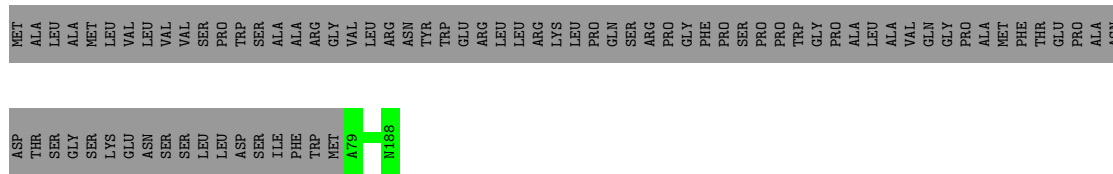




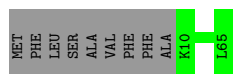
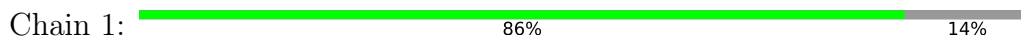
- Molecule 55: 39S ribosomal protein L30, mitochondrial



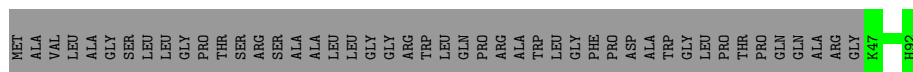
- Molecule 56: 39S ribosomal protein L32, mitochondrial



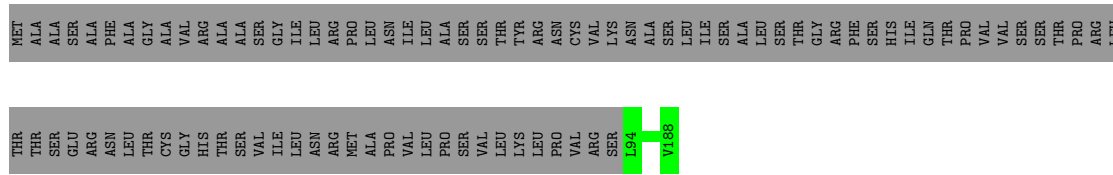
- Molecule 57: 39S ribosomal protein L33, mitochondrial



- Molecule 58: 39S ribosomal protein L34, mitochondrial



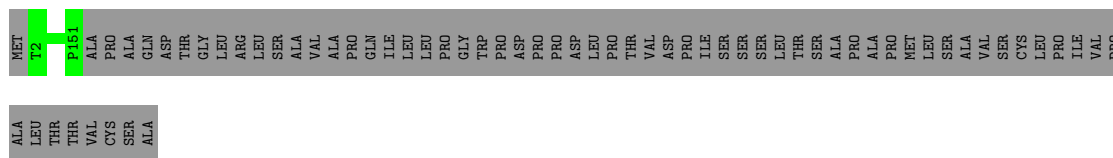
- Molecule 59: 39S ribosomal protein L35, mitochondrial




- Molecule 60: 39S ribosomal protein L36, mitochondrial

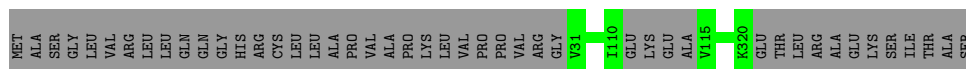
- Molecule 67: 39S ribosomal protein L43, mitochondrial

Chain b:  70% 30%




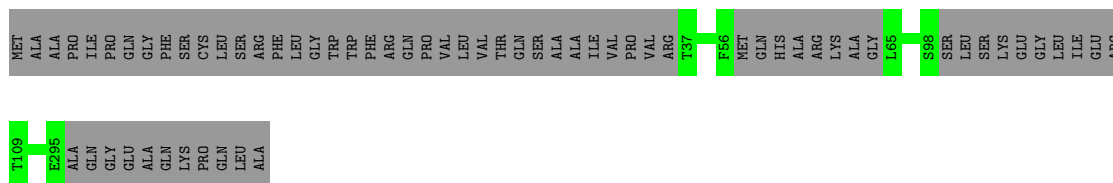
- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c:  86% 14%




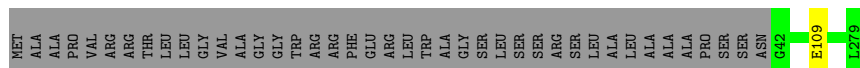
- Molecule 69: 39S ribosomal protein L45, mitochondrial

Chain d:  79% 21%



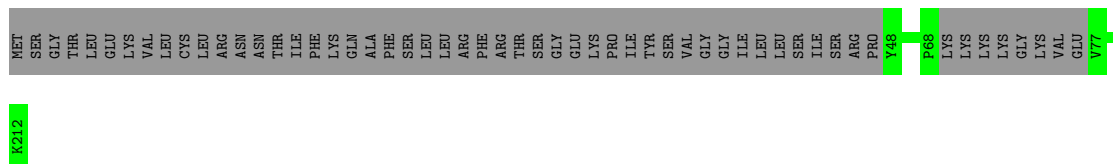
- Molecule 70: 39S ribosomal protein L46, mitochondrial

Chain e:  85% 15%




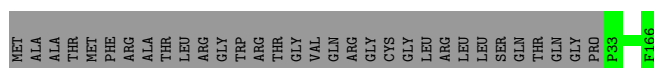
- Molecule 71: 39S ribosomal protein L48, mitochondrial

Chain f:  74% 26%



- Molecule 72: 39S ribosomal protein L49, mitochondrial

Chain g:  81% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82522	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)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
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: OMG, PUT, 5F0, ATP, PSU, MG, SAC, 5MU, GDP, 1MA, OMU, 5MC, 2MG, FES, NAD, AYA, K, B8T, MA6, ZN, SPM, THC, SPD

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	0.27	2/22537 (0.0%)	0.69	6/35085 (0.0%)
2	AB	0.24	0/1871	0.49	0/2531
3	AC	0.25	0/1113	0.48	0/1505
4	AD	0.24	0/2783	0.50	0/3724
5	AE	0.24	0/989	0.51	0/1335
6	AF	0.24	0/1767	0.46	0/2373
7	AG	0.24	0/2746	0.48	0/3681
8	AH	0.25	0/1178	0.47	0/1598
9	AI	0.25	0/1030	0.50	0/1386
10	AJ	0.25	0/855	0.55	0/1148
11	AK	0.22	0/880	0.58	0/1182
12	AL	0.24	0/1477	0.46	0/1974
13	AM	0.24	0/963	0.54	0/1295
14	AN	0.24	0/886	0.49	0/1199
15	AO	0.24	0/1648	0.48	0/2243
16	AP	0.25	0/798	0.44	0/1070
17	AQ	0.24	0/748	0.54	0/994
18	AR	0.24	0/2456	0.44	0/3317
19	AS	0.25	0/1138	0.50	0/1533
20	AT	0.25	0/1402	0.46	0/1883
21	AU	0.23	0/1510	0.53	0/2025
22	AV	0.24	0/3030	0.41	0/4093
23	AW	0.25	0/801	0.52	0/1079
24	AX	0.24	0/2921	0.44	0/3954
25	AZ	0.25	0/857	0.49	0/1141
26	A0	0.24	0/1834	0.53	0/2484
27	A1	0.24	0/2293	0.44	0/3102
28	A2	0.23	0/941	0.53	0/1257
29	A3	0.23	0/636	0.58	0/839
30	Aw	0.29	1/1603 (0.1%)	0.64	0/2488
31	Ax	0.31	1/1655 (0.1%)	0.65	0/2569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ay	0.28	1/1656 (0.1%)	0.65	0/2571
33	A	0.27	1/36876 (0.0%)	0.68	0/57402
34	B	0.35	1/1627 (0.1%)	0.67	0/2527
35	D	0.24	0/1896	0.57	0/2549
36	E	0.25	0/2475	0.46	0/3355
37	F	0.24	0/2090	0.50	0/2842
38	I	0.24	0/1731	0.48	0/2345
39	J	0.25	0/1348	0.47	0/1813
40	K	0.25	0/1490	0.47	0/2021
41	L	0.24	0/905	0.53	0/1218
42	M	0.25	0/2368	0.53	0/3195
43	N	0.25	0/1833	0.51	0/2468
44	O	0.24	0/1283	0.53	0/1727
45	P	0.24	0/1199	0.53	0/1623
46	Q	0.25	0/2027	0.50	0/2734
47	R	0.24	0/1175	0.54	0/1572
48	S	0.24	0/1320	0.52	0/1789
49	T	0.26	0/1403	0.51	0/1886
50	U	0.25	0/1274	0.54	0/1723
51	V	0.24	0/1721	0.51	0/2333
52	W	0.26	0/926	0.49	0/1244
53	X	0.25	0/2099	0.47	0/2837
54	Y	0.24	0/1593	0.50	0/2136
55	Z	0.23	0/1021	0.47	0/1378
56	0	0.24	0/913	0.52	0/1224
57	1	0.24	0/469	0.56	0/621
58	2	0.23	0/383	0.55	0/507
59	3	0.24	0/853	0.53	0/1136
60	4	0.24	0/350	0.56	0/461
61	5	0.24	0/3305	0.48	0/4502
62	6	0.26	0/3043	0.51	0/4140
63	7	0.24	0/2447	0.46	0/3310
64	8	0.24	0/1354	0.48	0/1819
65	9	0.26	0/1025	0.49	0/1379
66	a	0.25	0/866	0.50	0/1174
67	b	0.24	0/1211	0.54	0/1639
68	c	0.24	0/2347	0.46	0/3171
69	d	0.24	0/2039	0.47	0/2759
70	e	0.23	0/1970	0.47	0/2658
71	f	0.25	0/1273	0.44	0/1716
72	g	0.25	0/1151	0.49	0/1569
73	h	0.23	0/918	0.45	0/1249
74	i	0.24	0/850	0.52	0/1135

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	j	0.25	0/760	0.51	0/1023
76	k	0.23	0/777	0.52	0/1048
77	l	0.23	0/707	0.48	0/960
78	m	0.23	0/805	0.57	0/1081
79	o	0.24	0/819	0.57	0/1097
80	p	0.23	0/1223	0.50	0/1641
81	q	0.23	0/1422	0.51	0/1916
82	r	0.24	0/1362	0.52	0/1846
83	s	0.25	0/3239	0.51	0/4400
84	t	0.23	0/358	0.35	0/486
84	u	0.22	0/259	0.33	0/350
84	v	0.22	0/259	0.34	0/350
84	w	0.22	0/246	0.34	0/331
84	x	0.22	0/246	0.34	0/331
84	y	0.22	0/246	0.34	0/331
85	H	0.24	0/1698	0.49	0/2292
86	z	0.24	0/2067	0.46	0/2793
87	AY	0.25	0/1877	0.45	0/2524
88	A5	0.24	0/4737	0.43	0/6398
89	A4	0.24	0/4924	0.43	0/6663
90	A6	0.24	0/619	0.48	0/835
91	Az	0.18	0/981	0.69	0/1522
All	All	0.25	7/197080 (0.0%)	0.57	6/279762 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	1671	G	OP3-P	-10.77	1.48	1.61
31	Ax	1	U	OP3-P	-10.64	1.48	1.61
32	Ay	1	U	OP3-P	-10.56	1.48	1.61
30	Aw	1	U	OP3-P	-10.55	1.48	1.61
34	B	1	C	OP3-P	-10.51	1.48	1.61

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1179	G	C6-N1-C2	18.72	136.33	125.10
1	AA	1179	G	N1-C2-N3	-12.96	116.12	123.90
1	AA	1179	G	C5-C6-N1	-11.62	105.69	111.50
1	AA	1179	G	C2-N3-C4	8.23	116.02	111.90
1	AA	1179	G	N3-C4-C5	-7.12	125.04	128.60

There are no chirality outliers.

There are no planarity outliers.

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	
2	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
3	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
4	AD	341/430 (79%)	329 (96%)	12 (4%)	0	100	100
5	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
6	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
7	AG	323/396 (82%)	315 (98%)	8 (2%)	0	100	100
8	AH	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	22	50
9	AI	134/194 (69%)	131 (98%)	3 (2%)	0	100	100
10	AJ	106/138 (77%)	106 (100%)	0	0	100	100
11	AK	99/128 (77%)	99 (100%)	0	0	100	100
12	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
13	AM	117/137 (85%)	117 (100%)	0	0	100	100
14	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
15	AO	191/258 (74%)	187 (98%)	4 (2%)	0	100	100
16	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
17	AQ	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
18	AR	293/360 (81%)	283 (97%)	10 (3%)	0	100	100
19	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	AU	174/205 (85%)	174 (100%)	0	0	100	100
22	AV	358/414 (86%)	351 (98%)	7 (2%)	0	100	100
23	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
24	AX	350/398 (88%)	343 (98%)	7 (2%)	0	100	100
25	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
26	A0	213/217 (98%)	209 (98%)	4 (2%)	0	100	100
27	A1	275/323 (85%)	271 (98%)	4 (2%)	0	100	100
28	A2	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
29	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
35	D	236/305 (77%)	232 (98%)	4 (2%)	0	100	100
36	E	303/348 (87%)	298 (98%)	4 (1%)	1 (0%)	41	68
37	F	250/311 (80%)	244 (98%)	6 (2%)	0	100	100
38	I	210/261 (80%)	201 (96%)	9 (4%)	0	100	100
39	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
40	K	175/178 (98%)	173 (99%)	2 (1%)	0	100	100
41	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
42	M	287/296 (97%)	284 (99%)	3 (1%)	0	100	100
43	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
44	O	152/175 (87%)	148 (97%)	4 (3%)	0	100	100
45	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
46	Q	236/292 (81%)	234 (99%)	2 (1%)	0	100	100
47	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
48	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
49	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
50	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
51	V	203/216 (94%)	198 (98%)	5 (2%)	0	100	100
52	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
53	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
54	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
55	Z	120/161 (74%)	120 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	0	108/188 (57%)	108 (100%)	0	0	100	100
57	1	54/65 (83%)	54 (100%)	0	0	100	100
58	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
59	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
60	4	36/103 (35%)	36 (100%)	0	0	100	100
61	5	392/423 (93%)	383 (98%)	9 (2%)	0	100	100
62	6	352/380 (93%)	344 (98%)	8 (2%)	0	100	100
63	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
64	8	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
65	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
66	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
67	b	148/215 (69%)	145 (98%)	3 (2%)	0	100	100
68	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
69	d	235/306 (77%)	231 (98%)	4 (2%)	0	100	100
70	e	236/279 (85%)	222 (94%)	13 (6%)	1 (0%)	34	62
71	f	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
72	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
73	h	108/158 (68%)	108 (100%)	0	0	100	100
74	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
75	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
76	k	99/112 (88%)	99 (100%)	0	0	100	100
77	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
78	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
79	o	92/102 (90%)	92 (100%)	0	0	100	100
80	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
81	q	161/222 (72%)	160 (99%)	1 (1%)	0	100	100
82	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
83	s	382/439 (87%)	372 (97%)	10 (3%)	0	100	100
84	t	44/198 (22%)	44 (100%)	0	0	100	100
84	u	30/198 (15%)	30 (100%)	0	0	100	100
84	v	30/198 (15%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	w	29/198 (15%)	29 (100%)	0	0	100	100
84	x	29/198 (15%)	29 (100%)	0	0	100	100
84	y	29/198 (15%)	29 (100%)	0	0	100	100
85	H	200/267 (75%)	194 (97%)	6 (3%)	0	100	100
86	z	250/325 (77%)	240 (96%)	9 (4%)	1 (0%)	34	62
87	AY	219/395 (55%)	207 (94%)	11 (5%)	1 (0%)	29	57
88	A5	579/1394 (42%)	561 (97%)	17 (3%)	1 (0%)	47	75
89	A4	591/689 (86%)	577 (98%)	13 (2%)	1 (0%)	47	75
90	A6	72/109 (66%)	69 (96%)	3 (4%)	0	100	100
All	All	15426/20987 (74%)	15134 (98%)	285 (2%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AH	126	ILE
86	z	128	ASP
87	AY	233	ASP
36	E	150	LYS
70	e	109	GLU

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	
2	AB	198/249 (80%)	198 (100%)	0	100	100
3	AC	115/143 (80%)	115 (100%)	0	100	100
4	AD	286/357 (80%)	286 (100%)	0	100	100
5	AE	104/107 (97%)	104 (100%)	0	100	100
6	AF	185/209 (88%)	185 (100%)	0	100	100
7	AG	285/342 (83%)	285 (100%)	0	100	100
8	AH	130/180 (72%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AI	104/146 (71%)	104 (100%)	0	100	100
10	AJ	93/118 (79%)	93 (100%)	0	100	100
11	AK	91/113 (80%)	91 (100%)	0	100	100
12	AL	158/226 (70%)	158 (100%)	0	100	100
13	AM	97/113 (86%)	97 (100%)	0	100	100
14	AN	96/115 (84%)	96 (100%)	0	100	100
15	AO	174/230 (76%)	174 (100%)	0	100	100
16	AP	88/123 (72%)	88 (100%)	0	100	100
17	AQ	78/79 (99%)	78 (100%)	0	100	100
18	AR	264/318 (83%)	264 (100%)	0	100	100
19	AS	116/164 (71%)	116 (100%)	0	100	100
20	AT	153/157 (98%)	153 (100%)	0	100	100
21	AU	152/174 (87%)	152 (100%)	0	100	100
22	AV	325/364 (89%)	325 (100%)	0	100	100
23	AW	87/158 (55%)	87 (100%)	0	100	100
24	AX	311/351 (89%)	311 (100%)	0	100	100
25	AZ	90/95 (95%)	90 (100%)	0	100	100
26	A0	188/189 (100%)	188 (100%)	0	100	100
27	A1	255/291 (88%)	255 (100%)	0	100	100
28	A2	100/101 (99%)	100 (100%)	0	100	100
29	A3	65/166 (39%)	65 (100%)	0	100	100
35	D	192/245 (78%)	192 (100%)	0	100	100
36	E	260/290 (90%)	259 (100%)	1 (0%)	91	96
37	F	219/262 (84%)	219 (100%)	0	100	100
38	I	194/232 (84%)	194 (100%)	0	100	100
39	J	138/150 (92%)	138 (100%)	0	100	100
40	K	154/155 (99%)	154 (100%)	0	100	100
41	L	98/124 (79%)	98 (100%)	0	100	100
42	M	245/249 (98%)	245 (100%)	0	100	100
43	N	189/211 (90%)	189 (100%)	0	100	100
44	O	134/150 (89%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	P	126/155 (81%)	126 (100%)	0	100	100
46	Q	220/256 (86%)	220 (100%)	0	100	100
47	R	118/126 (94%)	118 (100%)	0	100	100
48	S	146/180 (81%)	146 (100%)	0	100	100
49	T	146/176 (83%)	146 (100%)	0	100	100
50	U	134/135 (99%)	134 (100%)	0	100	100
51	V	183/191 (96%)	183 (100%)	0	100	100
52	W	94/119 (79%)	94 (100%)	0	100	100
53	X	220/229 (96%)	220 (100%)	0	100	100
54	Y	163/223 (73%)	162 (99%)	1 (1%)	86	95
55	Z	113/147 (77%)	113 (100%)	0	100	100
56	0	99/164 (60%)	99 (100%)	0	100	100
57	1	53/60 (88%)	53 (100%)	0	100	100
58	2	40/72 (56%)	40 (100%)	0	100	100
59	3	88/166 (53%)	88 (100%)	0	100	100
60	4	37/89 (42%)	37 (100%)	0	100	100
61	5	353/368 (96%)	353 (100%)	0	100	100
62	6	313/332 (94%)	313 (100%)	0	100	100
63	7	270/303 (89%)	270 (100%)	0	100	100
64	8	146/190 (77%)	146 (100%)	0	100	100
65	9	104/112 (93%)	104 (100%)	0	100	100
66	a	96/133 (72%)	95 (99%)	1 (1%)	76	91
67	b	131/185 (71%)	131 (100%)	0	100	100
68	c	251/288 (87%)	251 (100%)	0	100	100
69	d	223/274 (81%)	223 (100%)	0	100	100
70	e	207/236 (88%)	207 (100%)	0	100	100
71	f	139/188 (74%)	139 (100%)	0	100	100
72	g	124/148 (84%)	124 (100%)	0	100	100
73	h	104/148 (70%)	104 (100%)	0	100	100
74	i	86/110 (78%)	86 (100%)	0	100	100
75	j	74/97 (76%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	k	83/90 (92%)	83 (100%)	0	100	100
77	l	76/116 (66%)	76 (100%)	0	100	100
78	m	85/113 (75%)	85 (100%)	0	100	100
79	o	80/87 (92%)	80 (100%)	0	100	100
80	p	135/181 (75%)	135 (100%)	0	100	100
81	q	142/178 (80%)	142 (100%)	0	100	100
82	r	147/169 (87%)	147 (100%)	0	100	100
83	s	340/381 (89%)	340 (100%)	0	100	100
84	t	40/158 (25%)	40 (100%)	0	100	100
84	u	31/158 (20%)	31 (100%)	0	100	100
84	v	31/158 (20%)	31 (100%)	0	100	100
84	w	30/158 (19%)	30 (100%)	0	100	100
84	x	30/158 (19%)	30 (100%)	0	100	100
84	y	30/158 (19%)	30 (100%)	0	100	100
85	H	182/228 (80%)	182 (100%)	0	100	100
86	z	226/287 (79%)	226 (100%)	0	100	100
87	AY	202/357 (57%)	202 (100%)	0	100	100
88	A5	515/1219 (42%)	515 (100%)	0	100	100
89	A4	532/609 (87%)	532 (100%)	0	100	100
90	A6	63/90 (70%)	63 (100%)	0	100	100
All	All	13812/18099 (76%)	13809 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	E	303	LYS
54	Y	198	ARG
66	a	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
54	Y	179	HIS
62	6	320	GLN

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Mol	Chain	Res	Type
89	A4	381	GLN
88	A5	201	GLN
54	Y	225	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	950/954 (99%)	135 (14%)	1 (0%)
30	Aw	67/68 (98%)	18 (26%)	0
31	Ax	68/70 (97%)	12 (17%)	0
32	Ay	68/70 (97%)	13 (19%)	0
33	A	1556/1561 (99%)	224 (14%)	3 (0%)
34	B	71/72 (98%)	12 (16%)	0
91	Az	41/42 (97%)	21 (51%)	0
All	All	2821/2837 (99%)	435 (15%)	4 (0%)

5 of 435 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	651	A
1	AA	673	U
1	AA	680	U
1	AA	688	A
1	AA	695	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1539	C
33	A	2030	U
33	A	2112	A
33	A	2245	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	AA	1076	1	19,22,23	0.63	0	28,32,35	1.21	3 (10%)
33	PSU	A	3067	33	18,21,22	0.79	0	22,30,33	2.55	5 (22%)
67	THC	b	2	67	8,9,10	0.28	0	9,11,13	0.52	0
1	B8T	AA	1486	1,95	19,22,23	0.30	0	26,31,34	0.35	0
34	2MG	B	10	34	18,26,27	1.15	2 (11%)	16,38,41	0.95	2 (12%)
1	MA6	AA	1584	1	18,26,27	0.76	0	19,38,41	0.60	0
40	SAC	K	2	40	7,8,9	0.21	0	8,9,11	0.55	0
33	OMG	A	3040	30,33	18,26,27	0.93	2 (11%)	19,38,41	0.61	0
34	1MA	B	9	34	16,25,26	1.16	3 (18%)	18,37,40	0.85	1 (5%)
1	5MC	AA	1488	1	18,22,23	0.32	0	26,32,35	0.42	0
1	MA6	AA	1583	1	18,26,27	0.75	0	19,38,41	0.54	0
33	OMG	A	2815	31,33,96	18,26,27	0.96	3 (16%)	19,38,41	0.61	0
17	AYA	AQ	2	17	6,7,8	0.78	0	5,8,10	0.43	0
33	OMU	A	3039	33,96	19,22,23	0.29	0	26,31,34	0.43	0
34	PSU	B	39	34	18,21,22	0.77	0	22,30,33	2.55	4 (18%)
50	AYA	U	2	50	6,7,8	0.77	0	5,8,10	0.58	0
76	AYA	k	2	76	6,7,8	0.82	0	5,8,10	0.50	0
28	AYA	A2	2	28	6,7,8	0.80	0	5,8,10	0.58	0
33	1MA	A	2617	33	16,25,26	1.17	3 (18%)	18,37,40	0.90	1 (5%)
9	5F0	AI	184	9	8,8,9	0.59	0	7,9,11	1.17	1 (14%)

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
1	5MU	AA	1076	1	-	0/7/25/26	0/2/2/2
33	PSU	A	3067	33	-	0/7/25/26	0/2/2/2
67	THC	b	2	67	-	0/8/10/12	-
1	B8T	AA	1486	1,95	-	1/7/27/28	0/2/2/2
34	2MG	B	10	34	-	0/5/27/28	0/3/3/3
1	MA6	AA	1584	1	-	2/7/29/30	0/3/3/3
40	SAC	K	2	40	-	0/7/8/10	-
33	OMG	A	3040	30,33	-	0/5/27/28	0/3/3/3
34	1MA	B	9	34	-	0/3/25/26	0/3/3/3
1	5MC	AA	1488	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	AA	1583	1	-	0/7/29/30	0/3/3/3
33	OMG	A	2815	31,33,96	-	0/5/27/28	0/3/3/3
17	AYA	AQ	2	17	-	0/4/6/8	-
33	OMU	A	3039	33,96	-	0/9/27/28	0/2/2/2
34	PSU	B	39	34	-	0/7/25/26	0/2/2/2
50	AYA	U	2	50	-	1/4/6/8	-
76	AYA	k	2	76	-	1/4/6/8	-
28	AYA	A2	2	28	-	0/4/6/8	-
33	1MA	A	2617	33	-	0/3/25/26	0/3/3/3
9	5F0	AI	184	9	-	0/9/9/10	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	2617	1MA	C6-N6	3.10	1.35	1.27
34	B	10	2MG	C8-N7	-3.08	1.29	1.35
34	B	9	1MA	C6-N6	3.07	1.35	1.27
34	B	10	2MG	C5-C6	-2.37	1.42	1.47
33	A	2815	OMG	C5-C6	-2.34	1.42	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	39	PSU	N1-C2-N3	8.07	124.27	115.13
33	A	3067	PSU	N1-C2-N3	8.04	124.24	115.13
34	B	39	PSU	C4-N3-C2	-6.57	116.87	126.34
33	A	3067	PSU	C4-N3-C2	-6.53	116.93	126.34
1	AA	1076	5MU	C4-N3-C2	-4.83	121.11	127.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1584	MA6	C5-C6-N6-C9
76	k	2	AYA	C-CA-N-CT
1	AA	1584	MA6	C4'-C5'-O5'-P
1	AA	1486	B8T	O4'-C4'-C5'-O5'
50	U	2	AYA	C-CA-N-CT

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 271 ligands modelled in this entry, 258 are monoatomic - leaving 13 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
93	SPM	AA	1702	-	13,13,13	0.25	0	12,12,12	0.99	0
101	PUT	A	3304	-	5,5,5	0.24	0	4,4,4	0.51	0
94	SPD	A	3303	-	9,9,9	0.26	0	8,8,8	1.18	0
98	FES	r	201	38,82	0,4,4	-	-	-		
98	FES	AT	201	13,20	0,4,4	-	-	-		
92	NAD	AA	1701	95	42,48,48	0.57	0	50,73,73	0.59	1 (2%)
100	GDP	AX	503	-	24,30,30	0.88	1 (4%)	30,47,47	0.60	0
94	SPD	A	3301	-	9,9,9	0.22	0	8,8,8	1.24	0
94	SPD	AA	1703	-	9,9,9	0.24	0	8,8,8	1.34	2 (25%)
98	FES	AP	201	16,5	0,4,4	-	-	-		
94	SPD	A	3302	-	9,9,9	0.25	0	8,8,8	1.15	0
99	ATP	AX	501	95	26,33,33	0.75	0	31,52,52	0.64	0
102	VAL	B	101	34	4,6,7	0.53	0	6,7,9	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPM	AA	1702	-	-	0/11/11/11	-
101	PUT	A	3304	-	-	0/3/3/3	-
94	SPD	A	3303	-	-	2/7/7/7	-
98	FES	r	201	38,82	-	-	0/1/1/1
98	FES	AT	201	13,20	-	-	0/1/1/1
92	NAD	AA	1701	95	-	0/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
100	GDP	AX	503	-	-	0/12/32/32	0/3/3/3
94	SPD	A	3301	-	-	1/7/7/7	-
94	SPD	AA	1703	-	-	0/7/7/7	-
98	FES	AP	201	16,5	-	-	0/1/1/1
94	SPD	A	3302	-	-	0/7/7/7	-
99	ATP	AX	501	95	-	0/18/38/38	0/3/3/3
102	VAL	B	101	34	-	0/5/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
100	AX	503	GDP	C5-C6	-2.16	1.43	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
94	AA	1703	SPD	C4-C5-N6	-2.33	105.86	112.14
92	AA	1701	NAD	C5A-C6A-N6A	2.28	123.81	120.35
94	AA	1703	SPD	C8-C7-N6	-2.10	106.46	112.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

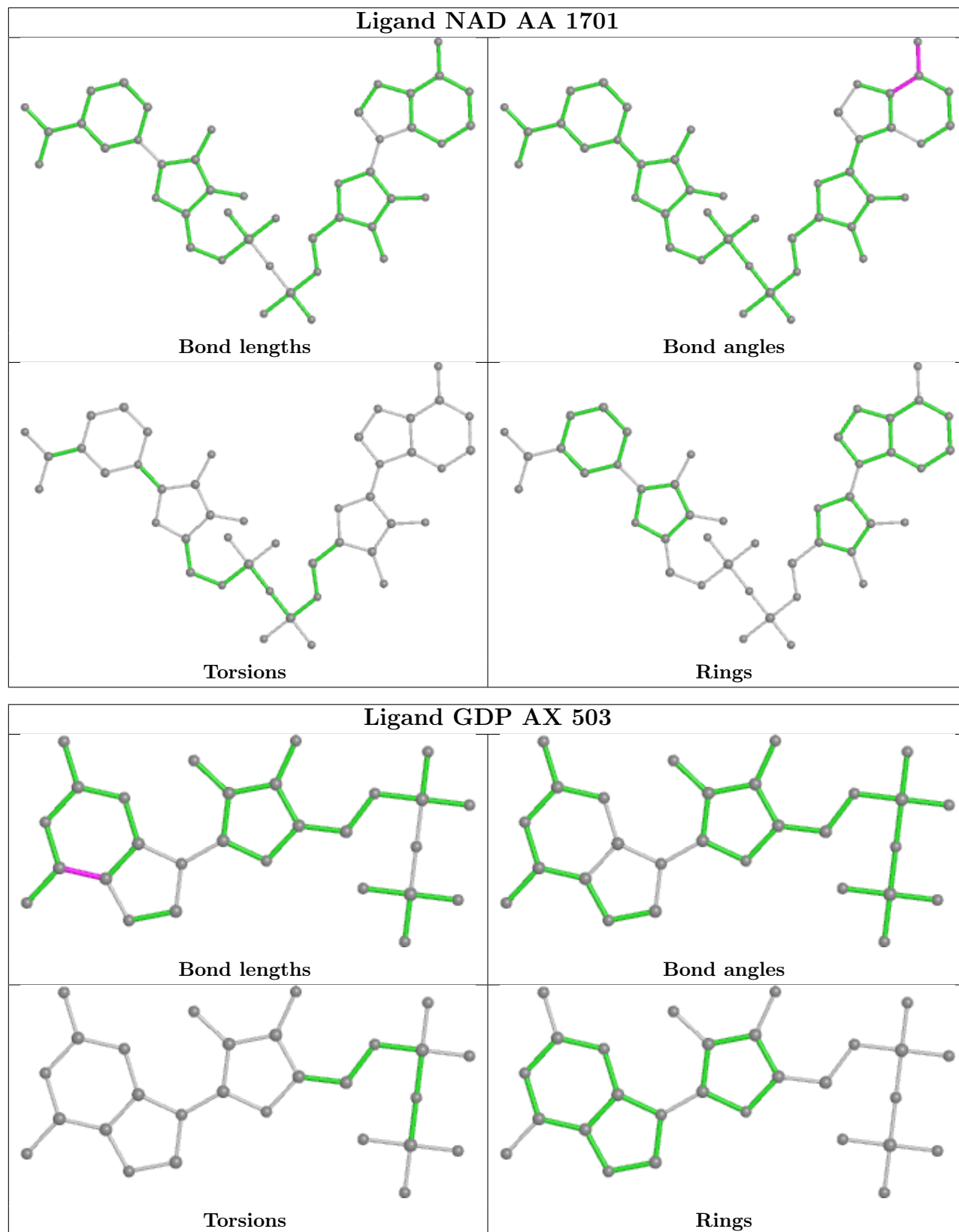
Mol	Chain	Res	Type	Atoms
94	A	3303	SPD	C4-C5-N6-C7
94	A	3303	SPD	C8-C7-N6-C5
94	A	3301	SPD	N6-C7-C8-C9

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
32	Ay	1
31	Ax	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ay	15:A	O3'	21:A	P	9.63
1	Ax	15:A	O3'	21:A	P	8.88

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15544. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

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.