



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:40 PM BST

PDB ID : 3J9M  
EMDB ID: : EMD-2876  
Title : Structure of the human mitochondrial ribosome (class 1)  
Authors : Amunts, A.; Brown, A.; Toots, J.; Scheres, S.H.; Ramakrishnan, V.  
Deposited on : 2015-02-08  
Resolution : 3.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

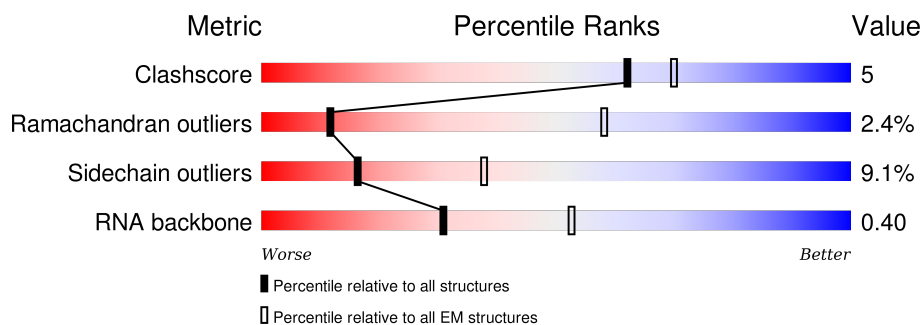
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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











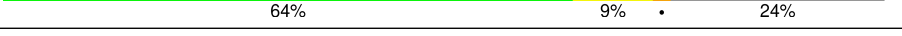

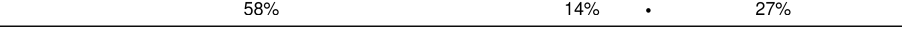
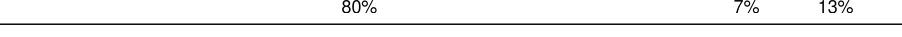

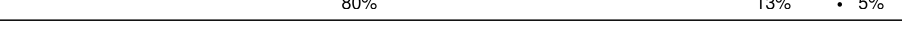


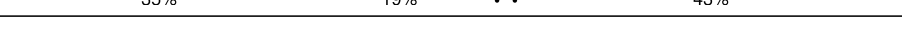

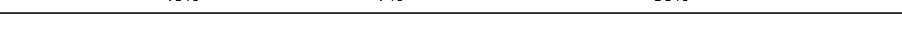






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	1559	48% 37% 9% 6%
2	B	73	40% 32% 5% 23%
3	D	305	62% 14% • 23%
4	E	348	70% 14% • 14%
5	F	311	61% 17% • 20%
6	H	267	31% • 64%
7	I	261	49% 11% 39%
8	J	192	63% 8% • 27%




















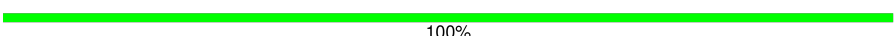





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Mol	Chain	Length	Quality of chain
9	K	178	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	179	
15	Q	292	
16	R	149	
17	S	205	
18	T	212	
19	U	153	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	
28	3	188	
29	4	103	
30	5	423	
31	6	380	
32	7	338	
33	8	206	




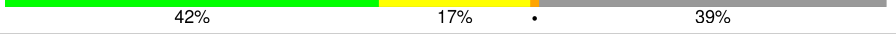



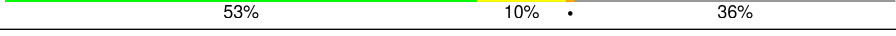
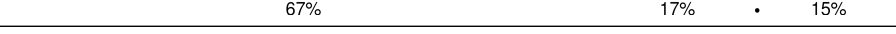








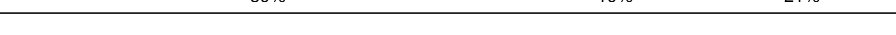


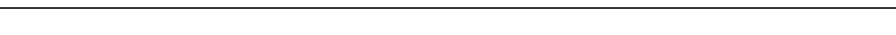




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Mol	Chain	Length	Quality of chain
34	9	137	
35	a	142	
36	b	155	
37	c	332	
38	d	306	
39	e	279	
40	f	194	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	t	28	
54	u	2	
55	AA	954	
56	AB	296	
57	AC	167	
58	AD	430	

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Mol	Chain	Length	Quality of chain
59	AE	125	
60	AF	242	
61	AG	396	
62	AH	201	
63	AI	194	
64	AJ	138	
65	AK	128	
66	AL	257	
67	AM	137	
68	AN	130	
69	AO	258	
70	AP	142	
71	AQ	87	
72	AR	360	
73	AS	190	
74	AT	173	
75	AU	205	
76	AV	414	
77	AW	187	
78	AX	398	
79	AY	395	
80	AZ	106	
81	A0	218	
82	A1	323	
83	A2	118	

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Mol	Chain	Length	Quality of chain
84	A3	199	<div><div></div><div>28%7%65%</div></div>
85	A4	579	<div><div></div><div>65%7%28%</div></div>

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 158384 atoms, of which 0 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1472	Total	C	N	O	P	0	0
			31261	14025	5642	10122	1472		

- Molecule 2 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 3 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 4 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	300	Total	C	N	O	S	0	0
			2365	1523	410	422	10		

- Molecule 5 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 6 is a protein called bL9m.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	95	Total	C	N	O	0	0
			784	498	152	134		

- Molecule 7 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 9 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 13 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called uL18m.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	133	Total	C	N	O	S	0	0
			1080	677	209	189	5		

- Molecule 15 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	219	Total	C	N	O	S	0	0
			1822	1168	322	323	9		

- Molecule 16 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 18 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	111	Total	C	N	O	S	0	0
			922	591	176	153	2		

- Molecule 20 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	189	Total	C	N	O	S	0	0
			1551	987	278	278	8		

- Molecule 21 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 22 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

- Molecule 23 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 28 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 30 is a protein called mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	376	Total	C	N	O	S	0	0
			3064	1987	529	538	10		

- Molecule 31 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	325	Total	C	N	O	S	0	0
			2636	1692	465	470	9		

- Molecule 32 is a protein called mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	266	Total	C	N	O	S	0	0
			2158	1383	371	388	16		

- Molecule 33 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 34 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	109	Total	C	N	O	S	0	0
			873	565	152	154	2		

- Molecule 35 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 36 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	162	Total	C	N	O	S	0	0
			1347	870	234	235	8		

- Molecule 39 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 40 is a protein called mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	131	Total	C	N	O	S	0	0
			1039	663	169	203	4		

- Molecule 41 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 42 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 43 is a protein called mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 44 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 45 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	84	Total	C	N	O	S	0	0
			655	407	122	121	5		

- Molecule 46 is a protein called mL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 47 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 48 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 49 is a protein called mL62 (ICT1).

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 50 is a protein called mL64 (CRIF1).

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 51 is a protein called mL66 (bS18a).

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 52 is a protein called mL65 (mS30).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 53 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	t	28	Total	C	N	O		
			140	84	28	28	0	0

- Molecule 54 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 55 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AA	923	Total	C	N	O	P	0	0
			19606	8790	3535	6358	923		

- Molecule 56 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AB	217	Total	C	N	O	S	0	0
			1768	1131	321	306	10		

- Molecule 57 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AC	132	Total	C	N	O	S	0	0
			1082	699	195	184	4		

- Molecule 58 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AD	322	Total	C	N	O	S	0	0
			2557	1611	476	457	13		

- Molecule 59 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 60 is a protein called uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AF	201	Total	C	N	O	S	0	0
			1668	1069	305	283	11		

- Molecule 61 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AG	305	Total	C	N	O	S	0	0
			2516	1599	448	455	14		

- Molecule 62 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AH	122	Total	C	N	O	S	0	0
			999	643	168	185	3		

- Molecule 63 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AI	136	Total	C	N	O	S	0	0
			1011	637	192	178	4		

- Molecule 64 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AJ	108	Total	C	N	O	S	0	0
			838	521	169	142	6		

- Molecule 65 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AK	101	Total	C	N	O	S	0	0
			861	537	179	140	5		

- Molecule 66 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AL	164	Total	C	N	O	S	0	0
			1382	883	257	235	7		

- Molecule 67 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AM	116	Total	C	N	O	S	0	0
			920	582	182	150	6		

- Molecule 68 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AN	107	Total	C	N	O	S	0	0
			846	549	153	141	3		

- Molecule 69 is a protein called mS40 (bS18b).

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AO	185	Total	C	N	O	S	0	0
			1528	970	285	267	6		

- Molecule 70 is a protein called bS18m (bS18c).



Mol	Chain	Residues	Atoms					AltConf	Trace
70	AP	96	Total	C	N	O	S	0	0
			774	498	133	135	8		

- Molecule 71 is a protein called bs21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AQ	86	Total	C	N	O	S	0	0
			740	458	150	124	8		

- Molecule 72 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AR	242	Total	C	N	O	S	0	0
			2008	1285	343	372	8		

- Molecule 73 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AS	126	Total	C	N	O	S	0	0
			1042	673	183	185	1		

- Molecule 74 is a protein called mS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AT	162	Total	C	N	O	S	0	0
			1330	850	231	238	11		

- Molecule 75 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AU	173	Total	C	N	O	S	0	0
			1461	900	294	263	4		

- Molecule 76 is a protein called mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AV	328	Total	C	N	O	S	0	0
			2702	1737	452	502	11		

- Molecule 77 is a protein called bs1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AW	97	Total	C	N	O	S	0	0
			766	486	137	139	4		

- Molecule 78 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AX	316	Total	C	N	O	S	0	0
			2531	1625	440	455	11		

- Molecule 79 is a protein called mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AY	108	Total	C	N	O	S	0	0
			914	593	150	169	2		

- Molecule 80 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AZ	87	Total	C	N	O	S	0	0
			740	473	133	130	4		

- Molecule 81 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	A0	201	Total	C	N	O	S	0	0
			1684	1065	322	292	5		

- Molecule 82 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	A1	256	Total	C	N	O	S	0	0
			2076	1321	350	395	10		

- Molecule 83 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	A2	116	Total	C	N	O	S	0	0
			925	574	181	162	8		

- Molecule 84 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	A3	69	Total	C	N	O	S	0	0
			610	393	130	86	1		

- Molecule 85 is a protein called mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	A4	414	Total	C	N	O	S	0	0
			2838	1805	490	529	14		

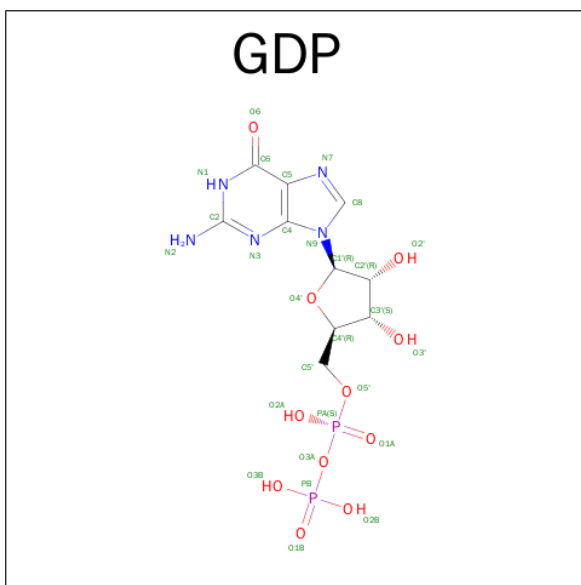
- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	g	1	Total	Mg	0
			1	1	
86	A	97	Total	Mg	0
			97	97	
86	AA	28	Total	Mg	0
			28	28	
86	M	1	Total	Mg	0
			1	1	

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	0	1	Total	Zn	0
			1	1	
87	AP	1	Total	Zn	0
			1	1	
87	AT	1	Total	Zn	0
			1	1	
87	AB	1	Total	Zn	0
			1	1	
87	4	1	Total	Zn	0
			1	1	
87	AO	1	Total	Zn	0
			1	1	
87	r	1	Total	Zn	0
			1	1	

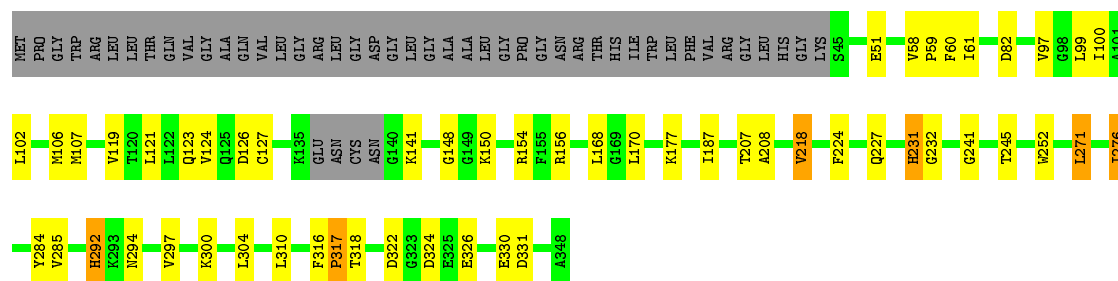
- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
88	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

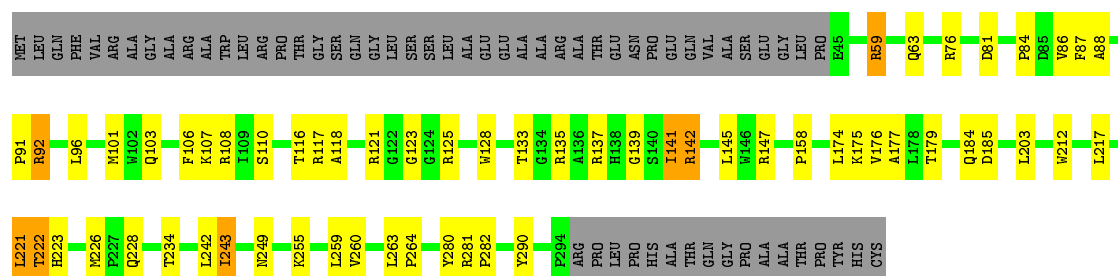






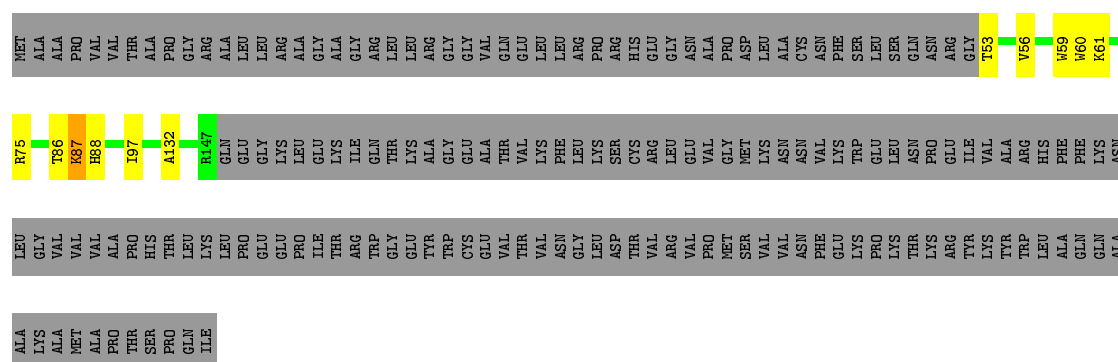
- Molecule 5: uL4m

Chain F: 61% 17% 20%



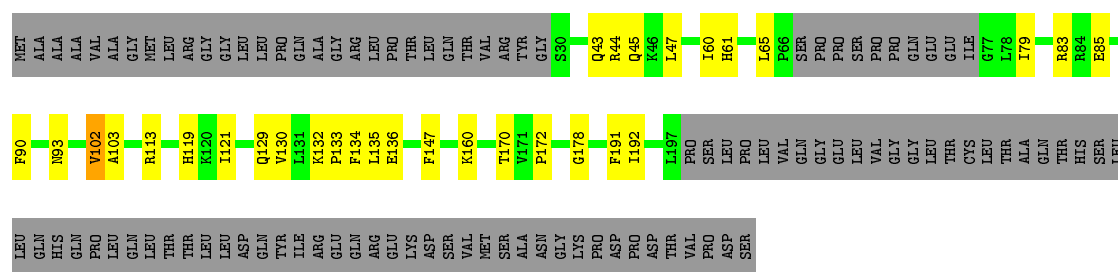
- Molecule 6: bL9m

Chain H: 31% 64%

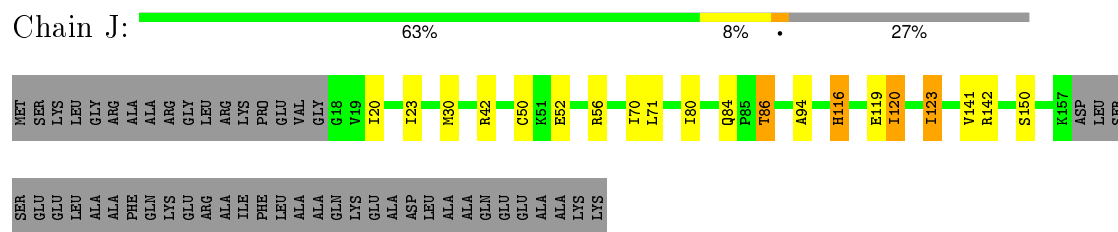


- Molecule 7: uL10m

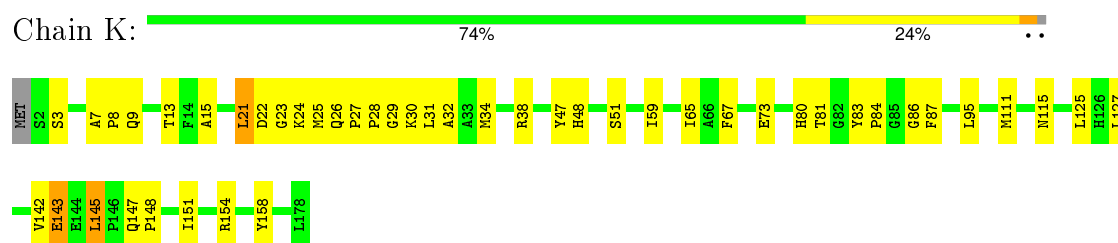
Chain I: 49% 11% 39%



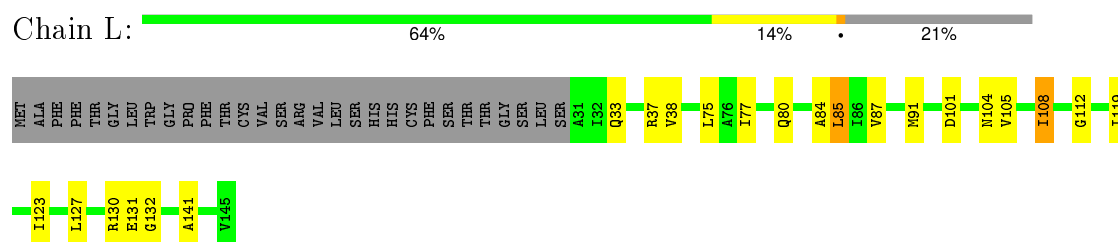
- Molecule 8: uL11m



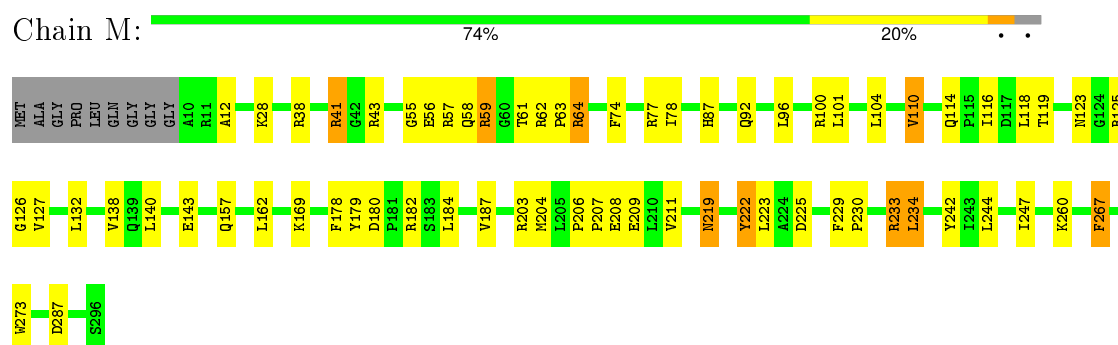
- Molecule 9: uL13m



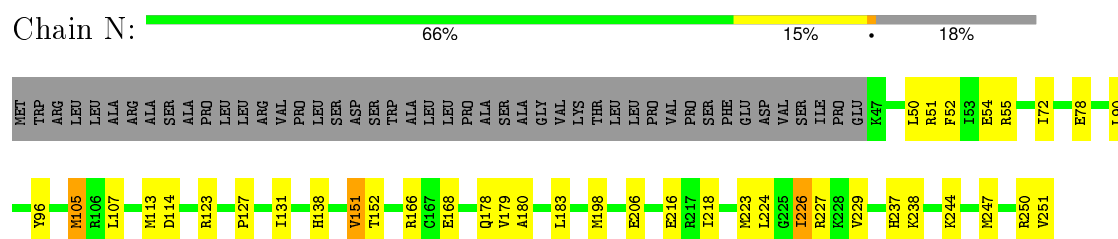
- Molecule 10: uL14m



- Molecule 11: uL15m



- Molecule 12: uL16m

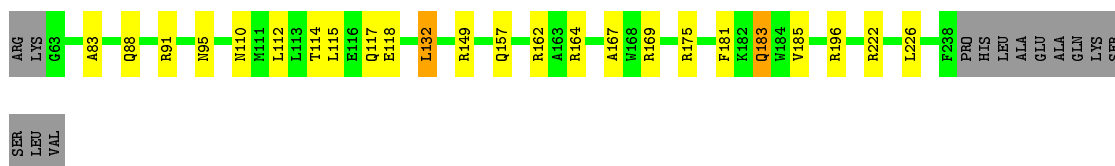


- Molecule 13: bL17m



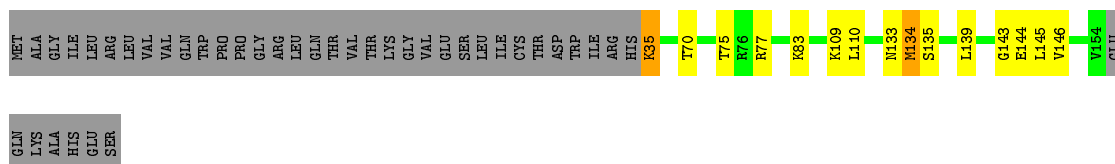






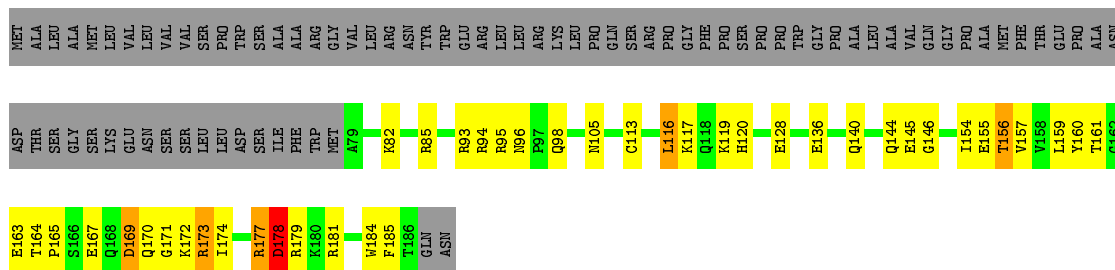
- Molecule 24: uL30m

Chain Z: 65% 8% 25%



- Molecule 25: bL32m

Chain 0: 35% 19% 43%



- Molecule 26: bL33m

Chain 1: 62% 17% 20%



- Molecule 27: bL34m

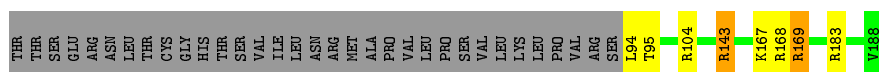
Chain 2: 40% 7% 50%



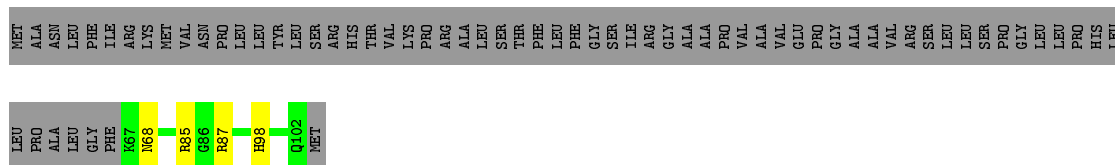
- Molecule 28: bL35m

Chain 3: 46% 49%

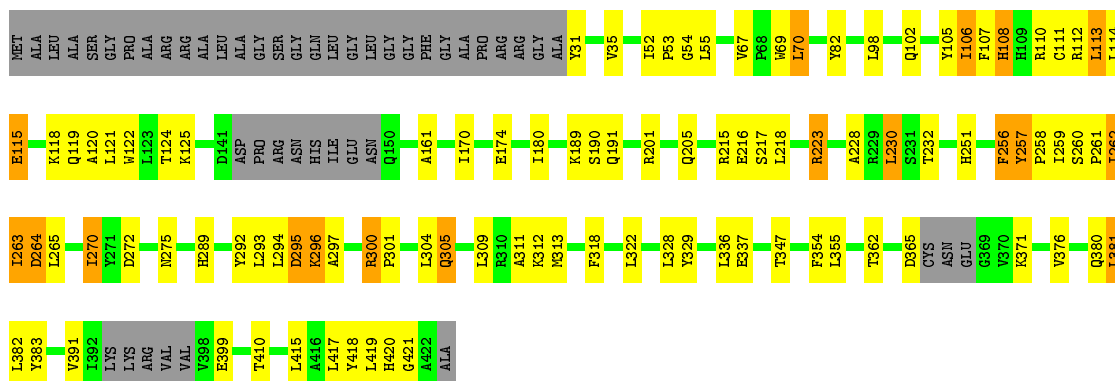




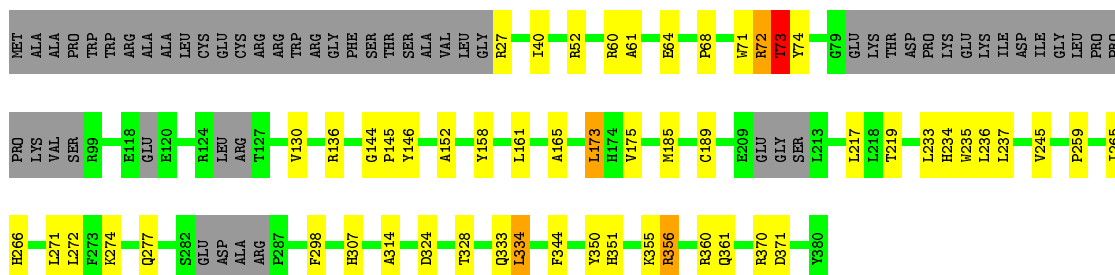
- Molecule 29: bL36m



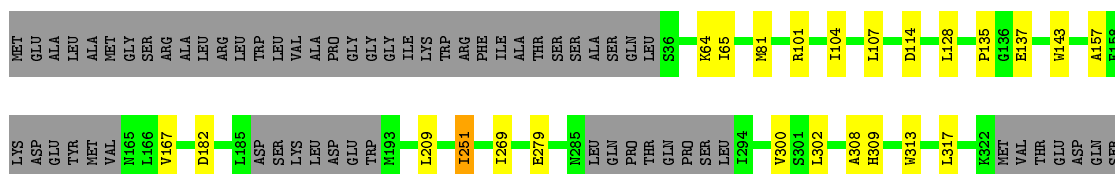
- Molecule 30: mL37



- Molecule 31: mL38



- Molecule 32: mL39



LYS  
ALA  
THR  
GLU  
GLU  
CYS  
THR  
SER  
THR

- Molecule 33: mL40

Chain 8:  46% 52%

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

ASP GLN GLU ALA LYS LEU ARG LYS LEU THR GLN THR TRP T83 L140 Q143 L150 F169 P170 P181 ILE PRO ASN TYR PHE GLN TRP PRO GLU LEU ILE ARG TYR ASN ASP SER ILE GLU THR LYS VAL ARG LYS LYS VAL PHE LYS ARG

- Molecule 34: mL41

Chain 9:  67% 12% 20%

MET GLY VAL LEU ALA ALA ALA ARG CYS LEU VAL ARG GLY A15 D16 R17 S23 R24 R25 G26 I41 S46 I53 F92 Y96 A97 P98 D103 PHE LYS ASP GLY THR PHE ASP PRO ASP ASN LEU LYS TYR G118 P121 T122 Q123 Y131 P132 R133 N134

F135 L136 R137


- Molecule 35: mL42

Chain a:  54% 42%

MET VAL VAL VAL LYS TRP VAL MET SER LYS THR ILE LEU LYS HIS LEU PHE PRO VAL GLN ASN GLY ALA TYR CYS VAL CYS HIS LYS SER T35 I44 R77 PRO ASP PHE VAL HIS ASN GLU GLU THR HIS ASP GLN VAL LEU LYS THR ARG LEU GLU

LYS VAL GLU HIS LEU E104 I109 E110 Q111 T118 R122 R142

- Molecule 36: mL43

Chain b:  86% 8% 5%

MET T2 R9 F10 L11 L15 L26 R49 R68 P69 C70 C71 R85 E96 K103 R116 K117 N135 Q149 ASP PRO ALA PRO ALA ALA GLN

- Molecule 37: mL44

Chain c:  75% 8% 17%

MET ALA SER GLY LEU VAL ARG LEU LEU GLN GLY HIS ARG CYS LEU LEU ALA PRO VAL ALA PRO LYS LEU VAL PRO VAL VAL ARG GLY Y31 R32 R33 Q34 F35 R40 E44 P64 N65 F83 L87 L88 G107 LEU GLY ILE GLU LYS LYS GLU ALA VAL LEU LEU ASN

L119 Q123 D147 E183 L191 T211 L241 V250 Q260 T264 P268 L269 Y270 F271 L280 E283 N310 R311 R312 P313 N314 F315 Y316 SER LYS LYS LYS THR LEU ARG ALA GLU LYS SER ILE THR ALA SER

- Molecule 38: mL45

Chain d:  49% 47%

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

ARG LYS ALA GLY LEU VAL ILE PRO PRO GLY LYS SER MET ASP ARG ARG SER ILE TRP HIS LEU ALA CYS THR ARG GLY ILE THR ASP PHE ASP ALA TYR VAL PRO PRO ILE GLY GLY ALA ALA ARG THR LYS GLY LEU ILE TYR GLN LYS ARG THR ARG ARG MET LYS LYS THR MET A117 R159

V164 T165 E166 E187 V195 C199 SER SER MET MET ASN GLN N207 V208 Y209 L231 L252 THR ASN P255 P268 P272 L287 LYS PRO GLU ALA ALA ARG THR LYS GLU TYR GLU GLU ALA ALA SER THR LYS LYS ARG PHE THR LYS GLN GLY GLU ALA GLN LYS PRO GLN LEU ALA

- Molecule 39: mL46

Chain e: 73% 5% 22%

MET ALA ALA PRO VAL ARG ARG THR LEU LEU GLY VAL VAL GLY GLY TRP ARG ARG PHE GLU ARG ALA TRP MET ARG THR GLY SER LEU SER SER ARG SER LEU D242 F243 S244 Q245 D258 L279

GLN ASP ILE L116 Q126 E139 D145 R151 L157 P174 F217 PRO GLN ALA MET ARG THR GLU SER ASN L227 D242 F243 S244 Q245 D258 L279

- Molecule 40: mL48

Chain f: 63% 32%

MET SER GLY THR LEU GLY VAL VAL CYS LEU ARG ARG ASN ASN THR ILE PHE LYS GLN ALA PHE SER LEU LEU ARG PHE ARG THR SER GLY GLY ILE LEU LEU SER SER ARG ARG Y48 K51 E66 GLU PRO LYS LYS LYS GLY LYS

VAL GLU V77 G83 V90 Q138 ASP GLN GLY SER LYS M144 A164 T165 F166 S185 E188 H189 T190 D193 PHE

- Molecule 41: mL49

Chain g: 69% 9% 22%

MET ALA ALA THR MET PHE ARG ALA THR LEU LEU ARG GLY TRP ARG THR GLY VAL GLN ARG GLY CYS GLY LEU ARG LEU LEU SER GLN THR GLN GLY PRO PRO ASP TYR PRO ARG F38 T55 S70 R76 I100 T101 N104 M107 R111 Q121 P136 V137 N141

G145 T146 L147 Q155 F166

- Molecule 42: mL50

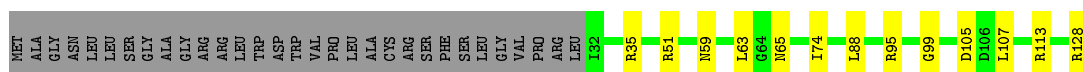
Chain h: 54% 9% 37%

MET ALA ALA ARG SER VAL SER GLY THR ARG ARG VAL PHE MET TRP THR VAL SER GLY THR PRO CYS ARG GLU PHE TRP SER ARG PHE ARG LYS PRO GLU VAL VAL VAL VAL GLU THR VAL VAL GLU LYS LYS GLU PRO ILE LEU VAL CYS PRO PRO LEU R56 D65 L66

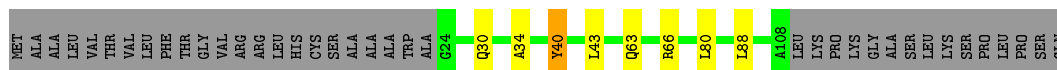
L70 Y73 F78 G79 L82 E92 L100 L117 M120 D125 M131 R137 S138 S146 M147 W156 S157 Y158

- Molecule 43: mL51

Chain i: 66% 10% 24%



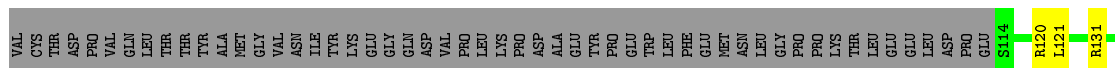
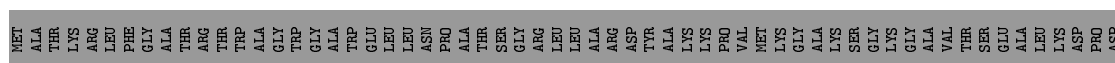
- Molecule 44: mL52



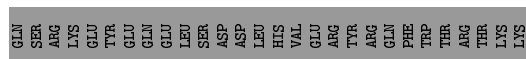
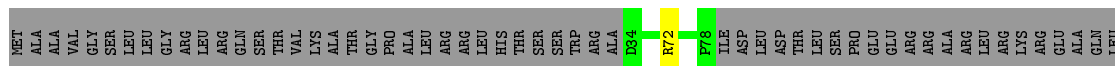
- Molecule 45: mL53



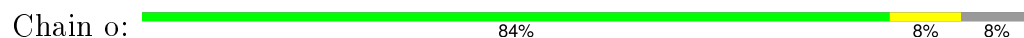
- Molecule 46: mL54



- Molecule 47: bL31m



- Molecule 48: mL63



- Molecule 49: mL62 (ICT1)



- Molecule 50: mL64 (CRIF1)



- Molecule 51: mL66 (bS18a)



- Molecule 52: mL65 (mS30)



- Molecule 53: Unknown protein/protein extension



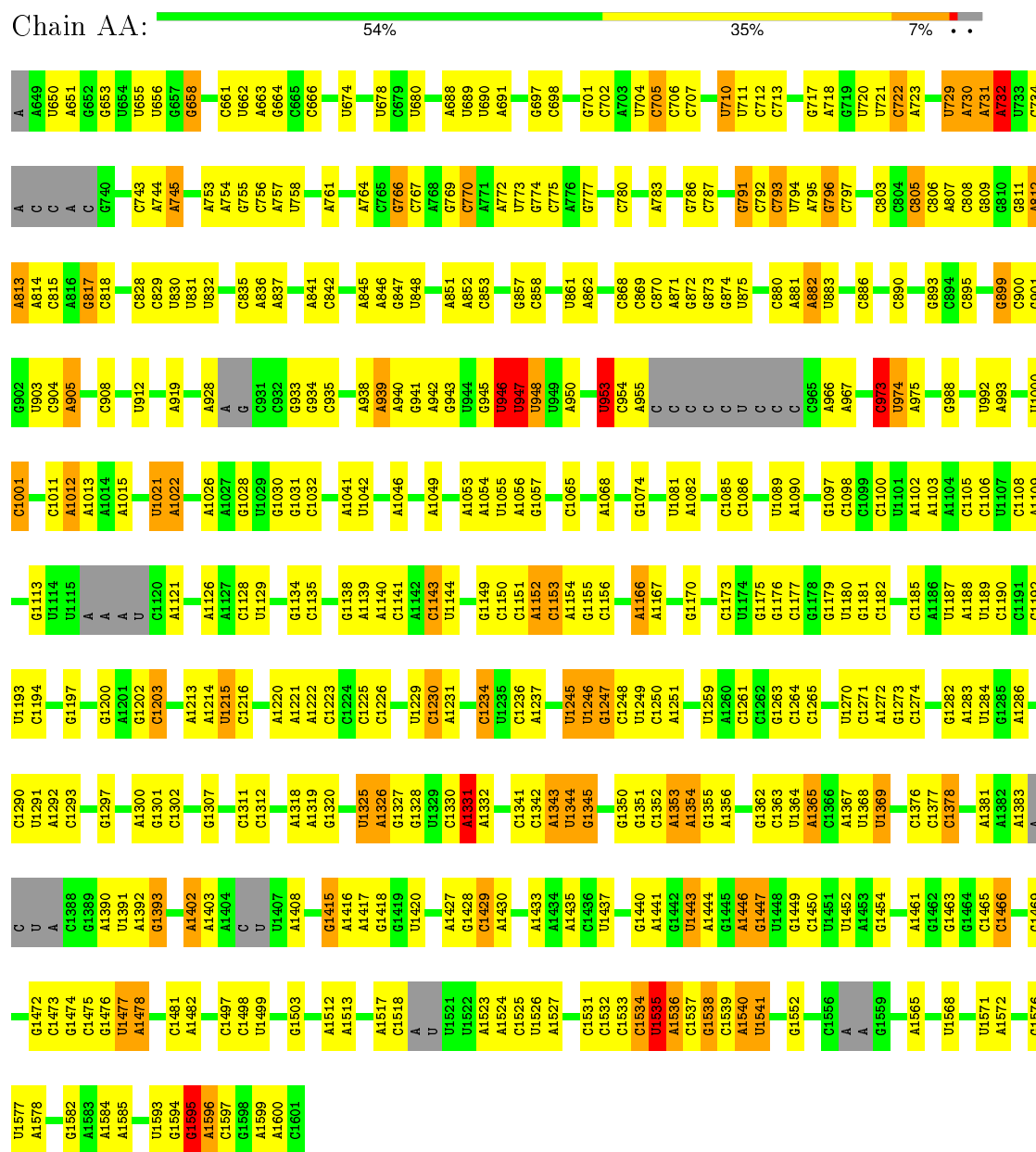
There are no outlier residues recorded for this chain.

- Molecule 54: E-site tRNA

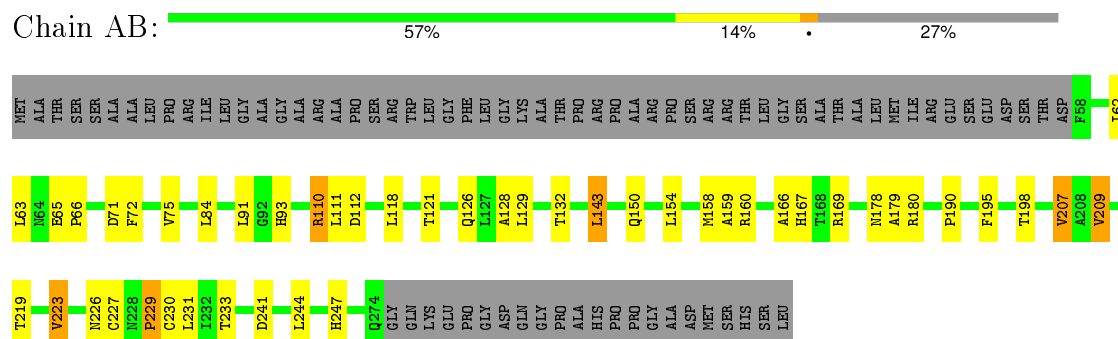




● Molecule 55: 12S rRNA

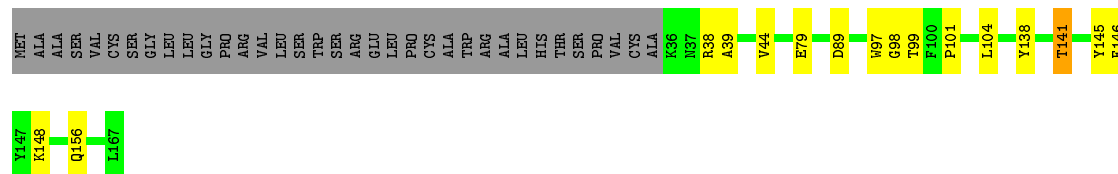


● Molecule 56: uS2m



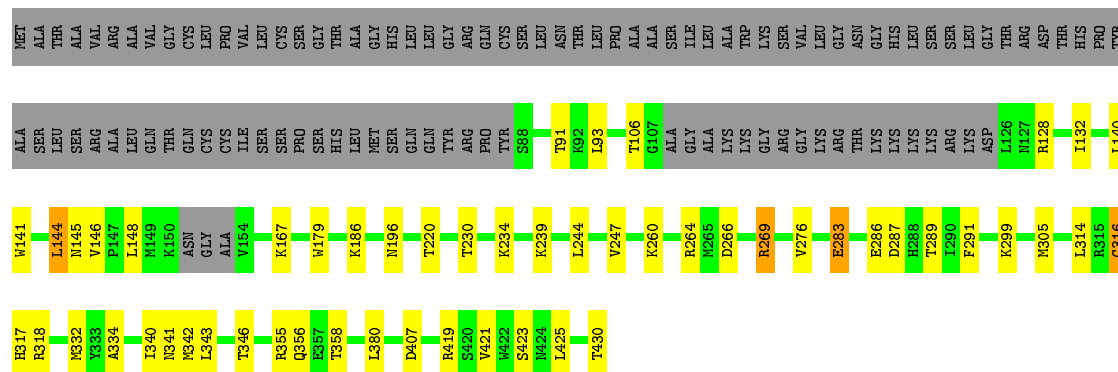
- Molecule 57: uS3m

Chain AC: 




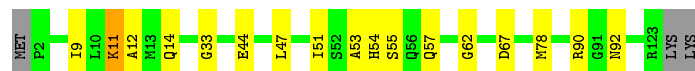
- Molecule 58: uS5m

Chain AD: 



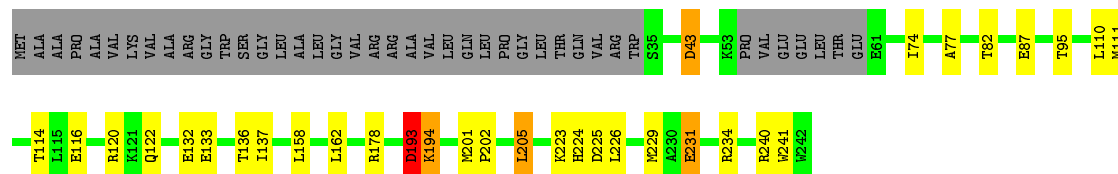
- Molecule 59: bS6m

Chain AE: 



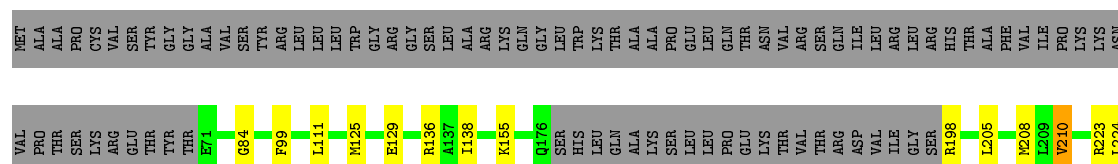
- Molecule 60: uS7m

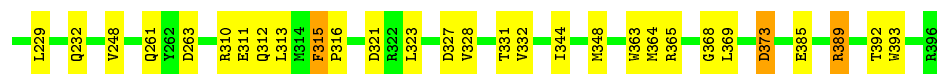
Chain AF: 



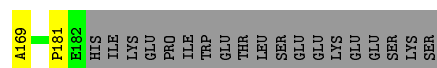
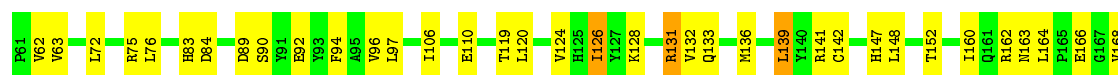
- Molecule 61: uS9m

Chain AG: 

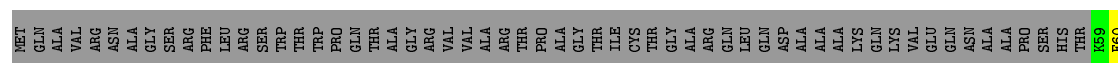




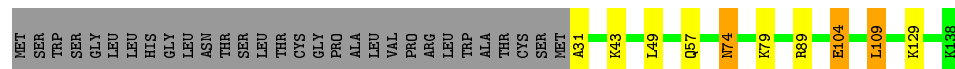
• Molecule 62: uS10m



• Molecule 63: uS11m



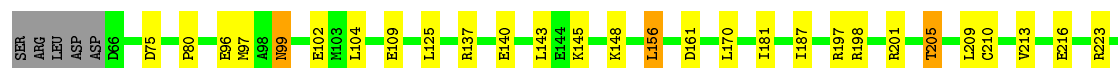
• Molecule 64: uS12m

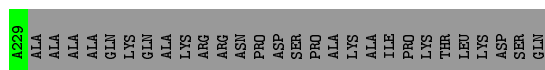


• Molecule 65: uS14m



• Molecule 66: uS15m





• Molecule 67: bS16m

Chain AM: 67% 17% 15%



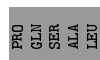
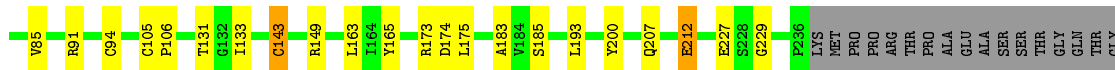
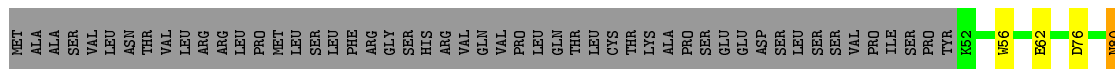
• Molecule 68: uS17m

Chain AN: 67% 15% 18%



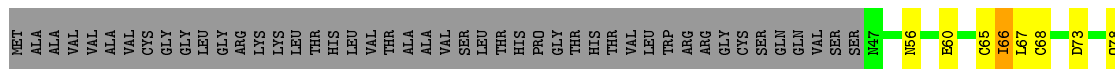
• Molecule 69: mS40 (bS18b)

Chain AO: 62% 9% 28%



• Molecule 70: bS18m (bS18c)

Chain AP: 54% 12% 32%



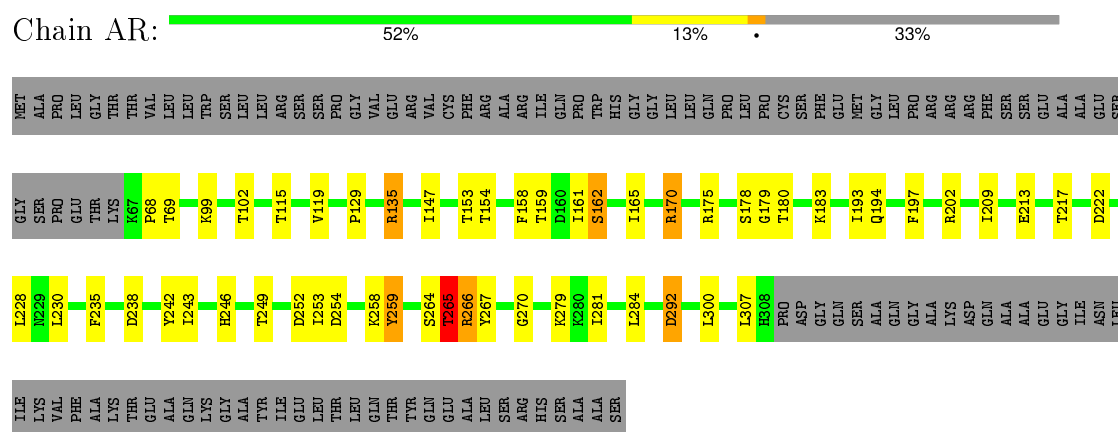
• Molecule 71: bS21m

Chain AQ: 86% 10% 2%



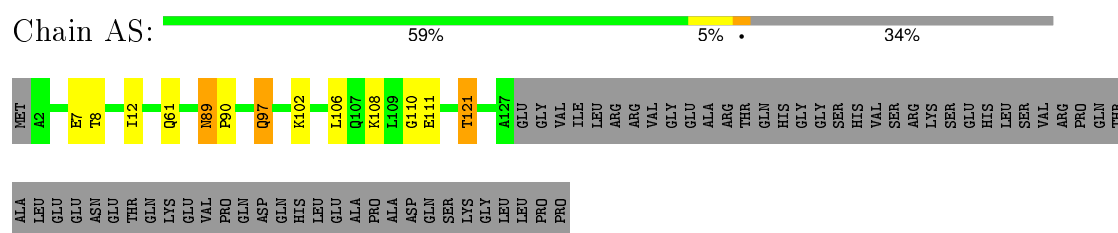
- Molecule 72: mS22

Chain AR:



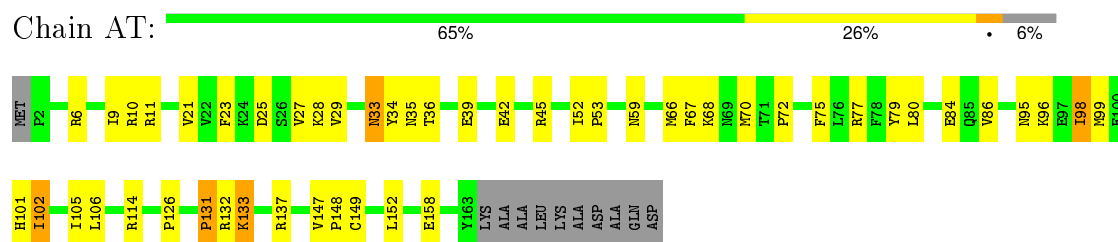
- Molecule 73: mS23

Chain AS:



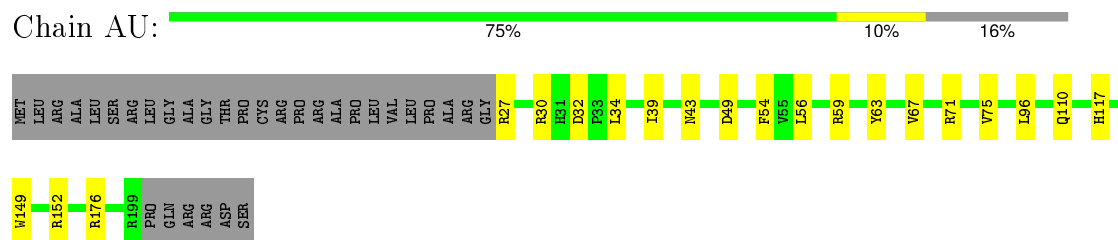
- Molecule 74: mS25

Chain AT:



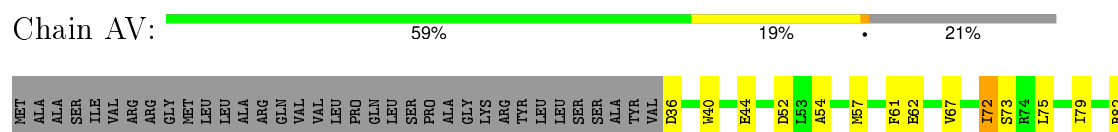
- Molecule 75: mS26

Chain AU:



- Molecule 76: mS27

Chain AV:







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

ASP  
ALA  
PRO  
GLN  
VAL  
ILE  
GLN  
CYS  
K128  
N139  
L146  
F152  
L153  
K165  
F169  
I176  
K179  
L182  
A185  
W189  
I194  
Y195  
L196  
ARG  
GLY  
LYS

● Molecule 85: mS39

Chain A4: 65% 7% 28%

MET  
ALA  
VAL  
VAL  
SER  
ALA  
VAL  
ARG  
TRP  
LEU  
GLY  
LEU  
ARG  
SER  
SER  
ARG  
GLY  
GLN  
PRO  
LEU  
THR  
GLY  
ARG  
ARG  
ALA  
GLY  
LEU  
CYS  
GLU  
GLN  
ALA  
ARG  
SER  
CYS  
ARG  
PHE  
TYR  
SER  
GLY  
SER  
ALA  
THR  
LEU  
SER  
LYS  
VAL  
GLU  
GLY  
THR  
THR  
ASP  
VAL  
THR  
GLY  
ILE  
GLU  
E56  
K61  
K67

V68  
L71  
V85  
D92  
P96  
S105  
E114  
I121  
I132  
A133  
GLU  
PRO  
HIS  
I137  
L140  
M141  
K266  
K275  
F379  
Q417  
M420  
S424  
S425  
I426  
ARG  
ASP  
LEU  
E430  
T441  
GLY  
ASP  
ASN  
TRP  
LYS  
PHE  
ILE  
P450  
R454  
Y457  
S459

K460  
M468  
GLU  
I471  
W477  
Y478  
S484  
ALA  
TYR  
PHE  
PRO  
HIS  
S490  
L500  
A503  
ASN  
ARG  
L506  
E507  
V508  
I509  
P510  
K511  
I512  
E518  
TYR  
GLY  
HIS  
THR  
PHE  
ARG  
S525  
D526  
L527  
L532  
R537  
ASP  
LYS  
HIS  
PRO  
PRO  
GLU  
L544  
I555  
S561  
GLN  
PRO  
ILE  
ARG

GLN  
THR  
ALA  
GLN  
ASP  
TRP  
PRO  
ALA  
T574  
S575  
L576  
I579  
F583  
A586  
GLY  
ARG  
THR  
Q590  
F599  
H602  
ASN  
LYS  
ILE  
PRO  
ARG  
SER  
GLU  
L610  
S621  
ASN  
SER  
PRO  
S625  
L639  
ILE  
CYS  
GLU  
GLY  
LEU  
THR  
GLN  
ARG  
VAL  
MET  
SER  
ASP  
PHE  
ALA  
ILE  
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GLN  
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ALA  
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SER  
ASN  
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THR  
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ASP  
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THR  
ASP  
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SER  
SER  
ASP  
SER  
ASP  
SER  
ASP  
SER  
THR  
SER  
GLY  
LYS



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	884122	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS, FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300, 300, 300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25, 25, 25, 25	Depositor
Minimum defocus (nm)	1500, 1500, 1500, 1500	Depositor
Maximum defocus (nm)	3500, 3500, 3500, 3500	Depositor
Magnification	59000, 59000, 59000, 59000	Depositor
Image detector	FEI FALCON II (4k x 4k), Not provided, Not provided, Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.27	0/34967	0.75	14/54407 (0.0%)
10	L	0.35	0/904	0.70	0/1218
11	M	0.44	0/2359	0.78	0/3185
12	N	0.38	0/1697	0.72	0/2281
13	O	0.42	0/1269	0.84	0/1708
14	P	0.42	0/1103	0.77	1/1491 (0.1%)
15	Q	0.43	0/1863	0.73	1/2509 (0.0%)
16	R	0.43	0/1174	0.86	0/1572
17	S	0.37	0/1276	0.71	0/1729
18	T	0.37	0/1402	0.73	0/1886
19	U	0.39	0/946	0.77	0/1283
2	B	0.22	0/1328	0.67	1/2056 (0.0%)
20	V	0.39	0/1590	0.67	0/2151
21	W	0.35	0/893	0.70	0/1204
22	X	0.42	0/2081	0.73	0/2812
23	Y	0.43	0/1552	0.80	0/2079
24	Z	0.36	0/1003	0.68	0/1354
25	0	0.44	0/895	0.80	0/1201
26	1	0.37	0/438	0.70	0/583
27	2	0.40	0/382	0.97	1/507 (0.2%)
28	3	0.39	0/852	0.74	1/1136 (0.1%)
29	4	0.36	0/329	0.71	0/435
3	D	0.39	1/1879 (0.1%)	0.73	0/2527
30	5	0.41	0/3154	0.75	1/4295 (0.0%)
31	6	0.41	0/2722	0.71	0/3709
32	7	0.39	0/2207	0.69	0/2978
33	8	0.42	0/855	0.73	0/1152
34	9	0.40	0/896	0.73	0/1205
35	a	0.40	0/709	0.61	0/963
36	b	0.39	0/1202	0.74	0/1626
37	c	0.42	0/2264	0.76	0/3059
38	d	0.40	0/1385	0.65	0/1877

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	e	0.40	0/1797	0.66	1/2422 (0.0%)
4	E	0.37	0/2433	0.69	0/3299
40	f	0.38	0/1055	0.61	0/1427
41	g	0.39	0/1102	0.69	0/1503
42	h	0.43	0/847	0.74	0/1150
43	i	0.42	0/849	0.86	0/1135
44	j	0.43	0/698	0.79	0/940
45	k	0.46	0/665	0.73	0/897
46	l	0.45	0/226	0.87	0/299
47	m	0.38	0/379	0.70	0/510
48	o	0.44	0/818	0.88	0/1097
49	p	0.38	0/1071	0.68	0/1433
5	F	0.39	0/2071	0.73	0/2817
50	q	0.46	0/1107	0.76	0/1498
51	r	0.39	0/1238	0.67	0/1676
52	s	0.40	0/3114	0.73	0/4225
54	u	0.29	0/46	1.12	0/69
55	AA	0.25	0/21926	0.76	17/34121 (0.0%)
56	AB	0.42	0/1811	0.79	0/2451
57	AC	0.41	0/1112	0.67	0/1505
58	AD	0.46	2/2607 (0.1%)	0.73	0/3498
59	AE	0.38	0/989	0.78	0/1335
6	H	0.41	0/798	0.72	0/1073
60	AF	0.42	0/1708	0.80	0/2291
61	AG	0.41	0/2570	0.75	0/3443
62	AH	0.39	0/1019	0.73	0/1379
63	AI	0.36	0/1031	0.69	0/1390
64	AJ	0.36	0/854	0.67	0/1148
65	AK	0.40	0/879	0.85	1/1182 (0.1%)
66	AL	0.43	0/1406	0.79	0/1878
67	AM	0.41	0/941	0.82	0/1265
68	AN	0.35	0/864	0.66	0/1169
69	AO	0.41	0/1580	0.73	0/2150
7	I	0.42	0/1308	0.79	0/1761
70	AP	0.42	0/791	0.71	0/1062
71	AQ	0.42	0/752	0.91	0/1001
72	AR	0.44	0/2050	0.82	4/2770 (0.1%)
73	AS	0.43	0/1069	0.75	0/1441
74	AT	0.40	0/1361	0.73	0/1829
75	AU	0.43	0/1482	0.84	0/1987
76	AV	0.45	0/2758	0.83	2/3724 (0.1%)
77	AW	0.41	0/778	0.74	0/1048
78	AX	0.44	0/2596	0.76	3/3519 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
79	AY	0.57	2/943 (0.2%)	0.71	0/1274
8	J	0.42	0/1077	0.73	0/1452
80	AZ	0.45	0/757	0.82	0/1011
81	A0	0.40	0/1727	0.78	1/2338 (0.0%)
82	A1	0.41	0/2121	0.70	1/2873 (0.0%)
83	A2	0.42	0/939	0.79	0/1256
84	A3	0.43	0/621	0.92	0/820
85	A4	0.42	0/2137	0.75	0/2872
9	K	0.45	0/1495	0.78	1/2029 (0.0%)
All	All	0.37	5/165949 (0.0%)	0.75	51/235920 (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
15	Q	0	1
58	AD	0	1
72	AR	0	1
74	AT	0	1
78	AX	0	2
8	J	0	1
80	AZ	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	AY	371	GLU	CD-OE1	8.47	1.34	1.25
79	AY	371	GLU	CD-OE2	7.81	1.34	1.25
58	AD	283	GLU	CD-OE2	7.25	1.33	1.25
58	AD	283	GLU	CD-OE1	6.94	1.33	1.25
3	D	115	GLU	CD-OE1	5.13	1.31	1.25

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	947	U	N1-C1'-C2'	-12.05	98.33	114.00
55	AA	946	U	N1-C1'-C2'	-9.06	102.04	112.00
55	AA	1596	A	N9-C1'-C2'	-8.73	102.40	112.00
72	AR	135	ARG	NE-CZ-NH2	7.44	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2507	A	C2'-C3'-O3'	7.32	125.61	109.50

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	AD	287	ASP	Peptide
72	AR	265	THR	Peptide
74	AT	147	VAL	Peptide
8	J	30	MET	Peptide
15	Q	215	VAL	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31261	0	15877	400	0
2	B	1191	0	607	11	0
3	D	1842	0	1896	26	0
4	E	2365	0	2378	21	0
5	F	2013	0	2044	35	0
6	H	784	0	832	4	0
7	I	1283	0	1369	13	0
8	J	1061	0	1141	7	0
9	K	1451	0	1448	36	0
10	L	889	0	941	8	0
11	M	2305	0	2378	41	0
12	N	1654	0	1681	21	0
13	O	1245	0	1283	19	0
14	P	1080	0	1081	30	0
15	Q	1822	0	1859	30	0
16	R	1153	0	1214	20	0
17	S	1251	0	1322	11	0
18	T	1368	0	1410	21	0
19	U	922	0	935	7	0
20	V	1551	0	1558	0	0
21	W	871	0	898	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	X	2027	0	2040	11	0
23	Y	1517	0	1561	8	0
24	Z	978	0	1030	3	0
25	0	880	0	903	69	0
26	1	433	0	475	4	0
27	2	376	0	406	15	0
28	3	831	0	883	7	0
29	4	322	0	344	0	0
30	5	3064	0	3059	70	0
31	6	2636	0	2450	32	0
32	7	2158	0	2173	6	0
33	8	836	0	844	1	0
34	9	873	0	878	7	0
35	a	686	0	658	0	0
36	b	1178	0	1180	0	0
37	c	2217	0	2220	0	0
38	d	1347	0	1343	0	0
39	e	1762	0	1767	0	0
40	f	1039	0	1044	0	0
41	g	1067	0	1056	0	0
42	h	827	0	806	0	0
43	i	827	0	857	0	0
44	j	684	0	673	0	0
45	k	655	0	656	0	0
46	l	221	0	227	0	0
47	m	372	0	387	0	0
48	o	797	0	804	0	0
49	p	1058	0	1083	0	0
50	q	1076	0	1049	0	0
51	r	1203	0	1221	0	0
52	s	3036	0	3022	0	0
53	t	140	0	30	0	0
54	u	42	0	23	0	0
55	AA	19606	0	9962	220	0
56	AB	1768	0	1765	17	0
57	AC	1082	0	1088	6	0
58	AD	2557	0	2596	15	0
59	AE	972	0	1000	14	0
60	AF	1668	0	1716	16	0
61	AG	2516	0	2503	13	0
62	AH	999	0	1024	18	0
63	AI	1011	0	1052	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	AJ	838	0	887	4	0
65	AK	861	0	885	9	0
66	AL	1382	0	1472	8	0
67	AM	920	0	951	11	0
68	AN	846	0	908	9	0
69	AO	1528	0	1488	5	0
70	AP	774	0	801	5	0
71	AQ	740	0	754	5	0
72	AR	2008	0	2031	16	0
73	AS	1042	0	1037	7	0
74	AT	1330	0	1344	20	0
75	AU	1461	0	1471	7	0
76	AV	2702	0	2690	35	0
77	AW	766	0	785	9	0
78	AX	2531	0	2520	38	0
79	AY	914	0	859	6	0
80	AZ	740	0	747	4	0
81	A0	1684	0	1685	6	0
82	A1	2076	0	2097	23	0
83	A2	925	0	962	9	0
84	A3	610	0	682	6	0
85	A4	2838	0	2263	19	0
86	A	97	0	0	0	0
86	AA	28	0	0	0	0
86	M	1	0	0	0	0
86	g	1	0	0	0	0
87	0	1	0	0	0	0
87	4	1	0	0	0	0
87	AB	1	0	0	0	0
87	AO	1	0	0	0	0
87	AP	1	0	0	0	0
87	AT	1	0	0	0	0
87	r	1	0	0	0	0
88	AX	28	0	12	0	0
All	All	158384	0	133341	1419	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1419 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2807:U:N3	1:A:2922:A:N6	1.61	1.47
25:0:156:THR:CG2	25:0:173:ARG:HH11	1.31	1.44
25:0:156:THR:HG21	25:0:173:ARG:NH1	1.38	1.35
25:0:154:ILE:HG21	25:0:171:GLY:O	1.27	1.34
1:A:2731:U:O4	1:A:2918:A:N1	1.60	1.34

There are no symmetry-related clashes.

## 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	D	234/305 (77%)	214 (92%)	18 (8%)	2 (1%)	21	68
4	E	296/348 (85%)	266 (90%)	20 (7%)	10 (3%)	5	39
5	F	248/311 (80%)	228 (92%)	13 (5%)	7 (3%)	6	43
6	H	93/267 (35%)	84 (90%)	8 (9%)	1 (1%)	17	63
7	I	154/261 (59%)	139 (90%)	11 (7%)	4 (3%)	7	45
8	J	138/192 (72%)	126 (91%)	11 (8%)	1 (1%)	26	72
9	K	175/178 (98%)	156 (89%)	11 (6%)	8 (5%)	3	29
10	L	113/145 (78%)	100 (88%)	11 (10%)	2 (2%)	11	53
11	M	285/296 (96%)	247 (87%)	34 (12%)	4 (1%)	14	58
12	N	203/251 (81%)	186 (92%)	16 (8%)	1 (0%)	34	78
13	O	150/175 (86%)	130 (87%)	16 (11%)	4 (3%)	6	44
14	P	129/179 (72%)	117 (91%)	9 (7%)	3 (2%)	8	48
15	Q	217/292 (74%)	186 (86%)	22 (10%)	9 (4%)	3	33
16	R	138/149 (93%)	126 (91%)	9 (6%)	3 (2%)	8	49
17	S	154/205 (75%)	141 (92%)	11 (7%)	2 (1%)	15	60
18	T	164/212 (77%)	154 (94%)	7 (4%)	3 (2%)	11	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	109/153 (71%)	95 (87%)	10 (9%)	4 (4%)	4	36
20	V	183/216 (85%)	159 (87%)	20 (11%)	4 (2%)	8	49
21	W	109/148 (74%)	100 (92%)	6 (6%)	3 (3%)	6	43
22	X	241/256 (94%)	211 (88%)	22 (9%)	8 (3%)	5	39
23	Y	174/250 (70%)	162 (93%)	9 (5%)	3 (2%)	11	54
24	Z	118/161 (73%)	110 (93%)	5 (4%)	3 (2%)	7	46
25	0	106/188 (56%)	93 (88%)	8 (8%)	5 (5%)	3	29
26	1	50/65 (77%)	44 (88%)	5 (10%)	1 (2%)	9	51
27	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	88 (95%)	4 (4%)	1 (1%)	17	63
29	4	34/103 (33%)	34 (100%)	0	0	100	100
30	5	368/423 (87%)	326 (89%)	32 (9%)	10 (3%)	6	44
31	6	313/380 (82%)	281 (90%)	25 (8%)	7 (2%)	8	49
32	7	258/338 (76%)	226 (88%)	28 (11%)	4 (2%)	12	55
33	8	97/206 (47%)	90 (93%)	6 (6%)	1 (1%)	19	66
34	9	105/137 (77%)	92 (88%)	10 (10%)	3 (3%)	6	42
35	a	78/142 (55%)	74 (95%)	3 (4%)	1 (1%)	15	60
36	b	146/155 (94%)	127 (87%)	16 (11%)	3 (2%)	9	50
37	c	271/332 (82%)	236 (87%)	28 (10%)	7 (3%)	7	45
38	d	156/306 (51%)	137 (88%)	12 (8%)	7 (4%)	3	30
39	e	211/279 (76%)	193 (92%)	14 (7%)	4 (2%)	10	51
40	f	125/194 (64%)	115 (92%)	6 (5%)	4 (3%)	5	40
41	g	127/166 (76%)	114 (90%)	8 (6%)	5 (4%)	4	34
42	h	96/158 (61%)	82 (85%)	9 (9%)	5 (5%)	2	25
43	i	95/128 (74%)	76 (80%)	16 (17%)	3 (3%)	5	40
44	j	83/123 (68%)	77 (93%)	4 (5%)	2 (2%)	7	47
45	k	82/112 (73%)	64 (78%)	12 (15%)	6 (7%)	1	16
46	l	21/138 (15%)	20 (95%)	1 (5%)	0	100	100
47	m	43/128 (34%)	39 (91%)	4 (9%)	0	100	100
48	o	92/102 (90%)	77 (84%)	12 (13%)	3 (3%)	5	39
49	p	119/206 (58%)	113 (95%)	4 (3%)	2 (2%)	11	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	q	126/222 (57%)	118 (94%)	8 (6%)	0	100	100
51	r	140/196 (71%)	124 (89%)	13 (9%)	3 (2%)	9	50
52	s	366/439 (83%)	332 (91%)	28 (8%)	6 (2%)	12	55
56	AB	215/296 (73%)	193 (90%)	18 (8%)	4 (2%)	10	51
57	AC	130/167 (78%)	117 (90%)	12 (9%)	1 (1%)	24	70
58	AD	316/430 (74%)	284 (90%)	28 (9%)	4 (1%)	15	60
59	AE	120/125 (96%)	114 (95%)	5 (4%)	1 (1%)	24	70
60	AF	197/242 (81%)	183 (93%)	12 (6%)	2 (1%)	19	66
61	AG	301/396 (76%)	265 (88%)	30 (10%)	6 (2%)	9	51
62	AH	120/201 (60%)	105 (88%)	11 (9%)	4 (3%)	5	39
63	AI	134/194 (69%)	116 (87%)	11 (8%)	7 (5%)	2	25
64	AJ	106/138 (77%)	91 (86%)	14 (13%)	1 (1%)	21	68
65	AK	99/128 (77%)	96 (97%)	2 (2%)	1 (1%)	19	66
66	AL	162/257 (63%)	148 (91%)	13 (8%)	1 (1%)	30	75
67	AM	114/137 (83%)	105 (92%)	9 (8%)	0	100	100
68	AN	105/130 (81%)	94 (90%)	8 (8%)	3 (3%)	6	42
69	AO	183/258 (71%)	157 (86%)	21 (12%)	5 (3%)	6	44
70	AP	94/142 (66%)	85 (90%)	6 (6%)	3 (3%)	5	40
71	AQ	84/87 (97%)	75 (89%)	6 (7%)	3 (4%)	4	37
72	AR	240/360 (67%)	202 (84%)	28 (12%)	10 (4%)	3	32
73	AS	124/190 (65%)	110 (89%)	14 (11%)	0	100	100
74	AT	160/173 (92%)	144 (90%)	8 (5%)	8 (5%)	3	27
75	AU	171/205 (83%)	163 (95%)	8 (5%)	0	100	100
76	AV	320/414 (77%)	283 (88%)	29 (9%)	8 (2%)	7	46
77	AW	95/187 (51%)	82 (86%)	9 (10%)	4 (4%)	3	32
78	AX	310/398 (78%)	263 (85%)	30 (10%)	17 (6%)	2	24
79	AY	106/395 (27%)	95 (90%)	8 (8%)	3 (3%)	6	43
80	AZ	85/106 (80%)	72 (85%)	8 (9%)	5 (6%)	2	22
81	A0	197/218 (90%)	175 (89%)	19 (10%)	3 (2%)	13	56
82	A1	252/323 (78%)	212 (84%)	34 (14%)	6 (2%)	7	47
83	A2	114/118 (97%)	97 (85%)	13 (11%)	4 (4%)	4	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	A3	67/199 (34%)	62 (92%)	4 (6%)	1 (2%)	13	56
85	A4	237/579 (41%)	230 (97%)	5 (2%)	2 (1%)	24	70
All	All	12628/17789 (71%)	11290 (89%)	1039 (8%)	299 (2%)	12	47

5 of 299 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	170	LEU
4	E	245	THR
5	F	223	HIS
7	I	102	VAL
8	J	70	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	190/245 (78%)	173 (91%)	17 (9%)	12	47
4	E	255/290 (88%)	233 (91%)	22 (9%)	13	49
5	F	217/262 (83%)	198 (91%)	19 (9%)	12	48
6	H	86/228 (38%)	83 (96%)	3 (4%)	43	78
7	I	145/232 (62%)	133 (92%)	12 (8%)	14	50
8	J	113/150 (75%)	103 (91%)	10 (9%)	12	48
9	K	155/156 (99%)	145 (94%)	10 (6%)	21	62
10	L	98/124 (79%)	88 (90%)	10 (10%)	9	40
11	M	245/249 (98%)	217 (89%)	28 (11%)	7	33
12	N	172/211 (82%)	152 (88%)	20 (12%)	7	33
13	O	133/150 (89%)	114 (86%)	19 (14%)	4	24
14	P	115/154 (75%)	102 (89%)	13 (11%)	7	34
15	Q	201/256 (78%)	187 (93%)	14 (7%)	19	59
16	R	118/126 (94%)	104 (88%)	14 (12%)	6	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	S	141/180 (78%)	130 (92%)	11 (8%)	16	53
18	T	146/182 (80%)	141 (97%)	5 (3%)	44	79
19	U	99/135 (73%)	89 (90%)	10 (10%)	9	40
20	V	169/191 (88%)	157 (93%)	12 (7%)	18	58
21	W	91/119 (76%)	85 (93%)	6 (7%)	21	61
22	X	217/227 (96%)	199 (92%)	18 (8%)	14	50
23	Y	159/223 (71%)	148 (93%)	11 (7%)	19	59
24	Z	111/147 (76%)	102 (92%)	9 (8%)	15	52
25	0	97/164 (59%)	81 (84%)	16 (16%)	3	16
26	1	49/60 (82%)	43 (88%)	6 (12%)	6	29
27	2	40/72 (56%)	37 (92%)	3 (8%)	17	55
28	3	88/166 (53%)	83 (94%)	5 (6%)	25	66
29	4	35/89 (39%)	31 (89%)	4 (11%)	7	33
30	5	337/368 (92%)	305 (90%)	32 (10%)	11	43
31	6	266/332 (80%)	242 (91%)	24 (9%)	12	46
32	7	242/303 (80%)	230 (95%)	12 (5%)	30	69
33	8	91/190 (48%)	88 (97%)	3 (3%)	45	79
34	9	91/112 (81%)	85 (93%)	6 (7%)	21	61
35	a	78/133 (59%)	74 (95%)	4 (5%)	29	69
36	b	130/135 (96%)	118 (91%)	12 (9%)	11	45
37	c	241/288 (84%)	220 (91%)	21 (9%)	13	48
38	d	151/274 (55%)	146 (97%)	5 (3%)	45	79
39	e	188/236 (80%)	178 (95%)	10 (5%)	28	67
40	f	117/173 (68%)	113 (97%)	4 (3%)	44	79
41	g	119/148 (80%)	109 (92%)	10 (8%)	14	50
42	h	95/148 (64%)	84 (88%)	11 (12%)	7	33
43	i	86/110 (78%)	76 (88%)	10 (12%)	7	33
44	j	68/97 (70%)	61 (90%)	7 (10%)	9	40
45	k	74/90 (82%)	68 (92%)	6 (8%)	15	52
46	l	23/116 (20%)	20 (87%)	3 (13%)	5	27
47	m	40/113 (35%)	39 (98%)	1 (2%)	55	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	o	80/87 (92%)	75 (94%)	5 (6%)	22	63
49	p	117/181 (65%)	107 (92%)	10 (8%)	13	49
50	q	110/178 (62%)	99 (90%)	11 (10%)	9	41
51	r	133/169 (79%)	124 (93%)	9 (7%)	20	60
52	s	326/381 (86%)	299 (92%)	27 (8%)	14	50
56	AB	191/249 (77%)	171 (90%)	20 (10%)	8	38
57	AC	115/143 (80%)	106 (92%)	9 (8%)	16	53
58	AD	269/357 (75%)	239 (89%)	30 (11%)	7	35
59	AE	104/107 (97%)	98 (94%)	6 (6%)	25	65
60	AF	178/209 (85%)	161 (90%)	17 (10%)	10	43
61	AG	265/342 (78%)	243 (92%)	22 (8%)	14	50
62	AH	112/180 (62%)	93 (83%)	19 (17%)	2	15
63	AI	104/147 (71%)	89 (86%)	15 (14%)	4	23
64	AJ	93/118 (79%)	86 (92%)	7 (8%)	17	55
65	AK	91/113 (80%)	82 (90%)	9 (10%)	10	41
66	AL	152/226 (67%)	131 (86%)	21 (14%)	4	25
67	AM	95/113 (84%)	82 (86%)	13 (14%)	4	25
68	AN	93/115 (81%)	86 (92%)	7 (8%)	17	55
69	AO	166/230 (72%)	150 (90%)	16 (10%)	10	43
70	AP	87/123 (71%)	75 (86%)	12 (14%)	4	25
71	AQ	78/79 (99%)	73 (94%)	5 (6%)	22	62
72	AR	224/318 (70%)	198 (88%)	26 (12%)	7	33
73	AS	109/164 (66%)	103 (94%)	6 (6%)	27	67
74	AT	150/157 (96%)	128 (85%)	22 (15%)	4	22
75	AU	149/174 (86%)	137 (92%)	12 (8%)	15	52
76	AV	295/364 (81%)	266 (90%)	29 (10%)	10	42
77	AW	84/158 (53%)	76 (90%)	8 (10%)	11	43
78	AX	275/351 (78%)	231 (84%)	44 (16%)	3	18
79	AY	99/357 (28%)	91 (92%)	8 (8%)	15	52
80	AZ	80/95 (84%)	72 (90%)	8 (10%)	9	41
81	A0	176/190 (93%)	158 (90%)	18 (10%)	9	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	A1	237/291 (81%)	218 (92%)	19 (8%)	15	52
83	A2	99/101 (98%)	84 (85%)	15 (15%)	3	21
84	A3	63/166 (38%)	58 (92%)	5 (8%)	15	53
85	A4	226/379 (60%)	211 (93%)	15 (7%)	21	61
All	All	11347/15266 (74%)	10314 (91%)	1033 (9%)	16	46

5 of 1033 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	g	141	ASN
56	AB	150	GLN
80	AZ	32	LYS
43	i	35	ARG
50	q	44	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
35	a	62	HIS
39	e	245	GLN
78	AX	66	GLN
36	b	27	GLN
37	c	172	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1459/1559 (93%)	470 (32%)	99 (6%)
2	B	51/73 (69%)	19 (37%)	3 (5%)
54	u	1/2 (50%)	1 (100%)	0
55	AA	914/954 (95%)	273 (29%)	57 (6%)
All	All	2425/2588 (93%)	763 (31%)	159 (6%)

5 of 763 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1672	C
1	A	1674	A

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Mol	Chain	Res	Type
1	A	1675	A
1	A	1676	A
1	A	1678	C

5 of 159 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2618	U
1	A	2989	G
55	AA	1415	G
1	A	2684	C
1	A	2846	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 134 are monoatomic - leaving 1 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	$\# Z  > 2$
88	GDP	AX	500	-	24,30,30	1.22	2 (8%)	26,47,47	1.93	5 (19%)

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
88	GDP	AX	500	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	AX	500	GDP	C5-C4	3.36	1.48	1.40
88	AX	500	GDP	C6-C5	3.76	1.48	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	AX	500	GDP	C5-C6-N1	-3.99	118.31	123.52
88	AX	500	GDP	N3-C2-N1	-3.72	122.49	127.56
88	AX	500	GDP	C6-C5-C4	-3.05	117.38	120.86
88	AX	500	GDP	O4'-C1'-N9	2.75	113.30	108.11
88	AX	500	GDP	C6-N1-C2	5.54	122.38	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.