wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Feb 8, 2017 – 01:42 PM EST

PDB ID	:	5MRF
EMDB ID:	:	EMD-3553
Title	:	Structure of the yeast mitochondrial ribosome - Class C
Authors	:	Desai, N.; Brown, A.; Amunts, A.; Ramakrishnan, V.
Deposited on	:	2016-12-22
Resolution	:	4.97 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

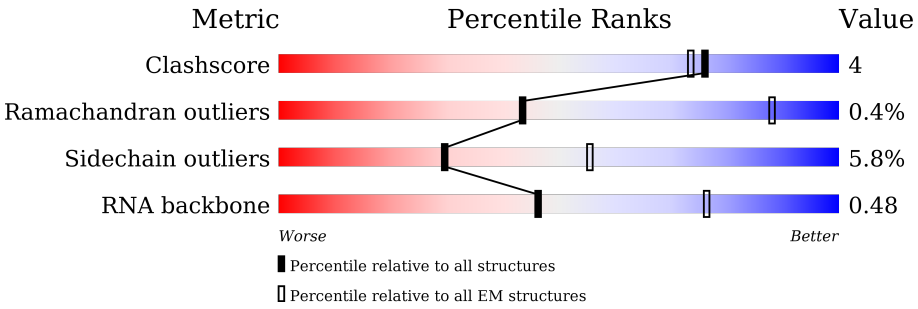
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.97 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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	3296	60% 20% • 18%
2	B	393	71% 10% • 18%
3	C	249	89% 10% •
4	D	252	88% 11% •
5	E	274	93% 7%
6	F	196	91% 9%
7	G	74	95% 5%
8	H	160	90% 10%

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Mol	Chain	Length	Quality of chain
9	I	138	84% 8% 8%
10	J	220	90% 10%
11	K	195	88% 12%
12	L	237	88% 8%
13	M	151	91% 8%
14	N	118	97%
15	O	225	92% 8%
16	P	207	94% 6%
17	Q	296	88% 7%
18	R	337	91% 7%
19	S	216	81% 14%
20	T	225	84% 12%
21	U	82	85% 15%
22	V	177	51% 47%
23	W	112	94% 6%
24	X	64	84% 16%
25	Y	46	91% 9%
26	Z	62	94% 6%
27	0	38	89% 11%
28	1	348	93% 7%
29	2	113	88% 12%
30	3	130	93% 7%
31	4	138	91% 9%
32	5	324	89% 11%
33	6	281	75% 8% 17%

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Mol	Chain	Length	Quality of chain
34	7	106	87% 13%
35	8	264	70% 5% 25%
36	9	215	86% 7% 6%
37	a	177	96%
38	b	155	97%
39	c	119	98%
40	d	215	94%
41	AA	344	55% 41%
42	BB	266	81% 17%
43	CC	398	71% 13% 15%
44	DD	486	50% 8% 41%
45	EE	293	86% 12%
46	FF	125	81% 18%
47	GG	161	93% 7%
48	HH	154	79% 18%
49	II	244	83% 9% 7%
50	JJ	186	84% 13%
51	KK	148	76% 18%
52	LL	124	82% 17%
53	MM	120	91% 8%
54	NN	115	81% 13% 5%
55	OO	253	80% 12% 6%
56	PP	119	89% 8%
57	QQ	237	74% 11% 14%
58	RR	99	85% 7% 8%

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Mol	Chain	Length	Quality of chain
59	SS	80	86% 13%
60	TT	92	88% 11%
61	UU	233	85% 14%
62	VV	233	93% 6%
63	WW	401	84% 15%
64	XX	96	93% 5%
65	YY	273	86% 12%
66	ZZ	91	67% 22% 5%
67	11	34	91% 9%
68	22	99	96%
69	33	255	84% 11%
70	44	321	79% 6% 16%
71	55	339	17% 83%
72	66	319	88% 8%
73	77	165	92% 8%
74	88	457	87% 11%
75	aa	1649	63% 27% 9%
76	bb	76	49% 51%
77	cc	94	100%
78	dd	151	100%

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 201462 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 21S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2709	57598	25914	10252	18729	2703	0	0

- Molecule 2 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	321	2527	1575	507	436	9	0	0

- Molecule 3 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	249	1932	1218	360	344	10	0	0

- Molecule 4 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	252	1991	1264	355	369	3	0	0

- Molecule 5 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	274	2187	1396	391	394	6	0	0

- Molecule 6 is a protein called uL6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	196	1524	967	273	280	4	0	0

- Molecule 7 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	74	Total	C	N	O	S	0	0
			617	393	110	113	1		

- Molecule 8 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	160	Total	C	N	O	S	0	0
			1275	807	240	224	4		

- Molecule 9 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			956	595	180	170	11		

- Molecule 10 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	220	Total	C	N	O	S	0	0
			1746	1119	326	298	3		

- Molecule 11 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	195	Total	C	N	O	S	0	0
			1573	1001	297	270	5		

- Molecule 12 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	229	Total	C	N	O	S	0	0
			1817	1140	333	336	8		

- Molecule 13 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	151	Total	C	N	O	S	0	0
			1206	766	220	217	3		

- Molecule 14 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	118	Total	C	N	O	S	0	0
			948	598	177	171	2		

- Molecule 15 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	225	Total	C	N	O	S	0	0
			1826	1169	332	320	5		

- Molecule 16 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	207	Total	C	N	O	S	0	0
			1729	1104	310	309	6		

- Molecule 17 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	284	Total	C	N	O	S	0	0
			2272	1451	396	417	8		

- Molecule 18 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	331	Total	C	N	O	S	0	0
			2738	1728	497	509	4		

- Molecule 19 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	185	Total	C	N	O	S	0	0
			1543	994	281	265	3		

- Molecule 20 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1792	1139	324	325	4		

- Molecule 21 is a protein called uL30m.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	82	Total 639	C 410	N 116	O 113	0	0

- Molecule 22 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	93	Total 729	C 456	N 145	O 127	S 1	0	0

- Molecule 23 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total 937	C 587	N 181	O 163	S 6	0	0

- Molecule 24 is a protein called bL33m.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	64	Total 512	C 330	N 96	O 86	0	0

- Molecule 25 is a protein called bL34m.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	46	Total 385	C 245	N 82	O 58	0	0

- Molecule 26 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	62	Total 508	C 322	N 111	O 74	S 1	0	0

- Molecule 27 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	38	Total 324	C 205	N 66	O 50	S 3	0	0

- Molecule 28 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	348	Total	C	N	O	S	0	0
			2875	1847	499	523	6		

- Molecule 29 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	113	Total	C	N	O	S	0	0
			944	597	174	168	5		

- Molecule 30 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	130	Total	C	N	O	S	0	0
			1046	671	189	183	3		

- Molecule 31 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	138	Total	C	N	O	S	0	0
			1117	700	219	193	5		

- Molecule 32 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	324	Total	C	N	O	S	0	0
			2552	1630	431	480	11		

- Molecule 33 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	234	Total	C	N	O	S	0	0
			1932	1250	327	353	2		

- Molecule 34 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	106	Total	C	N	O	S	0	0
			858	553	151	152	2		

- Molecule 35 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	199	Total	C	N	O	S	0	0
			1629	1032	278	315	4		

- Molecule 36 is a protein called mL57.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	202	Total	C	N	O	S	0	0
			1587	1014	279	289	5		

- Molecule 37 is a protein called mL58.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	177	Total	C	N	O	S	0	0
			1440	907	267	260	6		

- Molecule 38 is a protein called mL59.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	155	Total	C	N	O	S	0	0
			1299	850	225	221	3		

- Molecule 39 is a protein called mL60.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	119	Total	C	N	O	S	0	0
			1004	645	191	164	4		

- Molecule 40 is a protein called mL67.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	206	Total	C	N	O	S	0	0
			1746	1117	318	304	7		

- Molecule 41 is a protein called bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AA	203	Total	C	N	O	S	0	0
			1610	1032	285	288	5		

- Molecule 42 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BB	266	Total	C	N	O	S	0	0
			2085	1313	366	404	2		

- Molecule 43 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CC	339	Total	C	N	O	S	0	0
			2821	1772	502	517	30		

- Molecule 44 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	DD	287	Total	C	N	O	S	0	0
			2369	1542	420	403	4		

- Molecule 45 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	EE	288	Total	C	N	O	S	0	0
			2306	1473	408	417	8		

- Molecule 46 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	FF	125	Total	C	N	O	S	0	0
			1002	639	182	177	4		

- Molecule 47 is a protein called uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	GG	161	Total	C	N	O	S	0	0
			1282	811	238	228	5		

- Molecule 48 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	HH	154	Total	C	N	O	S	0	0
			1213	767	217	220	9		

- Molecule 49 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	II	226	Total	C	N	O	S	0	0
			1820	1167	332	316	5		

- Molecule 50 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	JJ	186	Total	C	N	O	S	0	0
			1508	964	259	281	4		

- Molecule 51 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	KK	142	Total	C	N	O	S	0	0
			1121	717	195	203	6		

- Molecule 52 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LL	124	Total	C	N	O	S	0	0
			948	585	194	165	4		

- Molecule 53 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	MM	120	Total	C	N	O	S	0	0
			942	596	179	161	6		

- Molecule 54 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	NN	115	Total	C	N	O	S	0	0
			953	612	182	154	5		

- Molecule 55 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	OO	238	Total	C	N	O	S	0	0
			1962	1227	371	356	8		

- Molecule 56 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	PP	116	Total	C	N	O	S	0	0
			919	586	172	159	2		

- Molecule 57 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	QQ	204	Total	C	N	O	S	0	0
			1683	1055	315	308	5		

- Molecule 58 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	RR	91	Total	C	N	O	S	0	0
			738	463	143	128	4		

- Molecule 59 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SS	80	Total	C	N	O	S	0	0
			636	408	115	111	2		

- Molecule 60 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	TT	92	Total	C	N	O	S	0	0
			760	475	150	130	5		

- Molecule 61 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	UU	233	Total	C	N	O	S	0	0
			1907	1211	331	358	7		

- Molecule 62 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	VV	233	Total	C	N	O	S	0	0
			1872	1189	338	342	3		

- Molecule 63 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	WW	401	Total	C	N	O	S	0	0
			3216	2072	540	596	8		

- Molecule 64 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	XX	96	Total	C	N	O	S	0	0
			774	496	140	135	3		

- Molecule 65 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	YY	269	Total	C	N	O	S	0	0
			2258	1429	404	421	4		

- Molecule 66 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ZZ	87	Total	C	N	O	S	0	0
			687	435	128	118	6		

- Molecule 67 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	11	34	Total	C	N	O	S	0	0
			303	183	75	43	2		

- Molecule 68 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	22	99	Total	C	N	O	S	0	0
			833	530	156	146	1		

- Molecule 69 is a protein called mS42.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	33	244	Total	C	N	O	S	0	0
			1953	1261	328	359	5		

- Molecule 70 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	44	270	Total	C	N	O	S	0	0
			2169	1380	370	412	7		

- Molecule 71 is a protein called mS44.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	55	59	Total	C	N	O	0	0
			508	338	84	86		

- Molecule 72 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	66	305	Total	C	N	O	S	0	0
			2488	1587	445	450	6		

- Molecule 73 is a protein called mS46.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	77	165	Total	C	N	O	S	0	0
			1330	854	214	259	3		

- Molecule 74 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	88	452	Total	C	N	O	S	0	0
			3573	2272	600	681	20		

- Molecule 75 is a RNA chain called 15S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	aa	1501	Total	C	N	O	P	0	0
			31883	14338	5633	10411	1501		

- Molecule 76 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	bb	76	Total	C	N	O	P	0	0
			1615	723	289	528	75		

- Molecule 77 is a protein called unknown protein sequence 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
77	cc	94	Total 470	C 282	N 94	O 94	0	0

- Molecule 78 is a protein called unknown protein sequence 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	dd	151	Total 755	C 453	N 151	O 151	0	0

- Molecule 79 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
79	BB	1	Total 1	Mg 1	0
79	WW	1	Total 1	Mg 1	0
79	LL	1	Total 1	Mg 1	0
79	MM	1	Total 1	Mg 1	0
79	PP	1	Total 1	Mg 1	0
79	OO	1	Total 1	Mg 1	0
79	A	182	Total 182	Mg 182	0
79	R	1	Total 1	Mg 1	0
79	aa	110	Total 110	Mg 110	0

- Molecule 80 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
80	B	1	Total 1	Na 1	0

- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	0	1	Total 1	Zn 1	0

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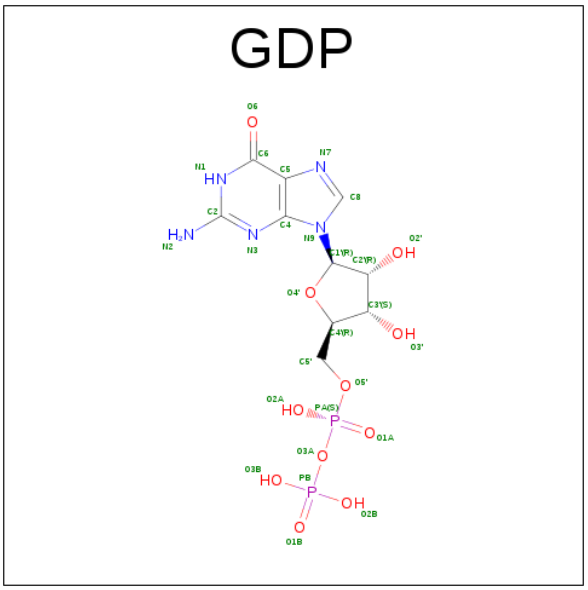
Mol	Chain	Residues	Atoms		AltConf
81	W	1	Total	Zn	0
			1	1	

- Molecule 82 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



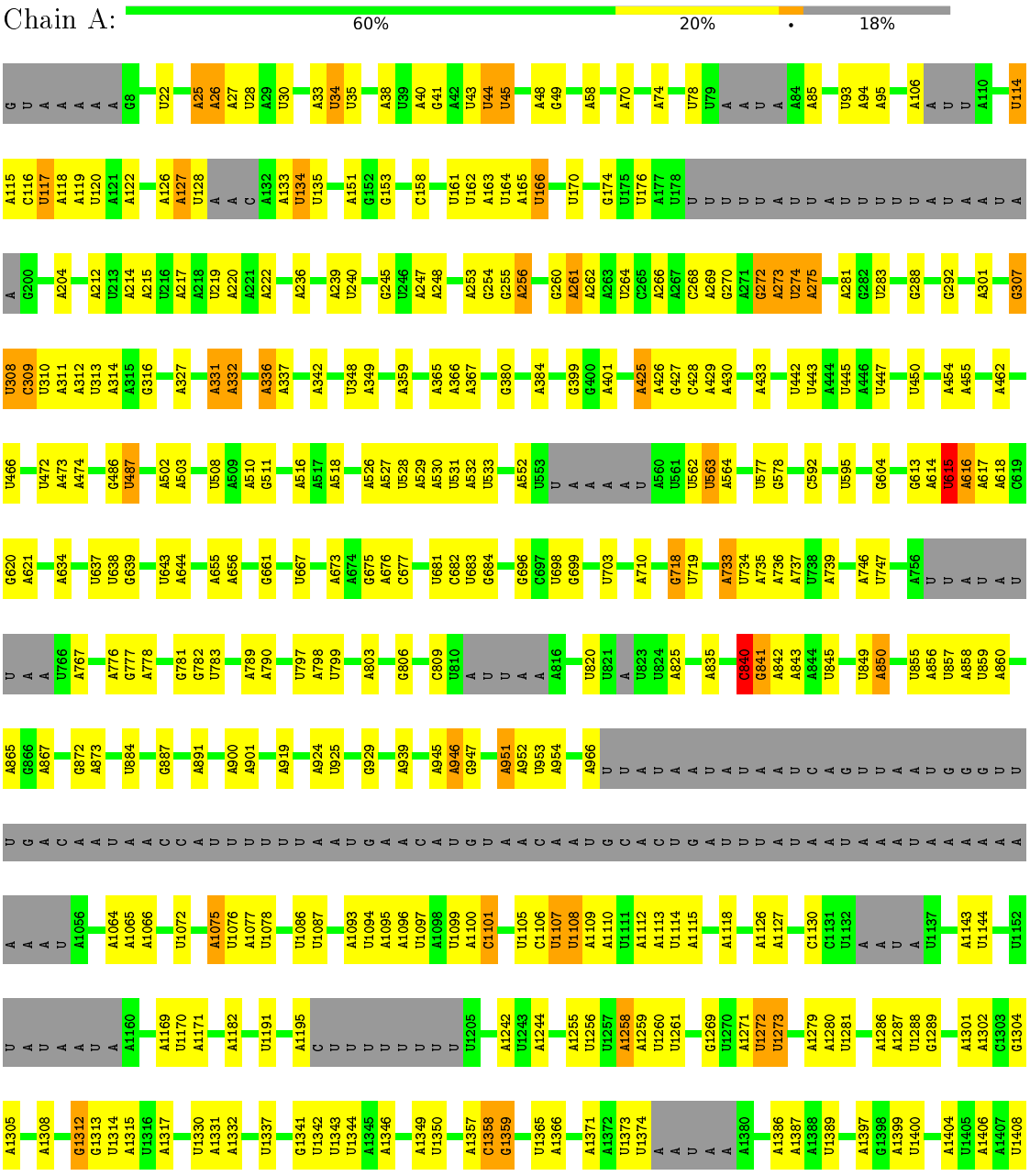
Mol	Chain	Residues	Atoms					AltConf
82	WW	1	Total	C	N	O	P	0
			28	10	5	11	2	

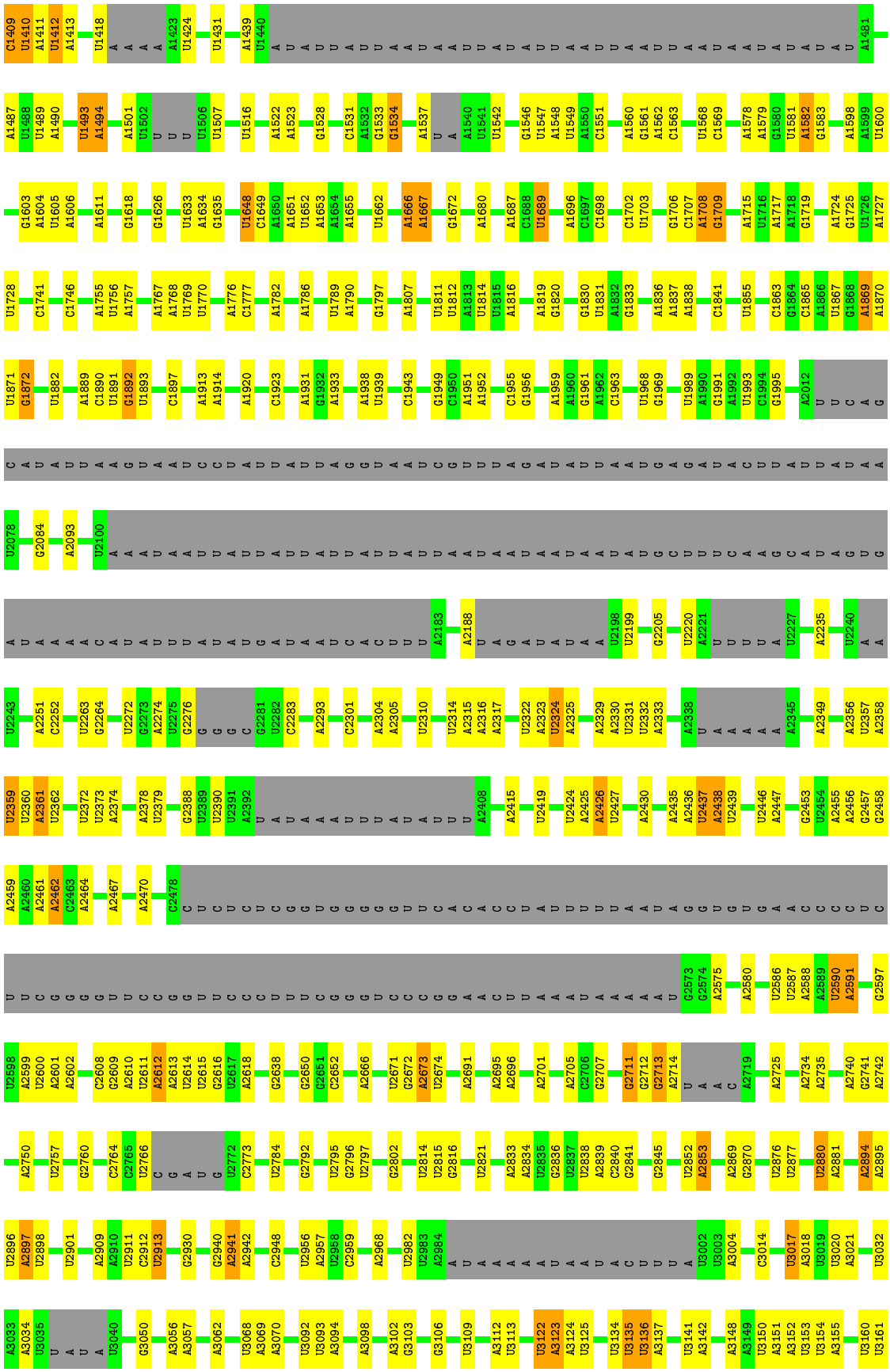
3 Residue-property plots (i)

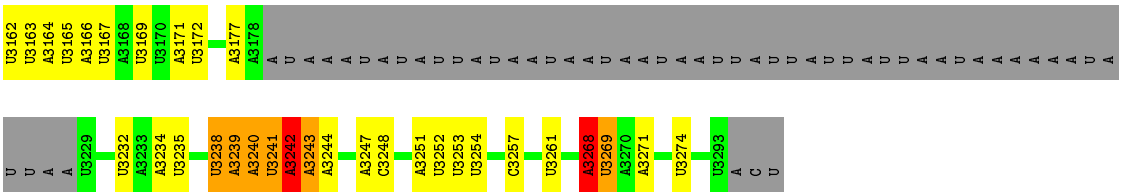
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: 21S RNA

Chain A:

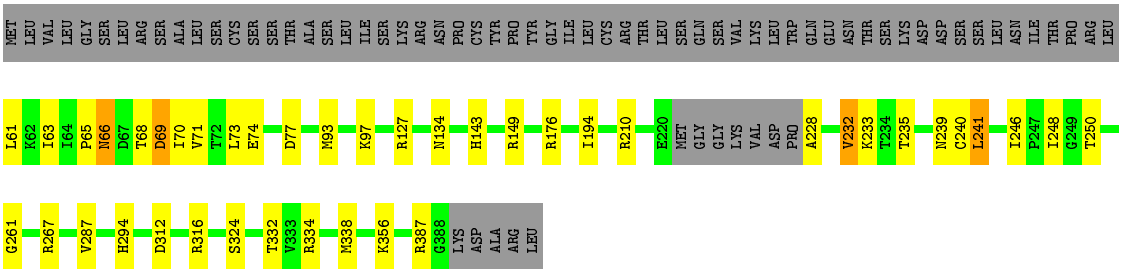






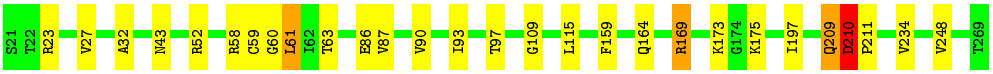
- Molecule 2: uL2m

Chain B:



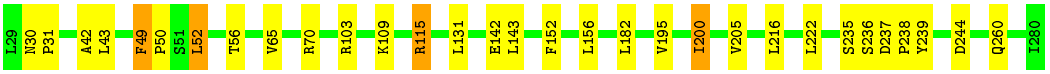
- Molecule 3: uL3m

Chain C:



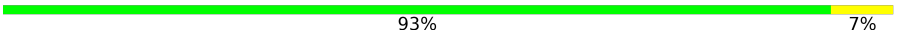
- Molecule 4: uL4m

Chain D:



- Molecule 5: uL5m

Chain E:

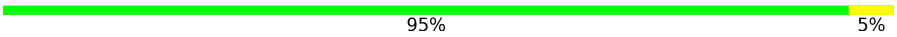


- Molecule 6: uL6m

Chain F:

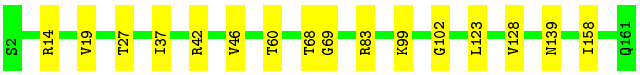
- Molecule 7: bL9m

Chain G:



- Molecule 8: uL13m

Chain H:

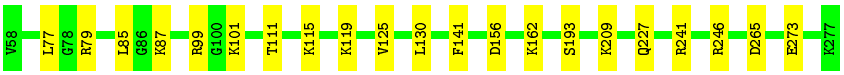


- Molecule 9: uL14m

Chain I:

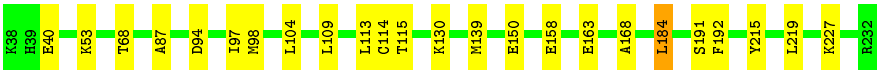
- Molecule 10: uL15m

Chain J:



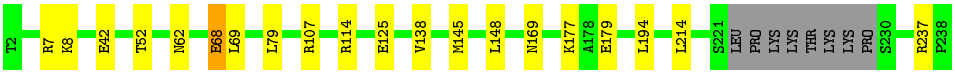
- Molecule 11: uL16m

Chain K:



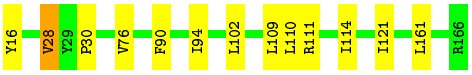
- Molecule 12: bL17m

Chain L:



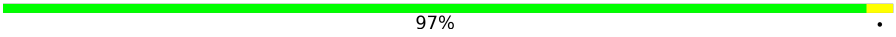
- Molecule 13: bL19m

Chain M:



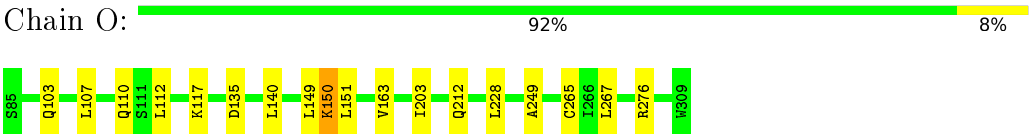
- Molecule 14: bL21m

Chain N:



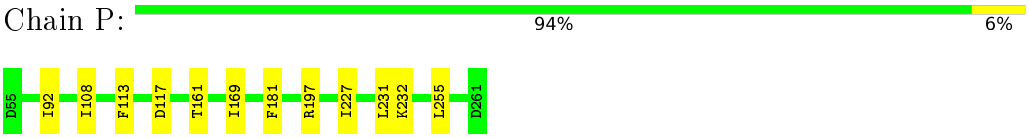
- Molecule 15: uL22m

Chain O:



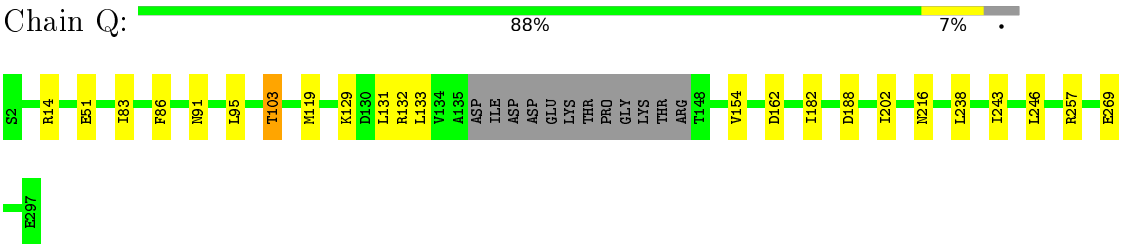
- Molecule 16: uL23m

Chain P:



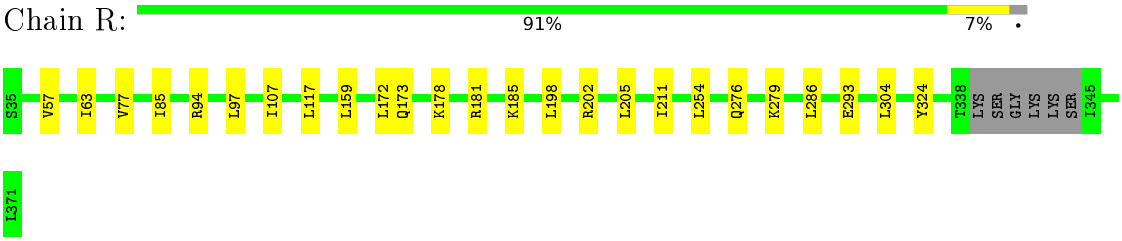
- Molecule 17: uL24m

Chain Q:



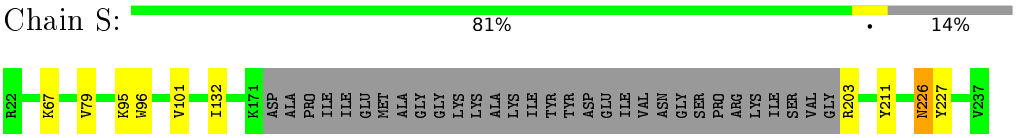
- Molecule 18: bL27m

Chain R:



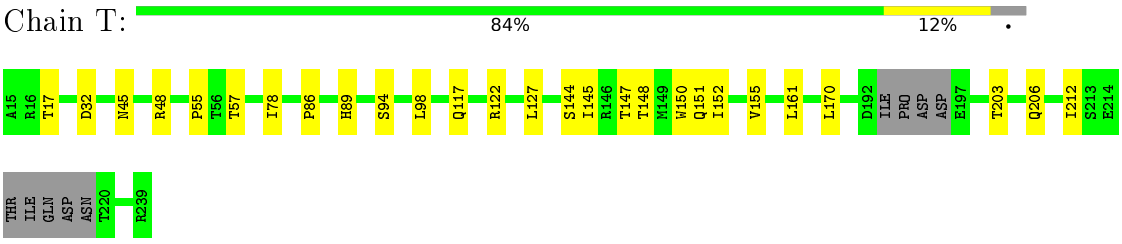
- Molecule 19: bL28m

Chain S:



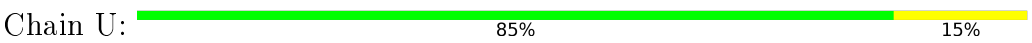
- Molecule 20: uL29m

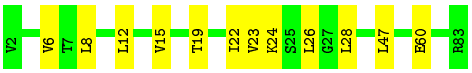
Chain T:



- Molecule 21: uL30m

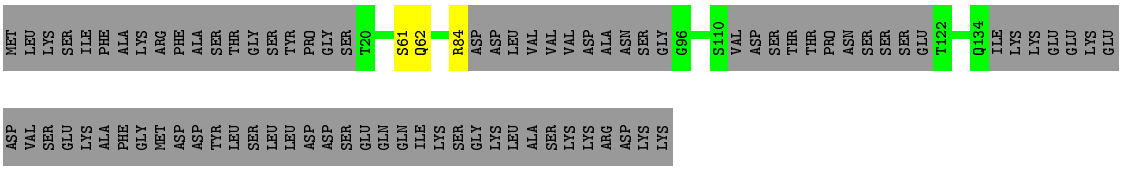
Chain U:





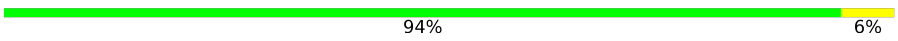
- Molecule 22: bL31m

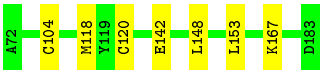
Chain V:



- Molecule 23: bL32m

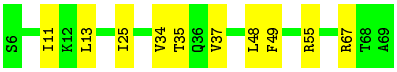
Chain W:





- Molecule 24: bL33m

Chain X:

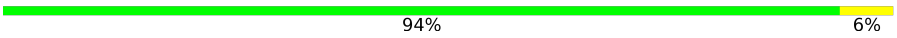


- Molecule 25: bL34m

Chain Y:

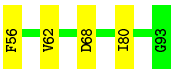
- Molecule 26: bL35m

Chain Z:



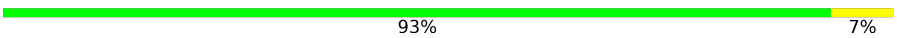
- Molecule 27: bL36m

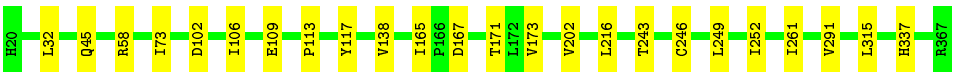
Chain 0:



- Molecule 28: mL38

Chain 1:



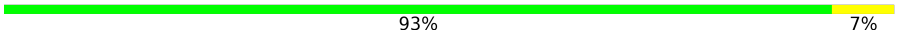


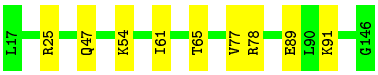
- Molecule 29: mL40

Chain 2:

- Molecule 30: mL41

Chain 3:



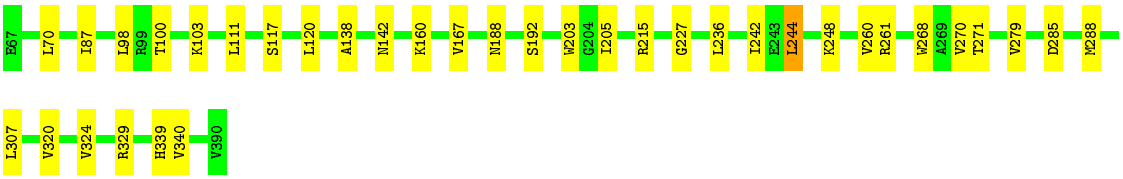


- Molecule 31: mL43

Chain 4:

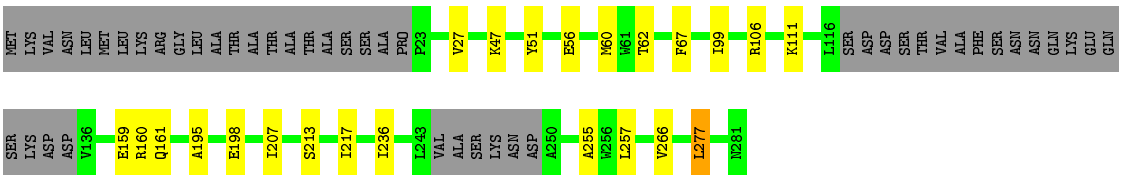
- Molecule 32: mL44

Chain 5:



- Molecule 33: mL46

Chain 6:



- Molecule 34: mL49

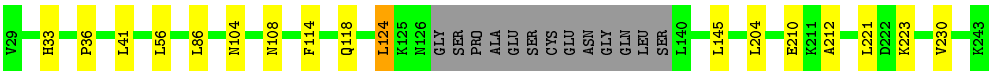
Chain 7:

- Molecule 35: mL50

Chain 8:

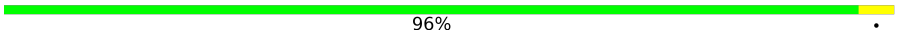
- Molecule 36: mL57

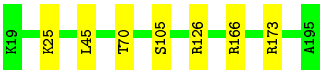
Chain 9:



- Molecule 37: mL58

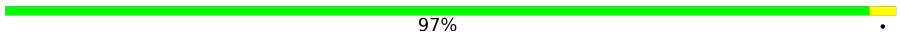
Chain a:

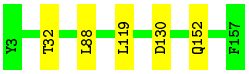




- Molecule 38: mL59

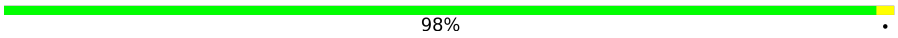
Chain b:





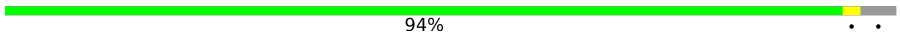
- Molecule 39: mL60

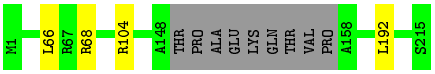
Chain c:



- Molecule 40: mL67

Chain d:



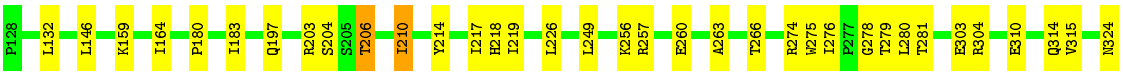


- Molecule 41: bS1m

Chain AA:

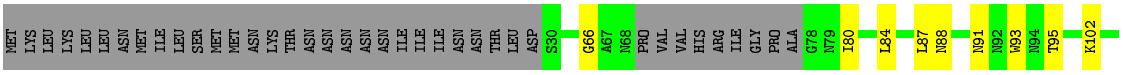
- Molecule 42: uS2m

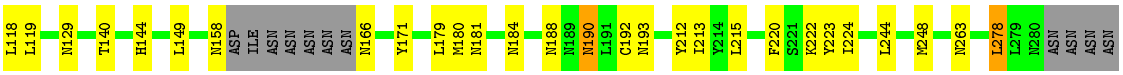
Chain BB:

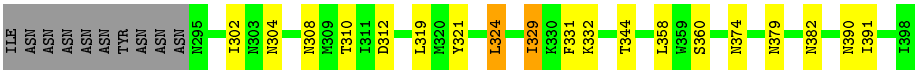


- Molecule 43: uS3m

Chain CC:

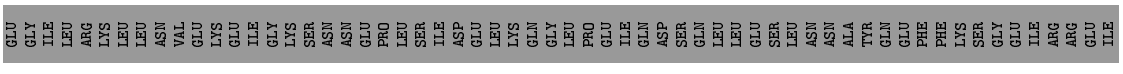


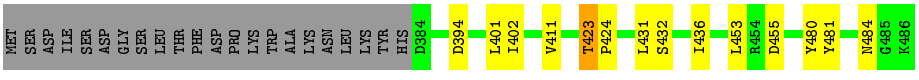




- Molecule 44: uS4m

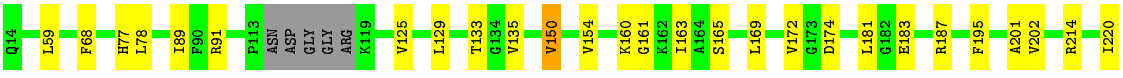
Chain DD:

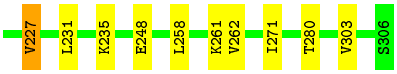




- Molecule 45: uS5m

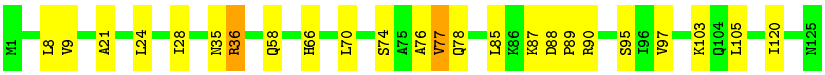
Chain EE:





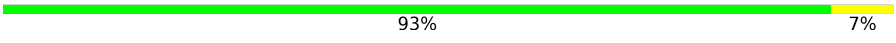
- Molecule 46: bS6m

Chain FF:



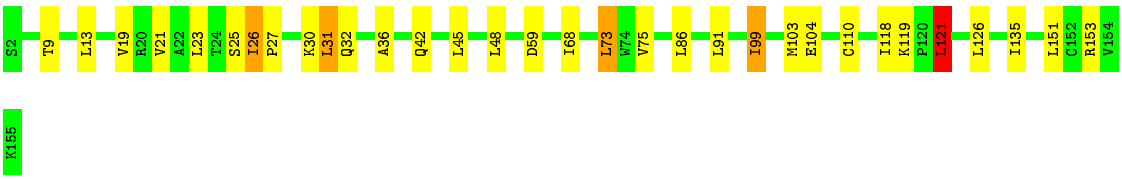
- Molecule 47: uS7m

Chain GG:



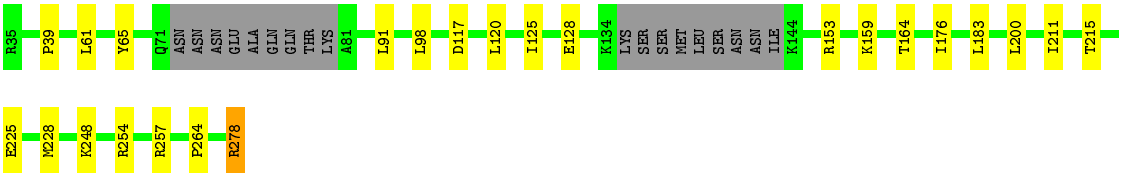
- Molecule 48: uS8m

Chain HH:



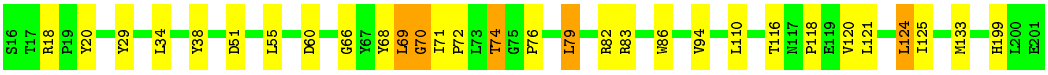
- Molecule 49: uS9m

Chain II:



- Molecule 50: uS10m

Chain JJ:

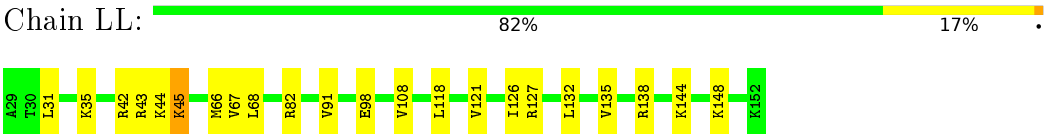


- Molecule 51: uS11m

Chain KK:

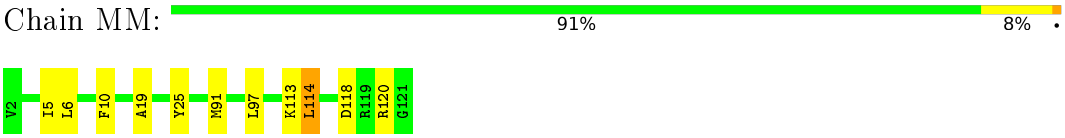
- Molecule 52: uS12m

Chain LL:



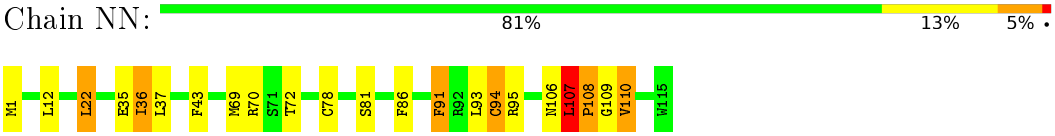
- Molecule 53: uS13m

Chain MM:



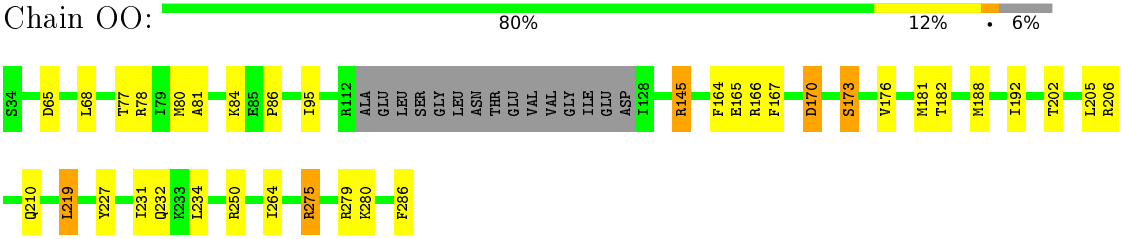
- Molecule 54: uS14m

Chain NN:



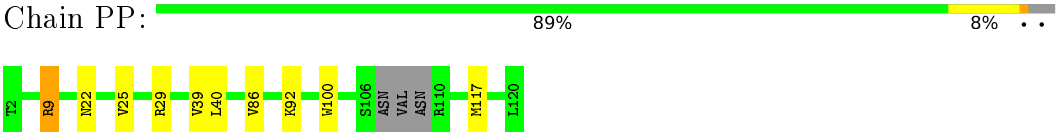
- Molecule 55: uS15m

Chain OO:



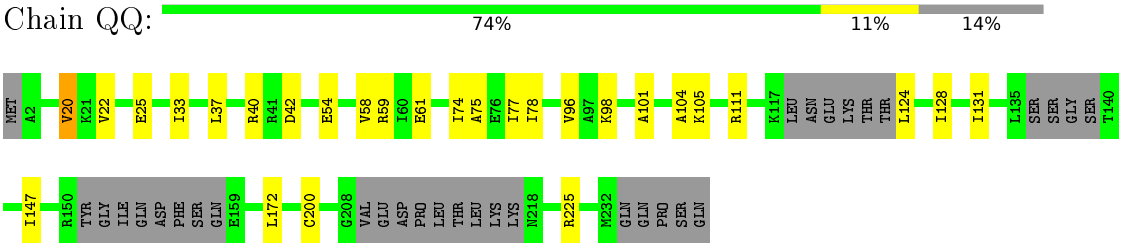
- Molecule 56: bS16m

Chain PP:



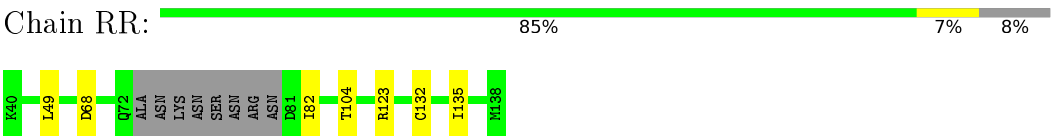
- Molecule 57: uS17m

Chain QQ:



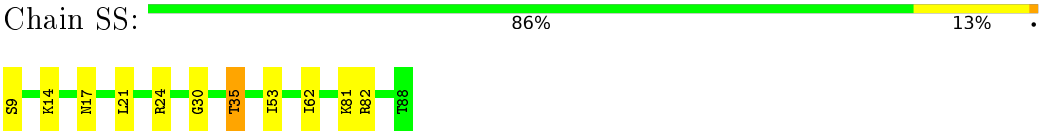
- Molecule 58: bS18m

Chain RR:



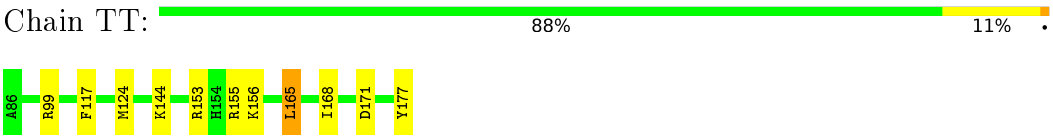
- Molecule 59: uS19m

Chain SS:



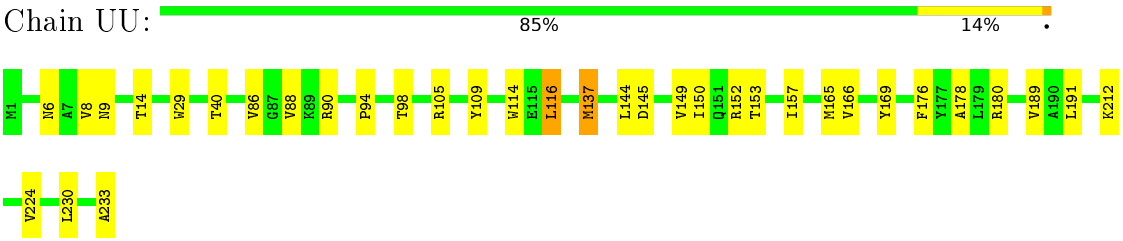
- Molecule 60: bS21m

Chain TT:



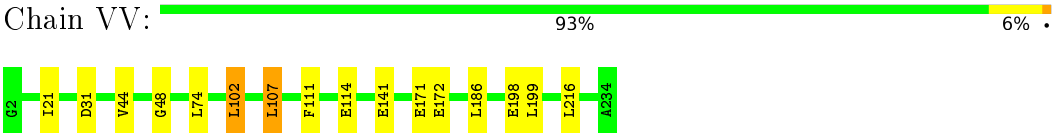
- Molecule 61: mS23

Chain UU:



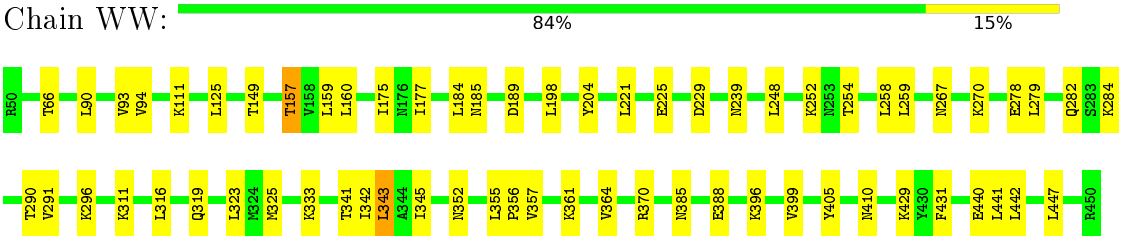
- Molecule 62: mS26

Chain VV:



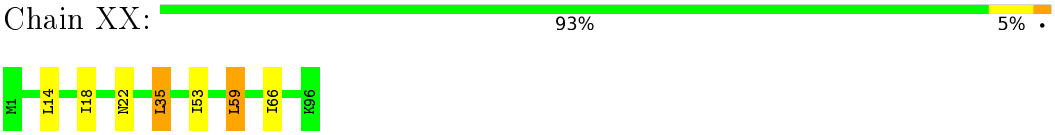
- Molecule 63: mS29

Chain WW:



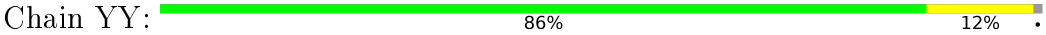
- Molecule 64: mS33

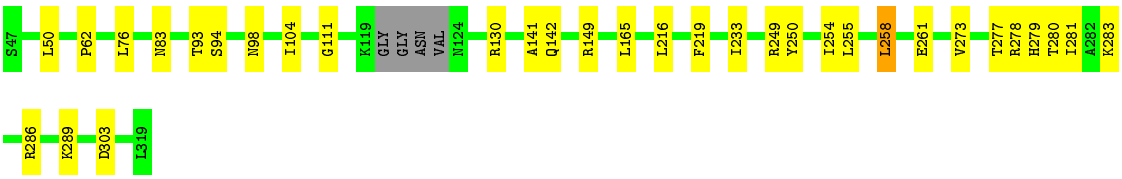
Chain XX:



- Molecule 65: mS35

Chain YY:



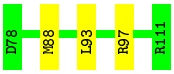


- Molecule 66: mS37

Chain ZZ:

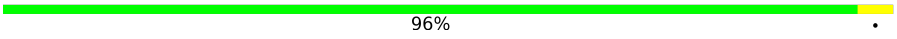
- Molecule 67: mS38

Chain 11:



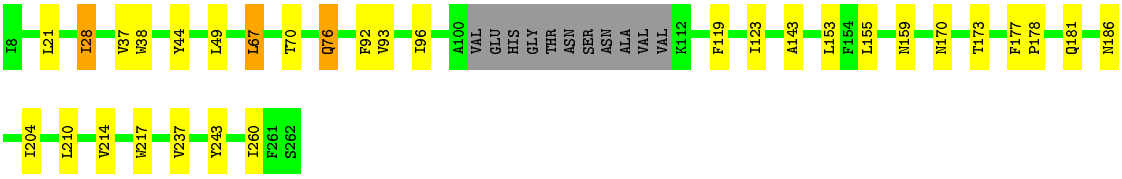
- Molecule 68: mS41

Chain 22:



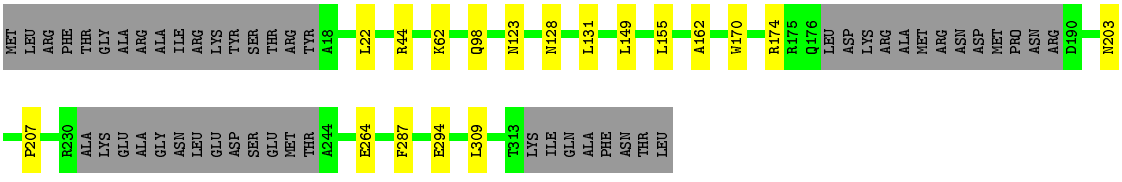
- Molecule 69: mS42

Chain 33:



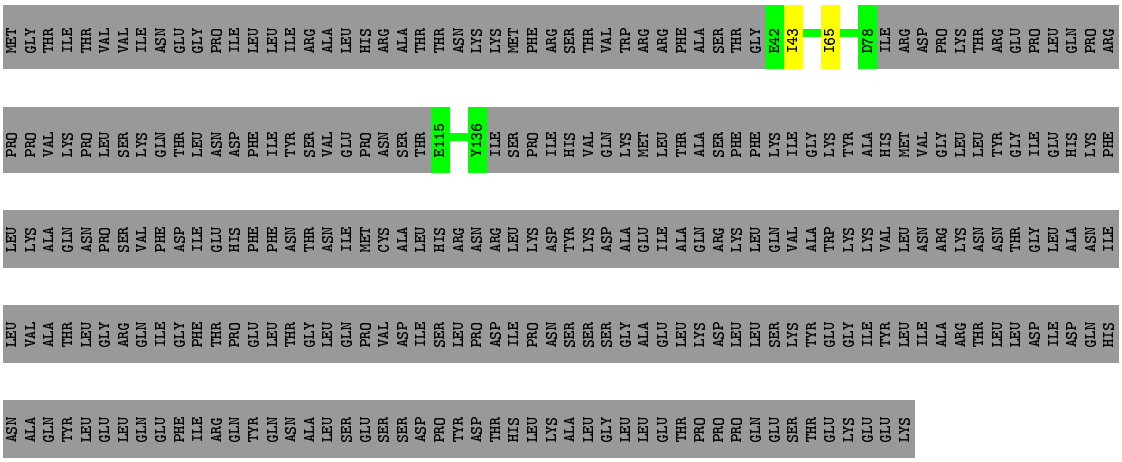
- Molecule 70: mS43

Chain 44:



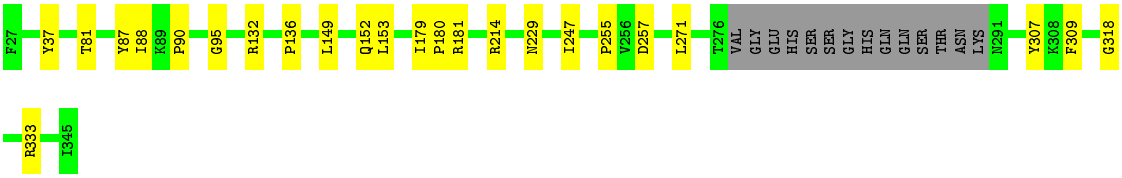
- Molecule 71: mS44

Chain 55:



- Molecule 72: mS45

Chain 66:

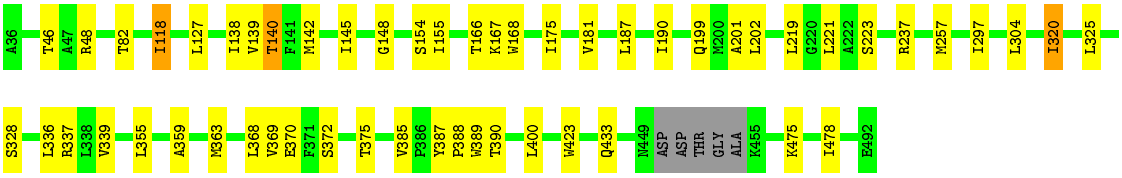


- Molecule 73: mS46

Chain 77:

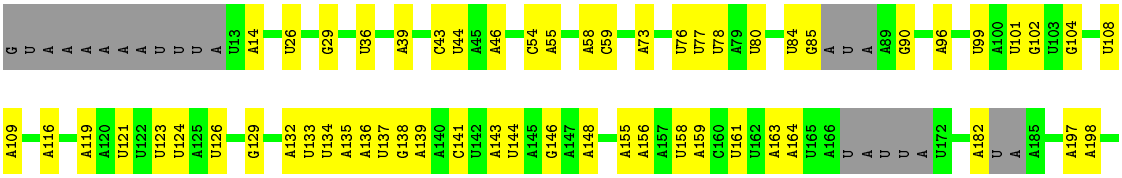
- Molecule 74: mS47

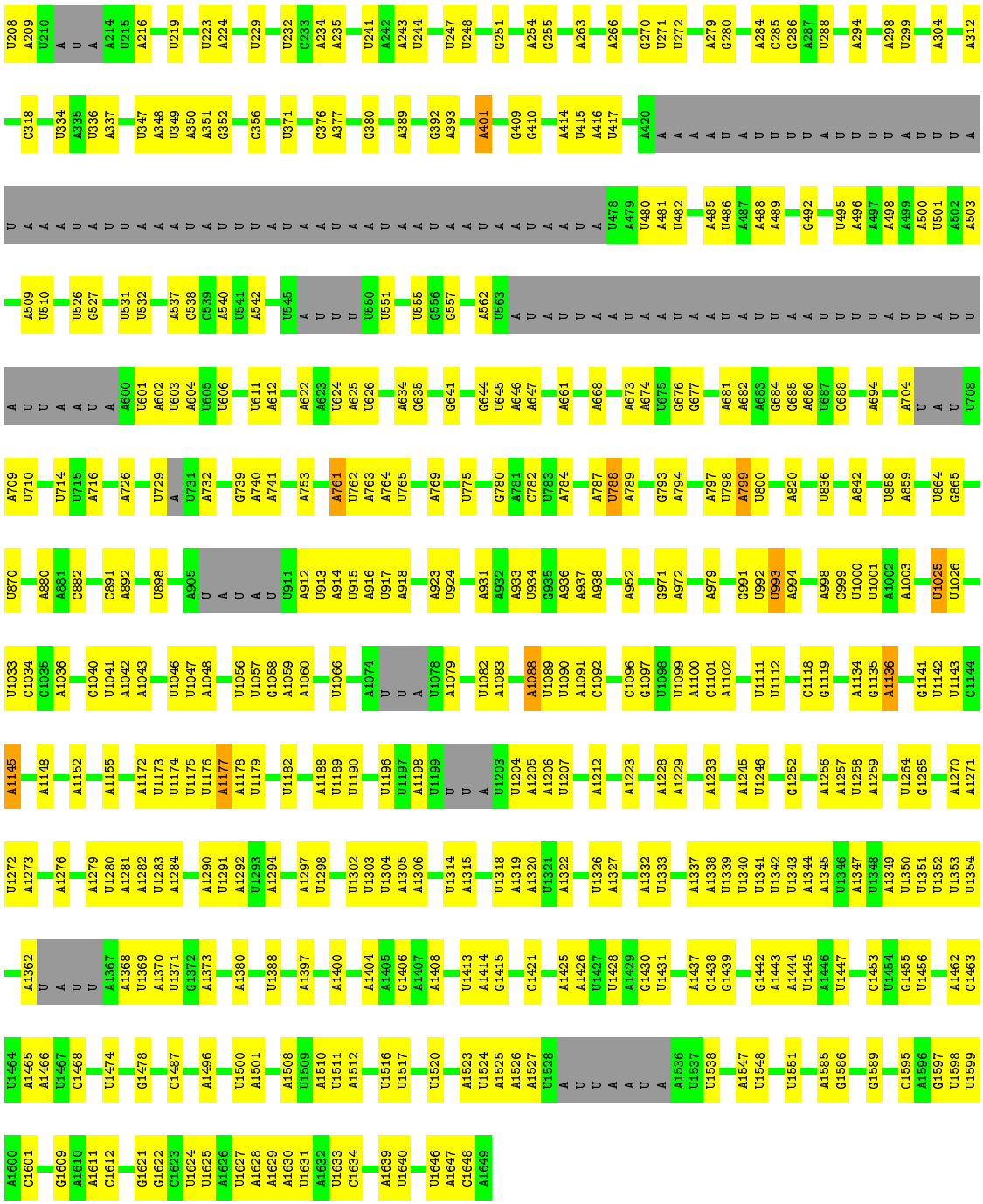
Chain 88:



- Molecule 75: 15S RNA

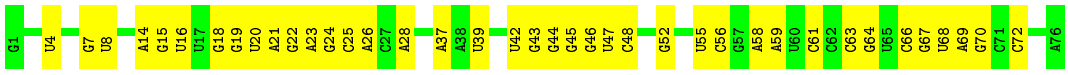
Chain aa:





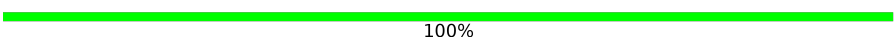
• Molecule 76: tRNA

Chain bb:



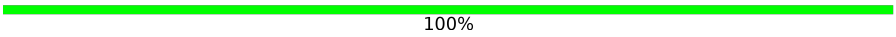
• Molecule 77: unknown protein sequence 1

Chain cc:



There are no outlier residues recorded for this chain.

- Molecule 78: unknown protein sequence 2

Chain dd: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	24632	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	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, NA, 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	0.23	0/64517	0.71	20/100359 (0.0%)
10	J	0.33	0/1783	0.64	0/2384
11	K	0.34	0/1606	0.66	0/2148
12	L	0.32	0/1845	0.63	0/2489
13	M	0.33	0/1224	0.66	0/1651
14	N	0.31	0/961	0.65	0/1295
15	O	0.32	0/1859	0.63	0/2495
16	P	0.33	0/1773	0.61	0/2390
17	Q	0.33	0/2323	0.57	0/3135
18	R	0.33	0/2783	0.64	0/3723
19	S	0.33	0/1576	0.61	0/2104
2	B	0.37	0/2573	0.73	1/3456 (0.0%)
20	T	0.34	0/1837	0.60	0/2486
21	U	0.34	0/648	0.61	0/870
22	V	0.35	0/741	0.61	0/995
23	W	0.31	0/955	0.59	0/1273
24	X	0.33	0/520	0.66	0/696
25	Y	0.35	0/392	0.73	0/515
26	Z	0.34	0/522	0.68	0/695
27	0	0.33	0/329	0.58	0/432
28	1	0.34	0/2949	0.59	0/3998
29	2	0.33	0/963	0.62	0/1295
3	C	0.32	0/1975	0.62	0/2657
30	3	0.34	0/1072	0.61	0/1442
31	4	0.34	0/1138	0.70	0/1526
32	5	0.32	0/2604	0.60	0/3526
33	6	0.34	0/1978	0.59	0/2664
34	7	0.35	0/873	0.62	0/1170
35	8	0.33	0/1659	0.56	0/2230
36	9	0.34	0/1616	0.57	0/2177
37	a	0.34	0/1471	0.65	0/1976
38	b	0.33	0/1333	0.58	0/1783

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
39	c	0.33	0/1028	0.62	0/1372
4	D	0.35	0/2031	0.67	0/2751
40	d	0.33	0/1791	0.62	0/2415
41	AA	0.33	0/1645	0.61	0/2218
42	BB	0.35	0/2128	0.69	0/2892
43	CC	0.34	0/2864	0.58	0/3853
44	DD	0.35	0/2434	0.64	0/3281
45	EE	0.33	0/2360	0.60	0/3180
46	FF	0.43	0/1014	0.70	1/1358 (0.1%)
47	GG	0.35	0/1305	0.62	0/1763
48	HH	0.33	0/1232	0.71	1/1660 (0.1%)
49	II	0.34	0/1855	0.62	0/2492
5	E	0.32	0/2244	0.56	0/3033
50	JJ	0.33	0/1544	0.63	0/2091
51	KK	0.36	0/1136	0.64	0/1515
52	LL	0.34	0/963	0.69	0/1292
53	MM	0.33	0/957	0.65	0/1277
54	NN	0.35	0/972	0.98	1/1300 (0.1%)
55	OO	0.36	0/1985	0.70	2/2647 (0.1%)
56	PP	0.33	0/934	0.64	0/1260
57	QQ	0.34	0/1694	0.65	0/2252
58	RR	0.37	0/749	0.67	0/998
59	SS	0.35	0/652	0.64	0/882
6	F	0.33	0/1551	0.57	0/2093
60	TT	0.37	0/771	0.64	0/1019
61	UU	0.33	0/1950	0.63	0/2636
62	VV	0.32	0/1900	0.60	0/2540
63	WW	0.34	0/3282	0.58	0/4438
64	XX	0.35	0/786	0.64	0/1046
65	YY	0.35	0/2313	0.62	0/3119
66	ZZ	0.32	0/702	0.61	0/945
67	11	0.33	0/303	0.80	0/386
68	22	0.34	0/852	0.56	0/1142
69	33	0.35	0/2002	0.58	0/2721
7	G	0.33	0/628	0.58	0/844
70	44	0.34	0/2214	0.58	0/2990
71	55	0.35	0/521	0.57	0/701
72	66	0.34	0/2547	0.59	0/3438
73	77	0.35	0/1358	0.56	0/1839
74	88	0.35	0/3646	0.58	0/4935
75	aa	0.25	0/35686	0.74	26/55477 (0.0%)
76	bb	0.42	0/1805	0.80	4/2811 (0.1%)
8	H	0.34	0/1302	0.63	0/1749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
9	I	0.31	0/962	0.66	0/1285
All	All	0.30	0/212996	0.68	56/307971 (0.0%)

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	NN	107	LEU	C-N-CD	-26.29	62.77	120.60
1	A	3242	A	N9-C1'-C2'	-8.66	102.48	112.00
1	A	2897	A	C2'-C3'-O3'	8.34	127.85	109.50
1	A	840	C	C2'-C3'-O3'	8.32	127.81	109.50
1	A	3242	A	C2'-C3'-O3'	-8.01	91.88	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	57598	0	28893	259	0
2	B	2527	0	2649	142	0
3	C	1932	0	1969	20	0
4	D	1991	0	2032	9	0
5	E	2187	0	2203	8	0
6	F	1524	0	1587	4	0
7	G	617	0	626	1	0
8	H	1275	0	1310	18	0
9	I	956	0	1037	4	0
10	J	1746	0	1840	5	0
11	K	1573	0	1629	5	0
12	L	1817	0	1878	10	0
13	M	1206	0	1283	6	0
14	N	948	0	1006	1	0
15	O	1826	0	1933	13	0
16	P	1729	0	1724	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	2272	0	2334	6	0
18	R	2738	0	2811	6	0
19	S	1543	0	1621	13	0
20	T	1792	0	1782	12	0
21	U	639	0	699	5	0
22	V	729	0	711	0	0
23	W	937	0	975	5	0
24	X	512	0	563	3	0
25	Y	385	0	423	3	0
26	Z	508	0	539	0	0
27	0	324	0	344	3	0
28	1	2875	0	2881	12	0
29	2	944	0	969	9	0
30	3	1046	0	1071	6	0
31	4	1117	0	1142	7	0
32	5	2552	0	2600	19	0
33	6	1932	0	1950	12	0
34	7	858	0	908	6	0
35	8	1629	0	1633	3	0
36	9	1587	0	1628	7	0
37	a	1440	0	1473	0	0
38	b	1299	0	1367	0	0
39	c	1004	0	1065	0	0
40	d	1746	0	1743	0	0
41	AA	1610	0	1639	5	0
42	BB	2085	0	2094	40	0
43	CC	2821	0	2829	39	0
44	DD	2369	0	2433	21	0
45	EE	2306	0	2324	23	0
46	FF	1002	0	1086	74	0
47	GG	1282	0	1342	5	0
48	HH	1213	0	1277	12	0
49	II	1820	0	1906	8	0
50	JJ	1508	0	1505	15	0
51	KK	1121	0	1172	32	0
52	LL	948	0	1003	12	0
53	MM	942	0	1001	3	0
54	NN	953	0	1007	37	0
55	OO	1962	0	2036	67	0
56	PP	919	0	982	4	0
57	QQ	1683	0	1769	42	0
58	RR	738	0	771	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	SS	636	0	654	2	0
60	TT	760	0	791	4	0
61	UU	1907	0	1898	21	0
62	VV	1872	0	1978	7	0
63	WW	3216	0	3315	15	0
64	XX	774	0	821	4	0
65	YY	2258	0	2229	10	0
66	ZZ	687	0	719	48	0
67	11	303	0	357	1	0
68	22	833	0	839	1	0
69	33	1953	0	1913	16	0
70	44	2169	0	2155	6	0
71	55	508	0	524	0	0
72	66	2488	0	2520	9	0
73	77	1330	0	1350	6	0
74	88	3573	0	3576	22	0
75	aa	31883	0	16010	0	0
76	bb	1615	0	821	0	0
77	cc	470	0	102	0	0
78	dd	755	0	167	0	0
79	A	182	0	0	0	0
79	BB	1	0	0	0	0
79	LL	1	0	0	0	0
79	MM	1	0	0	0	0
79	OO	1	0	0	0	0
79	PP	1	0	0	0	0
79	R	1	0	0	0	0
79	WW	1	0	0	0	0
79	aa	110	0	0	0	0
80	B	1	0	0	0	0
81	0	1	0	0	0	0
81	W	1	0	0	1	0
82	WW	28	0	12	1	0
All	All	201462	0	157758	977	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 4.

The worst 5 of 977 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)
2:B:63:ILE:HD11	57:QQ:104:ALA:CB	1.20	1.61
2:B:232:VAL:CG2	46:FF:87:LYS:HD2	1.30	1.59
2:B:73:LEU:HD23	46:FF:77:VAL:CG2	1.29	1.57
2:B:232:VAL:HG21	46:FF:87:LYS:CD	1.34	1.55
19:S:211:TYR:CE2	19:S:227:TYR:CE1	2.00	1.47

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
2	B	317/393 (81%)	302 (95%)	14 (4%)	1 (0%)	46 83
3	C	247/249 (99%)	234 (95%)	10 (4%)	3 (1%)	16 62
4	D	250/252 (99%)	237 (95%)	9 (4%)	4 (2%)	12 57
5	E	272/274 (99%)	254 (93%)	16 (6%)	2 (1%)	26 71
6	F	194/196 (99%)	182 (94%)	11 (6%)	1 (0%)	34 77
7	G	72/74 (97%)	70 (97%)	2 (3%)	0	100 100
8	H	158/160 (99%)	152 (96%)	6 (4%)	0	100 100
9	I	123/138 (89%)	114 (93%)	9 (7%)	0	100 100
10	J	218/220 (99%)	203 (93%)	14 (6%)	1 (0%)	34 77
11	K	193/195 (99%)	184 (95%)	9 (5%)	0	100 100
12	L	225/237 (95%)	218 (97%)	7 (3%)	0	100 100
13	M	149/151 (99%)	139 (93%)	10 (7%)	0	100 100
14	N	116/118 (98%)	108 (93%)	8 (7%)	0	100 100
15	O	223/225 (99%)	211 (95%)	12 (5%)	0	100 100
16	P	205/207 (99%)	196 (96%)	9 (4%)	0	100 100
17	Q	280/296 (95%)	268 (96%)	12 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	327/337 (97%)	314 (96%)	12 (4%)	1 (0%)	46	83
19	S	181/216 (84%)	172 (95%)	9 (5%)	0	100	100
20	T	210/225 (93%)	199 (95%)	11 (5%)	0	100	100
21	U	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
22	V	87/177 (49%)	83 (95%)	4 (5%)	0	100	100
23	W	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
24	X	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	Y	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
26	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
27	0	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
28	1	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
29	2	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
30	3	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
31	4	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
32	5	322/324 (99%)	306 (95%)	16 (5%)	0	100	100
33	6	228/281 (81%)	221 (97%)	7 (3%)	0	100	100
34	7	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
35	8	195/264 (74%)	192 (98%)	3 (2%)	0	100	100
36	9	198/215 (92%)	186 (94%)	12 (6%)	0	100	100
37	a	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
38	b	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
39	c	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	21	67
40	d	202/215 (94%)	189 (94%)	13 (6%)	0	100	100
41	AA	197/344 (57%)	190 (96%)	7 (4%)	0	100	100
42	BB	264/266 (99%)	247 (94%)	15 (6%)	2 (1%)	24	69
43	CC	331/398 (83%)	303 (92%)	26 (8%)	2 (1%)	30	74
44	DD	281/486 (58%)	264 (94%)	16 (6%)	1 (0%)	39	80
45	EE	284/293 (97%)	262 (92%)	20 (7%)	2 (1%)	26	71
46	FF	123/125 (98%)	112 (91%)	11 (9%)	0	100	100
47	GG	159/161 (99%)	147 (92%)	11 (7%)	1 (1%)	30	74
48	HH	152/154 (99%)	144 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
49	II	220/244 (90%)	207 (94%)	11 (5%)	2 (1%)	21 67
50	JJ	184/186 (99%)	163 (89%)	15 (8%)	6 (3%)	5 42
51	KK	138/148 (93%)	124 (90%)	12 (9%)	2 (1%)	14 58
52	LL	122/124 (98%)	110 (90%)	10 (8%)	2 (2%)	12 57
53	MM	118/120 (98%)	109 (92%)	9 (8%)	0	100 100
54	NN	113/115 (98%)	106 (94%)	4 (4%)	3 (3%)	6 46
55	OO	234/253 (92%)	222 (95%)	12 (5%)	0	100 100
56	PP	112/119 (94%)	105 (94%)	7 (6%)	0	100 100
57	QQ	194/237 (82%)	184 (95%)	9 (5%)	1 (0%)	34 77
58	RR	87/99 (88%)	81 (93%)	6 (7%)	0	100 100
59	SS	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	15 60
60	TT	90/92 (98%)	86 (96%)	4 (4%)	0	100 100
61	UU	231/233 (99%)	223 (96%)	8 (4%)	0	100 100
62	VV	231/233 (99%)	220 (95%)	11 (5%)	0	100 100
63	WW	399/401 (100%)	368 (92%)	28 (7%)	3 (1%)	24 69
64	XX	91/96 (95%)	88 (97%)	3 (3%)	0	100 100
65	YY	265/273 (97%)	244 (92%)	18 (7%)	3 (1%)	17 64
66	ZZ	83/91 (91%)	70 (84%)	12 (14%)	1 (1%)	16 62
67	11	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
68	22	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	19 65
69	33	240/255 (94%)	225 (94%)	14 (6%)	1 (0%)	39 80
70	44	264/321 (82%)	251 (95%)	10 (4%)	3 (1%)	17 64
71	55	55/339 (16%)	53 (96%)	2 (4%)	0	100 100
72	66	301/319 (94%)	291 (97%)	10 (3%)	0	100 100
73	77	163/165 (99%)	146 (90%)	16 (10%)	1 (1%)	30 74
74	88	448/457 (98%)	414 (92%)	31 (7%)	3 (1%)	26 71
All	All	13235/14689 (90%)	12462 (94%)	718 (5%)	55 (0%)	43 80

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	DD	423	THR
51	KK	141	TYR

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Mol	Chain	Res	Type
52	LL	45	LYS
52	LL	98	GLU
54	NN	108	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	272/337 (81%)	254 (93%)	18 (7%)	21	59
3	C	210/210 (100%)	200 (95%)	10 (5%)	31	68
4	D	218/218 (100%)	199 (91%)	19 (9%)	13	48
5	E	242/242 (100%)	231 (96%)	11 (4%)	34	70
6	F	172/172 (100%)	164 (95%)	8 (5%)	32	69
7	G	68/68 (100%)	66 (97%)	2 (3%)	50	79
8	H	138/138 (100%)	131 (95%)	7 (5%)	29	67
9	I	108/117 (92%)	104 (96%)	4 (4%)	41	74
10	J	181/181 (100%)	166 (92%)	15 (8%)	14	51
11	K	167/167 (100%)	151 (90%)	16 (10%)	10	43
12	L	203/211 (96%)	194 (96%)	9 (4%)	35	70
13	M	136/136 (100%)	130 (96%)	6 (4%)	35	70
14	N	107/107 (100%)	105 (98%)	2 (2%)	65	86
15	O	200/200 (100%)	188 (94%)	12 (6%)	24	62
16	P	185/185 (100%)	181 (98%)	4 (2%)	60	84
17	Q	256/267 (96%)	242 (94%)	14 (6%)	27	65
18	R	303/308 (98%)	291 (96%)	12 (4%)	38	72
19	S	167/191 (87%)	161 (96%)	6 (4%)	42	75
20	T	204/213 (96%)	196 (96%)	8 (4%)	39	73
21	U	73/73 (100%)	70 (96%)	3 (4%)	37	72
22	V	74/161 (46%)	71 (96%)	3 (4%)	37	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	W	104/104 (100%)	101 (97%)	3 (3%)	50 79
24	X	56/56 (100%)	52 (93%)	4 (7%)	18 57
25	Y	40/40 (100%)	39 (98%)	1 (2%)	55 82
26	Z	50/50 (100%)	46 (92%)	4 (8%)	15 52
27	0	36/36 (100%)	35 (97%)	1 (3%)	51 79
28	1	323/323 (100%)	311 (96%)	12 (4%)	41 74
29	2	106/106 (100%)	99 (93%)	7 (7%)	21 59
30	3	112/112 (100%)	109 (97%)	3 (3%)	52 80
31	4	121/121 (100%)	118 (98%)	3 (2%)	55 82
32	5	284/284 (100%)	278 (98%)	6 (2%)	61 85
33	6	213/252 (84%)	205 (96%)	8 (4%)	40 74
34	7	95/95 (100%)	91 (96%)	4 (4%)	36 71
35	8	182/240 (76%)	173 (95%)	9 (5%)	31 68
36	9	176/186 (95%)	168 (96%)	8 (4%)	34 70
37	a	158/158 (100%)	151 (96%)	7 (4%)	35 70
38	b	144/144 (100%)	139 (96%)	5 (4%)	43 76
39	c	110/110 (100%)	109 (99%)	1 (1%)	84 93
40	d	191/199 (96%)	187 (98%)	4 (2%)	61 85
41	AA	177/309 (57%)	168 (95%)	9 (5%)	29 67
42	BB	233/233 (100%)	206 (88%)	27 (12%)	7 34
43	CC	328/385 (85%)	296 (90%)	32 (10%)	10 42
44	DD	256/437 (59%)	227 (89%)	29 (11%)	7 35
45	EE	249/252 (99%)	237 (95%)	12 (5%)	31 68
46	FF	114/114 (100%)	105 (92%)	9 (8%)	15 53
47	GG	138/138 (100%)	132 (96%)	6 (4%)	35 71
48	HH	141/141 (100%)	125 (89%)	16 (11%)	7 35
49	II	196/215 (91%)	185 (94%)	11 (6%)	26 65
50	JJ	167/167 (100%)	152 (91%)	15 (9%)	12 46
51	KK	122/127 (96%)	107 (88%)	15 (12%)	6 32
52	LL	103/103 (100%)	91 (88%)	12 (12%)	7 34
53	MM	100/100 (100%)	94 (94%)	6 (6%)	24 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	NN	103/103 (100%)	91 (88%)	12 (12%)	7 34
55	OO	208/220 (94%)	198 (95%)	10 (5%)	31 68
56	PP	101/104 (97%)	95 (94%)	6 (6%)	24 63
57	QQ	187/218 (86%)	178 (95%)	9 (5%)	31 68
58	RR	80/87 (92%)	74 (92%)	6 (8%)	17 55
59	SS	69/69 (100%)	62 (90%)	7 (10%)	9 40
60	TT	81/81 (100%)	73 (90%)	8 (10%)	10 41
61	UU	208/208 (100%)	196 (94%)	12 (6%)	25 63
62	VV	208/210 (99%)	199 (96%)	9 (4%)	35 71
63	WW	368/368 (100%)	328 (89%)	40 (11%)	8 37
64	XX	84/84 (100%)	79 (94%)	5 (6%)	24 62
65	YY	248/250 (99%)	231 (93%)	17 (7%)	19 58
66	ZZ	78/82 (95%)	67 (86%)	11 (14%)	4 27
67	11	32/32 (100%)	31 (97%)	1 (3%)	47 78
68	22	90/90 (100%)	89 (99%)	1 (1%)	80 91
69	33	216/231 (94%)	203 (94%)	13 (6%)	24 62
70	44	238/281 (85%)	229 (96%)	9 (4%)	40 74
71	55	53/303 (18%)	51 (96%)	2 (4%)	40 74
72	66	277/289 (96%)	269 (97%)	8 (3%)	50 79
73	77	158/158 (100%)	152 (96%)	6 (4%)	40 74
74	88	401/404 (99%)	376 (94%)	25 (6%)	23 61
All	All	11997/13111 (92%)	11302 (94%)	695 (6%)	29 63

5 of 695 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BB	382	ARG
46	FF	36	ARG
69	33	210	LEU
43	CC	179	LEU
44	DD	51	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2677/3296 (81%)	613 (22%)	109 (4%)
75	aa	1473/1649 (89%)	445 (30%)	0
76	bb	75/76 (98%)	36 (48%)	0
All	All	4225/5021 (84%)	1094 (25%)	109 (2%)

5 of 1094 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	22	U
1	A	26	A
1	A	27	A
1	A	28	U
1	A	30	U

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1522	A
1	A	2301	C
1	A	3177	A
1	A	1547	U
1	A	1707	C

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 303 ligands modelled in this entry, 302 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	$\#\|Z\| > 2$
82	GDP	WW	501	79	24,30,30	1.22	2 (8%)	26,47,47	1.90	6 (23%)

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
82	GDP	WW	501	79	-	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)
82	WW	501	GDP	C5-C4	3.39	1.48	1.40
82	WW	501	GDP	C6-C5	3.74	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WW	501	GDP	C5-C6-N1	-3.92	118.39	123.52
82	WW	501	GDP	N3-C2-N1	-3.46	122.85	127.56
82	WW	501	GDP	C4'-O4'-C1'	-2.77	106.71	109.64
82	WW	501	GDP	C6-C5-C4	-2.74	117.73	120.86
82	WW	501	GDP	O4'-C1'-N9	3.42	114.57	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	WW	501	GDP	1	0

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
75	aa	13
78	dd	7
77	cc	3
64	XX	2

The worst 5 of 25 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	dd	115:UNK	C	151:UNK	N	40.49
1	dd	220:UNK	C	265:UNK	N	35.54
1	dd	170:UNK	C	202:UNK	N	27.03
1	cc	59:UNK	C	76:UNK	N	22.66
1	cc	93:UNK	C	105:UNK	N	20.49