wwPDB EM Validation Summary Report (i)

Mar 6, 2025 – 06:36 pm GMT

PDB ID	:	7PJT
EMDB ID	:	EMD-13459
Title	:	Structure of the 70S ribosome with tRNAs in hybrid state 1 (H1)
Authors	:	Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on	:	2021-08-24
Resolution	:	6.00 Å(reported)
Based on initial models	:	5LZD, 6YSS, 4AQY

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

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

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

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

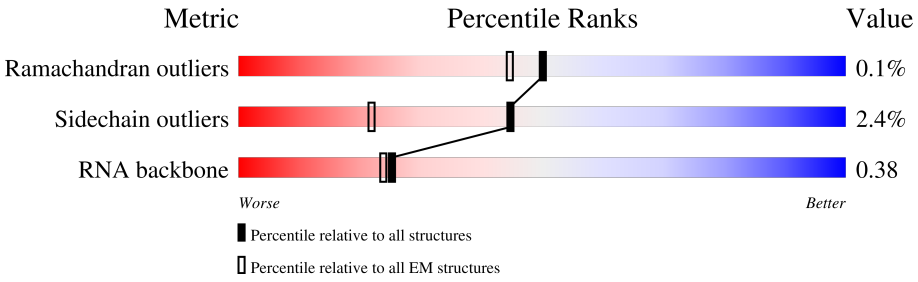
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 6.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	0	57	95%
2	1	55	91% 9%
3	2	46	98%
4	3	65	89% 9%
5	4	38	95% 5%
6	5	165	79% 21%
7	6	70	84% 10% 6%
8	A	2903	57% 40%
9	B	120	60% 39%

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Mol	Chain	Length	Quality of chain
10	C	273	99%
11	D	209	99%
12	E	201	100%
13	F	179	95%
14	G	177	98%
15	H	149	99%
16	I	142	99%
17	J	142	97%
18	K	123	99%
19	L	144	97%
20	M	136	99%
21	N	127	94% 6%
22	O	117	95%
23	P	115	97%
24	Q	118	97%
25	R	103	95% 5%
26	S	110	95% 5%
27	T	100	91% 7%
28	U	104	96%
29	V	94	100%
30	W	85	87% 12%
31	X	78	96%
32	Y	63	92% 8%
33	Z	59	98%
34	a	1542	60% 38%

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Mol	Chain	Length	Quality of chain
35	b	240	90% 9%
36	c	233	87% 12%
37	d	206	97%
38	e	167	93% 6%
39	f	135	73% 26%
40	g	179	83% 16%
41	h	130	98%
42	i	130	94%
43	j	103	94% 5%
44	k	129	88% 10%
45	l	124	98%
46	m	118	95%
47	n	102	95%
48	o	89	97%
49	p	82	100%
50	q	84	94% 5%
51	r	75	85% 13%
52	s	92	83% 7% 11%
53	t	87	98%
54	u	71	89% 8%
55	v	77	55% 38% 8%
56	w	76	50% 45% 5%
57	y	2	100%
58	z	33	15% 18% 67%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 147222 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 protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2902	Total	C	N	O	P	0	0
			62317	27806	11469	20140	2902		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 12 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	I	141	Total	C	N	O	0	0
			693	411	141	141		

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 29 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	94	Total 753	C 479	N 137	O 134	S 3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total 575	C 356	N 116	O 102	S 1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total 509	C 313	N 99	O 95	S 2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	58	Total 449	C 281	N 87	O 79	S 2	0	0

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total 33050	C 14748	N 6057	O 10705	P 1540	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

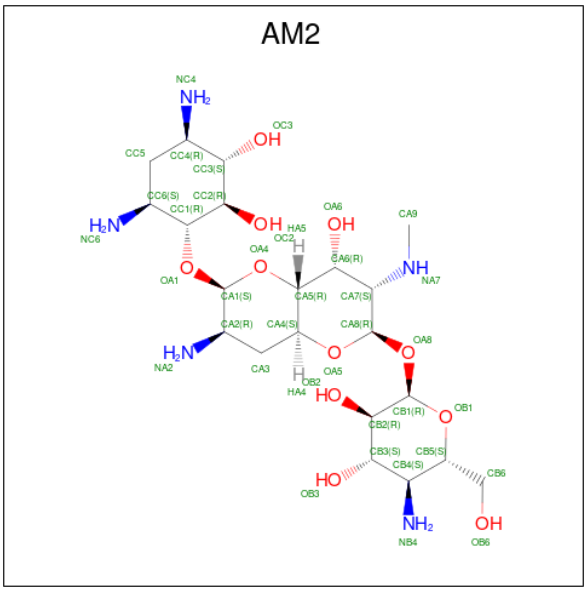
- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	11	Total	C	N	O	P	0	0
			230	103	35	81	11		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	4	1	Total	Zn	0
			1	1	
59	6	1	Total	Zn	0
			1	1	

- Molecule 60 is APRAMYCIN (three-letter code: AM2) (formula: $C_{21}H_{41}N_5O_{11}$).



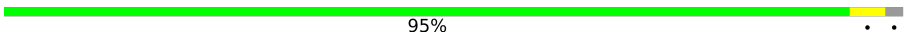
Mol	Chain	Residues	Atoms				AltConf
60	a	1	Total	C	N	O	0
			37	21	5	11	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

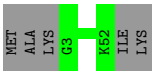
• Molecule 1: 50S ribosomal protein L32

Chain 0:



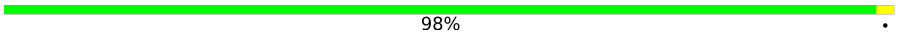
• Molecule 2: 50S ribosomal protein L33

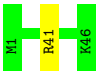
Chain 1:



• Molecule 3: 50S ribosomal protein L34

Chain 2:



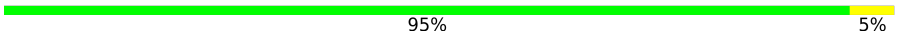


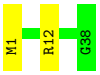
• Molecule 4: 50S ribosomal protein L35

Chain 3:

• Molecule 5: 50S ribosomal protein L36

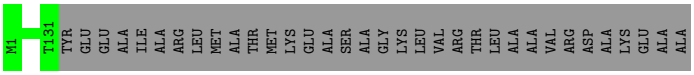
Chain 4:





• Molecule 6: 50S ribosomal protein L10

Chain 5:

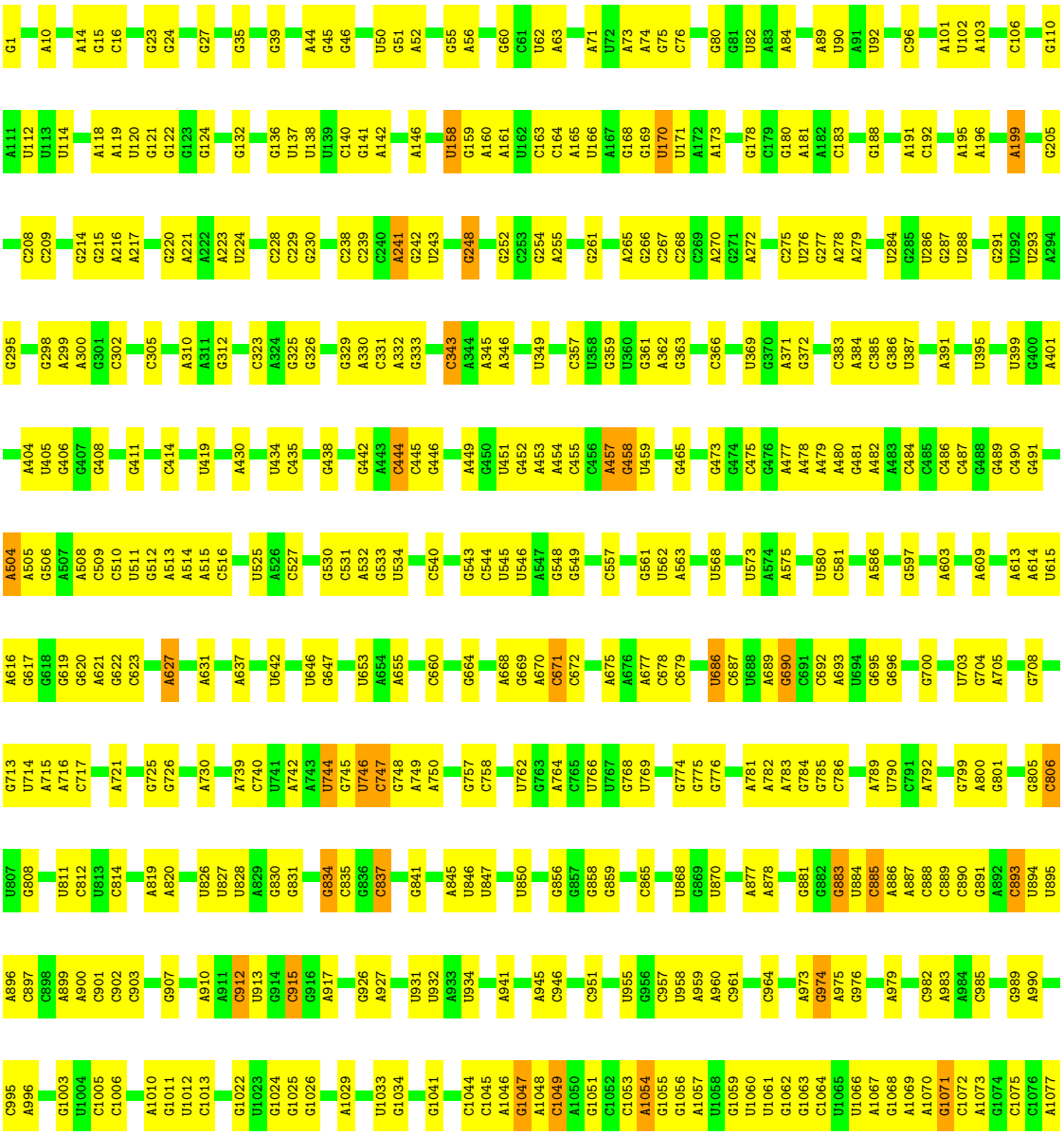


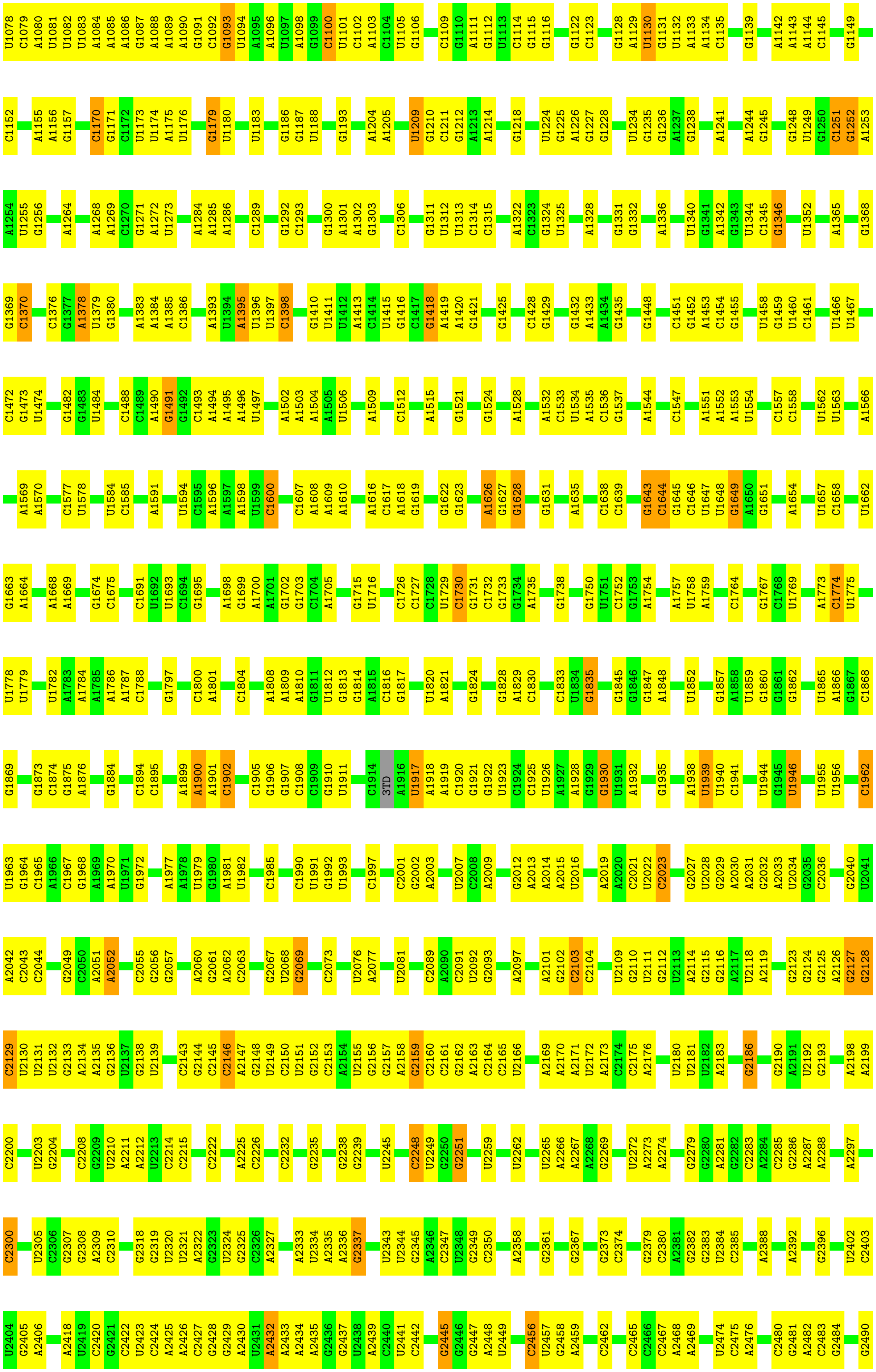
• Molecule 7: 50S ribosomal protein L31

Chain 6:

• Molecule 8: 23S ribosomal RNA

Chain A:

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C1152 A1155 A1156 G1157 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1179 U1180 U1183 G1186 G1187 U1188 G1193 A1204 A1205 U1209 G1210 C1211 G1212 A1213 A1214 G1218 U1224 G1225 A1226 G1227 G1228 U1234 G1235 G1236 A1237 G1238 A1241 A1244 G1245 G1248 U1249 G1250 C1251 G1252 A1253
A1254 U1255 G1256 A1264 A1268 A1269 C1270 G1271 A1272 U1273 A1284 A1285 A1286 C1289 G1292 C1293 G1300 A1301 A1302 G1303 C1306 G1311 U1312 U1313 C1314 C1315 A1322 C1323 G1324 U1325 A1328 G1331 G1332 A1336 U1340 G1341 A1342 G1343 U1344 C1345 G1346 U1352 A1365 G1368
G1369 C1370 C1376 G1377 A1378 U1379 G1380 A1383 A1384 A1385 C1386 A1393 U1394 A1395 U1396 U1397 C1398 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1425 C1428 G1429 G1432 A1433 A1434 G1435 G1448 C1451 G1452 A1453 C1454 G1455 U1458 G1459 U1460 C1461 U1466 U1467
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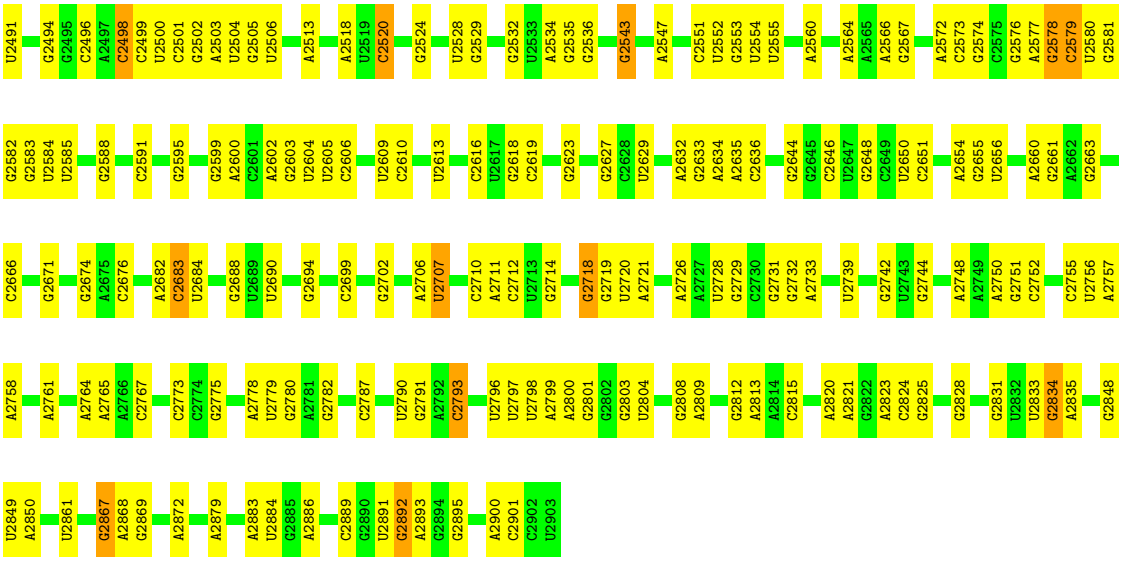
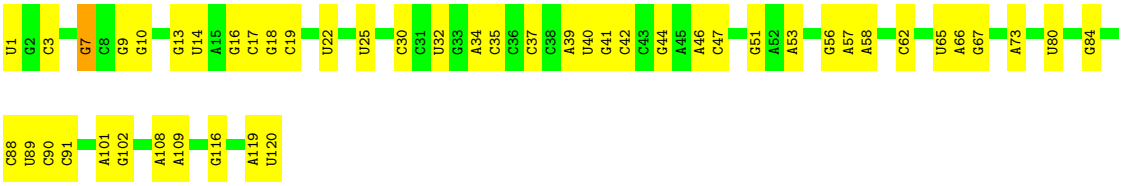


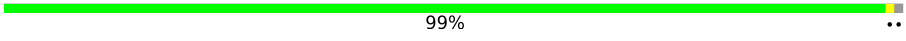
• Molecule 9: 5S ribosomal RNA

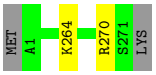
Chain B:



• Molecule 10: 50S ribosomal protein L2

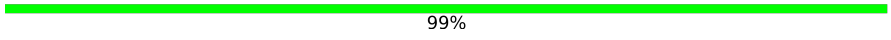
Chain C:

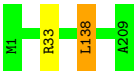




• Molecule 11: 50S ribosomal protein L3

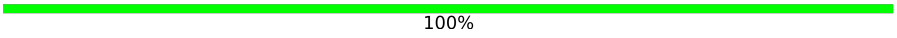
Chain D:





• Molecule 12: 50S ribosomal protein L4

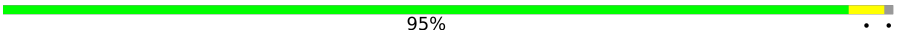
Chain E:



There are no outlier residues recorded for this chain.

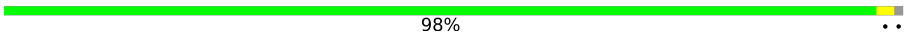
• Molecule 13: 50S ribosomal protein L5

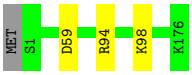
Chain F:



• Molecule 14: 50S ribosomal protein L6

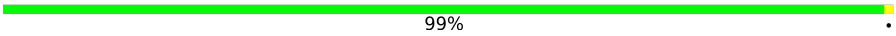
Chain G:





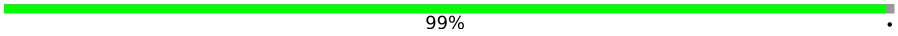
• Molecule 15: 50S ribosomal protein L9

Chain H:



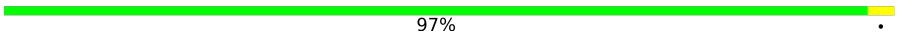
• Molecule 16: 50S ribosomal protein L11

Chain I:



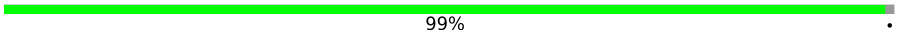
• Molecule 17: 50S ribosomal protein L13

Chain J:



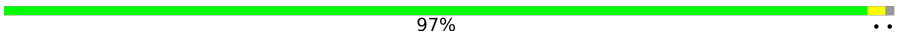
• Molecule 18: 50S ribosomal protein L14

Chain K:



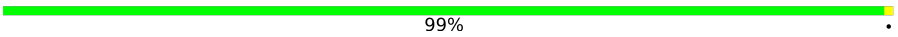
• Molecule 19: 50S ribosomal protein L15

Chain L:



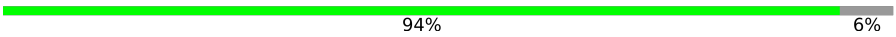
• Molecule 20: 50S ribosomal protein L16

Chain M:



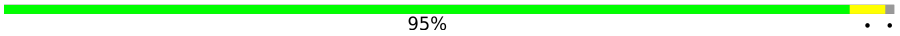
• Molecule 21: 50S ribosomal protein L17

Chain N:



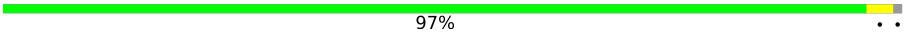
• Molecule 22: 50S ribosomal protein L18

Chain O:



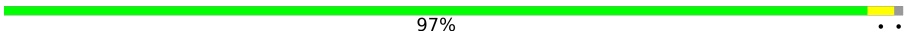
• Molecule 23: 50S ribosomal protein L19

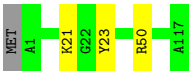
Chain P:



• Molecule 24: 50S ribosomal protein L20

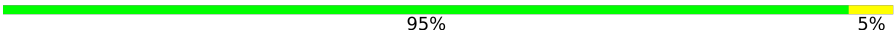
Chain Q:

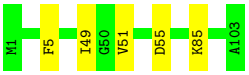




• Molecule 25: 50S ribosomal protein L21

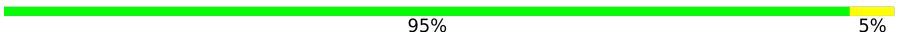
Chain R:

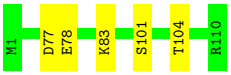




• Molecule 26: 50S ribosomal protein L22

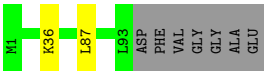
Chain S:





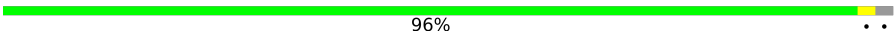
• Molecule 27: 50S ribosomal protein L23

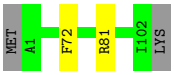
Chain T:



• Molecule 28: 50S ribosomal protein L24

Chain U:





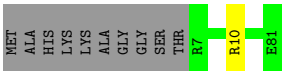
• Molecule 29: 50S ribosomal protein L25

Chain V:

There are no outlier residues recorded for this chain.

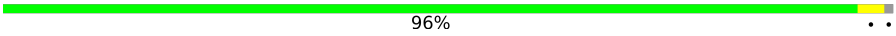
• Molecule 30: 50S ribosomal protein L27

Chain W:



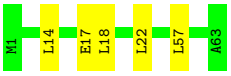
• Molecule 31: 50S ribosomal protein L28

Chain X:



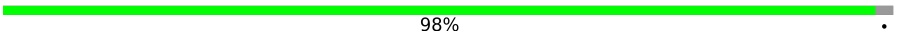
• Molecule 32: 50S ribosomal protein L29

Chain Y:



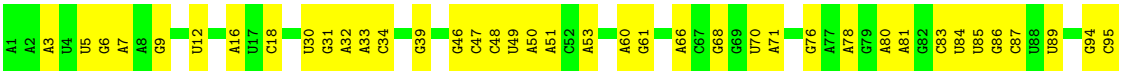
• Molecule 33: 50S ribosomal protein L30

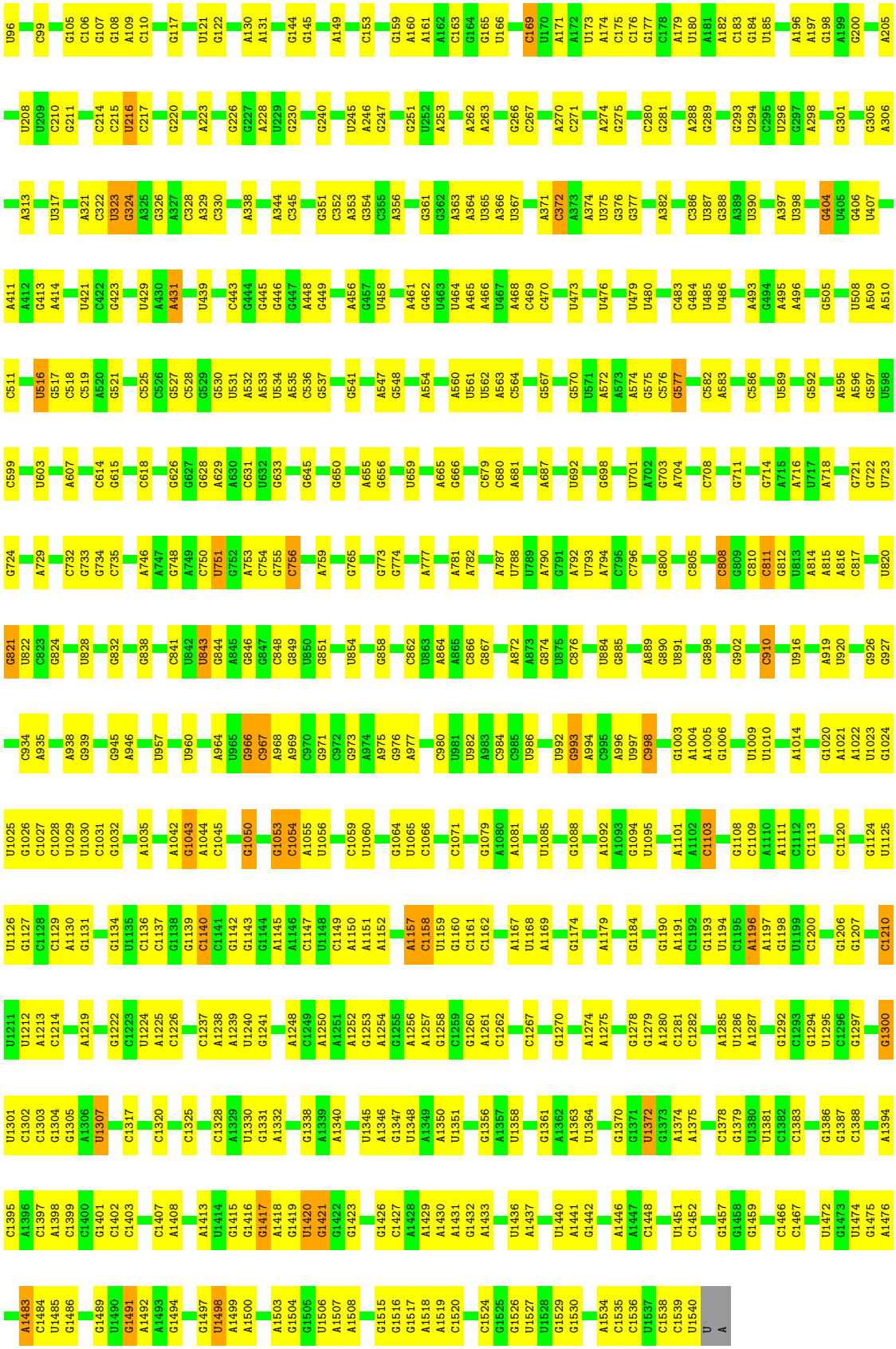
Chain Z:



• Molecule 34: 16S ribosomal RNA

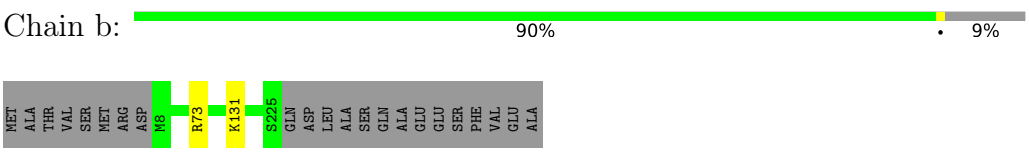
Chain a:





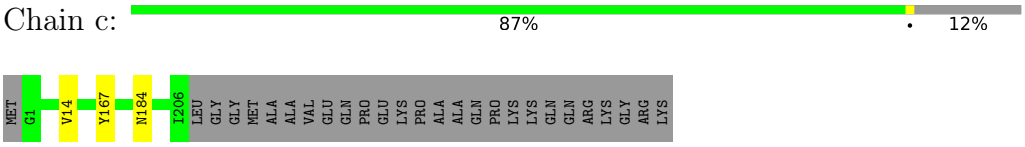
• Molecule 35: 30S ribosomal protein S2

Chain b:



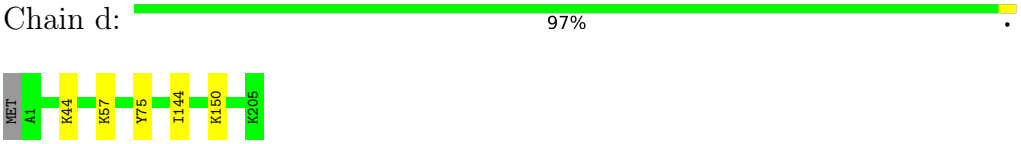
• Molecule 36: 30S ribosomal protein S3

Chain c:



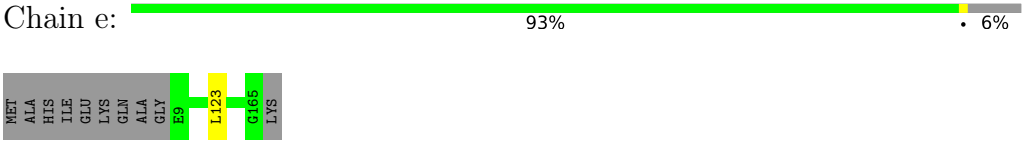
• Molecule 37: 30S ribosomal protein S4

Chain d:



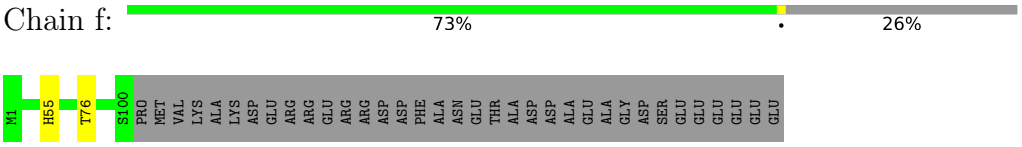
• Molecule 38: 30S ribosomal protein S5

Chain e:



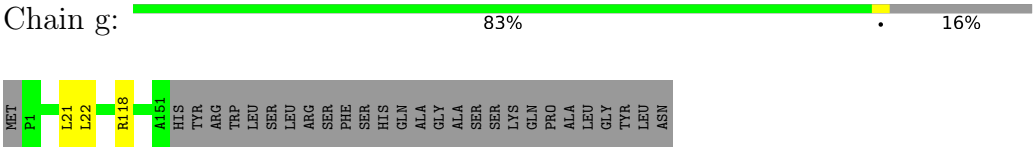
• Molecule 39: 30S ribosomal protein S6

Chain f:



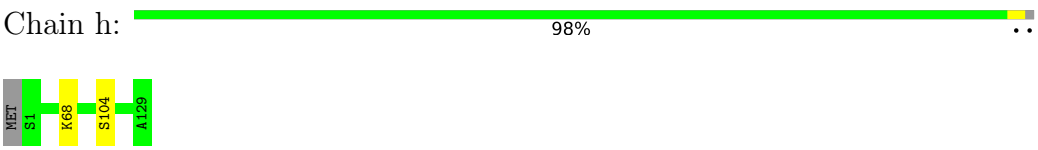
• Molecule 40: 30S ribosomal protein S7

Chain g:



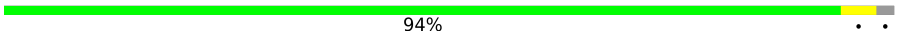
• Molecule 41: 30S ribosomal protein S8

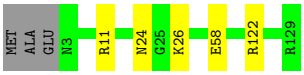
Chain h:



• Molecule 42: 30S ribosomal protein S9

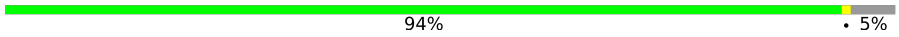
Chain i:

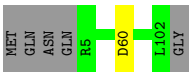




• Molecule 43: 30S ribosomal protein S10

Chain j:



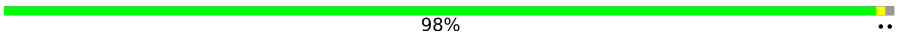


• Molecule 44: 30S ribosomal protein S11

Chain k:

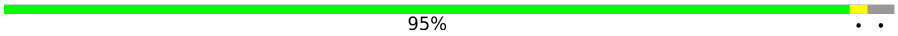
• Molecule 45: 30S ribosomal protein S12

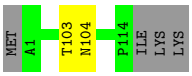
Chain l:



• Molecule 46: 30S ribosomal protein S13

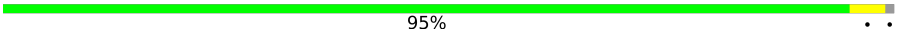
Chain m:

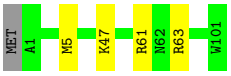




• Molecule 47: 30S ribosomal protein S14

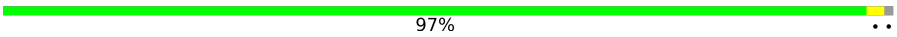
Chain n:

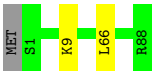




• Molecule 48: 30S ribosomal protein S15

Chain o:





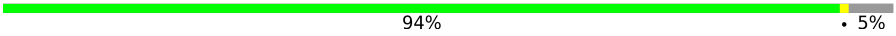
• Molecule 49: 30S ribosomal protein S16

Chain p:

There are no outlier residues recorded for this chain.

• Molecule 50: 30S ribosomal protein S17

Chain q:

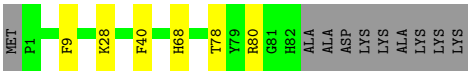


• Molecule 51: 30S ribosomal protein S18

Chain r:

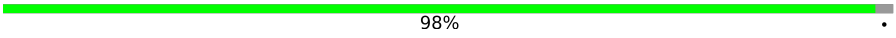
• Molecule 52: 30S ribosomal protein S19

Chain s:



• Molecule 53: 30S ribosomal protein S20

Chain t:

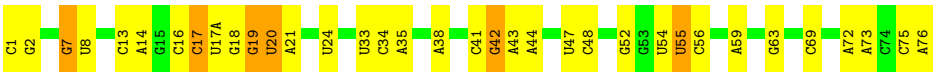


• Molecule 54: 30S ribosomal protein S21

Chain u:

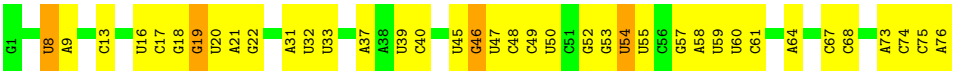
• Molecule 55: P-site tRNA(fMet)

Chain v:



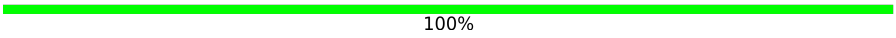
• Molecule 56: P-site fMet-Phe-tRNA(Phe)

Chain w:



• Molecule 57: Dipeptide (FME-PHE)

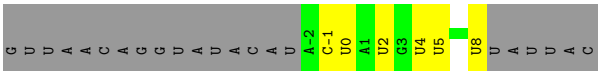
Chain y:



There are no outlier residues recorded for this chain.

• Molecule 58: mRNA

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 1MG, UR3, 4SU, MIA, AM2, 6MZ, OMG, FME, OMC, 5MC, OMU, 2MG, 4OC, PSU, MA6, ZN, 2MA, 5MU, G7M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.53	0/450	0.60	0/599
2	1	0.39	0/416	0.52	0/554
3	2	0.46	0/380	0.66	0/498
4	3	0.50	0/513	0.69	0/676
5	4	0.43	0/303	0.60	0/397
6	5	0.26	0/646	0.51	0/898
7	6	0.49	0/531	0.73	0/709
8	A	1.04	22/69266 (0.0%)	1.20	242/108055 (0.2%)
9	B	0.87	2/2873 (0.1%)	1.10	1/4478 (0.0%)
10	C	0.48	0/2121	0.62	0/2852
11	D	0.47	0/1586	0.62	0/2134
12	E	0.46	0/1571	0.60	0/2113
13	F	0.43	0/1434	0.59	0/1926
14	G	0.40	0/1343	0.57	0/1816
15	H	0.38	0/1122	0.61	0/1515
16	I	0.26	0/692	0.50	0/960
17	J	0.50	0/1152	0.55	0/1551
18	K	0.43	0/947	0.61	0/1268
19	L	0.48	0/1054	0.69	1/1403 (0.1%)
20	M	0.46	0/1093	0.57	0/1460
21	N	0.42	0/973	0.62	0/1301
22	O	0.43	0/902	0.61	0/1209
23	P	0.47	0/929	0.63	2/1242 (0.2%)
24	Q	0.50	0/960	0.60	1/1278 (0.1%)
25	R	0.47	0/829	0.64	0/1107
26	S	0.44	0/864	0.61	0/1156
27	T	0.42	0/744	0.62	0/994
28	U	0.46	0/787	0.61	0/1051
29	V	0.46	0/766	0.57	0/1025
30	W	0.45	0/582	0.63	0/769
31	X	0.44	0/635	0.66	1/848 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Y	0.41	0/510	0.64	0/677
33	Z	0.40	0/453	0.55	0/605
34	a	0.91	3/36725 (0.0%)	1.17	121/57285 (0.2%)
35	b	0.37	0/1735	0.57	0/2338
36	c	0.43	0/1651	0.56	1/2225 (0.0%)
37	d	0.39	0/1665	0.59	0/2227
38	e	0.42	0/1154	0.58	0/1554
39	f	0.38	0/835	0.56	0/1128
40	g	0.37	0/1195	0.54	0/1602
41	h	0.41	0/989	0.59	0/1326
42	i	0.42	0/1034	0.60	0/1375
43	j	0.37	0/796	0.62	0/1077
44	k	0.43	0/885	0.61	0/1195
45	l	0.44	0/969	0.60	0/1300
46	m	0.37	0/892	0.60	0/1193
47	n	0.45	0/811	0.69	0/1081
48	o	0.40	0/722	0.63	1/964 (0.1%)
49	p	0.40	0/659	0.58	0/884
50	q	0.41	0/657	0.59	0/881
51	r	0.42	0/544	0.60	0/731
52	s	0.46	0/675	0.69	0/908
53	t	0.38	0/671	0.51	0/888
54	u	0.40	0/512	0.56	0/683
55	v	0.83	1/1745 (0.1%)	1.17	7/2716 (0.3%)
56	w	0.69	0/1650	1.17	5/2569 (0.2%)
57	y	0.63	0/11	0.43	0/13
58	z	0.53	0/255	0.95	0/394
All	All	0.86	28/158864 (0.0%)	1.07	383/237661 (0.2%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	1	C	OP3-P	-10.75	1.48	1.61
9	B	1	U	OP3-P	-10.74	1.48	1.61
8	A	1	G	OP3-P	-10.73	1.48	1.61
8	A	1786	A	N9-C4	-7.76	1.33	1.37
8	A	195	A	N9-C4	-6.71	1.33	1.37

The worst 5 of 383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1054	C	O5'-P-OP1	14.14	127.67	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1196	A	C2'-C3'-O3'	9.93	131.35	109.50
34	a	1053	G	O3'-P-O5'	-9.74	85.50	104.00
34	a	1421	G	N9-C4-C5	9.61	109.24	105.40
34	a	1421	G	C8-N9-C1'	9.46	139.30	127.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	42 (78%)	12 (22%)	0	100	100
2	1	48/55 (87%)	38 (79%)	10 (21%)	0	100	100
3	2	44/46 (96%)	27 (61%)	17 (39%)	0	100	100
4	3	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
5	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
6	5	129/165 (78%)	100 (78%)	29 (22%)	0	100	100
7	6	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
10	C	269/273 (98%)	213 (79%)	56 (21%)	0	100	100
11	D	207/209 (99%)	172 (83%)	34 (16%)	1 (0%)	25	65
12	E	199/201 (99%)	165 (83%)	34 (17%)	0	100	100
13	F	175/179 (98%)	153 (87%)	22 (13%)	0	100	100
14	G	174/177 (98%)	149 (86%)	25 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	H	147/149 (99%)	117 (80%)	30 (20%)	0	100	100
16	I	139/142 (98%)	104 (75%)	35 (25%)	0	100	100
17	J	140/142 (99%)	109 (78%)	31 (22%)	0	100	100
18	K	120/123 (98%)	101 (84%)	19 (16%)	0	100	100
19	L	141/144 (98%)	108 (77%)	33 (23%)	0	100	100
20	M	134/136 (98%)	109 (81%)	24 (18%)	1 (1%)	19	57
21	N	118/127 (93%)	87 (74%)	31 (26%)	0	100	100
22	O	114/117 (97%)	101 (89%)	13 (11%)	0	100	100
23	P	112/115 (97%)	98 (88%)	14 (12%)	0	100	100
24	Q	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
25	R	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
26	S	108/110 (98%)	89 (82%)	19 (18%)	0	100	100
27	T	91/100 (91%)	74 (81%)	17 (19%)	0	100	100
28	U	100/104 (96%)	81 (81%)	19 (19%)	0	100	100
29	V	92/94 (98%)	79 (86%)	13 (14%)	0	100	100
30	W	73/85 (86%)	56 (77%)	17 (23%)	0	100	100
31	X	75/78 (96%)	63 (84%)	12 (16%)	0	100	100
32	Y	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
33	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
35	b	216/240 (90%)	184 (85%)	32 (15%)	0	100	100
36	c	204/233 (88%)	181 (89%)	23 (11%)	0	100	100
37	d	203/206 (98%)	160 (79%)	42 (21%)	1 (0%)	25	65
38	e	155/167 (93%)	119 (77%)	36 (23%)	0	100	100
39	f	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
40	g	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
41	h	127/130 (98%)	107 (84%)	20 (16%)	0	100	100
42	i	125/130 (96%)	98 (78%)	27 (22%)	0	100	100
43	j	96/103 (93%)	76 (79%)	19 (20%)	1 (1%)	13	49
44	k	114/129 (88%)	92 (81%)	22 (19%)	0	100	100
45	l	121/124 (98%)	96 (79%)	25 (21%)	0	100	100
46	m	112/118 (95%)	99 (88%)	13 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	n	99/102 (97%)	87 (88%)	12 (12%)	0	100 100
48	o	86/89 (97%)	74 (86%)	12 (14%)	0	100 100
49	p	80/82 (98%)	61 (76%)	19 (24%)	0	100 100
50	q	78/84 (93%)	68 (87%)	10 (13%)	0	100 100
51	r	63/75 (84%)	49 (78%)	14 (22%)	0	100 100
52	s	80/92 (87%)	70 (88%)	10 (12%)	0	100 100
53	t	83/87 (95%)	66 (80%)	17 (20%)	0	100 100
54	u	63/71 (89%)	50 (79%)	13 (21%)	0	100 100
All	All	5850/6220 (94%)	4809 (82%)	1037 (18%)	4 (0%)	50 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	j	60	ASP
37	d	144	ILE
11	D	138	LEU
20	M	59	ARG

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
1	0	47/48 (98%)	45 (96%)	2 (4%)	25 46
2	1	45/49 (92%)	45 (100%)	0	100 100
3	2	38/38 (100%)	37 (97%)	1 (3%)	41 59
4	3	51/52 (98%)	45 (88%)	6 (12%)	4 16
5	4	34/34 (100%)	32 (94%)	2 (6%)	16 38
7	6	59/62 (95%)	52 (88%)	7 (12%)	4 16
10	C	216/218 (99%)	214 (99%)	2 (1%)	75 83
11	D	164/164 (100%)	162 (99%)	2 (1%)	67 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	141 (95%)	7 (5%)	22	44
14	G	137/138 (99%)	134 (98%)	3 (2%)	47	65
15	H	114/114 (100%)	113 (99%)	1 (1%)	75	83
17	J	116/116 (100%)	112 (97%)	4 (3%)	32	51
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	100 (98%)	2 (2%)	50	68
20	M	109/109 (100%)	108 (99%)	1 (1%)	75	83
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	81 (94%)	5 (6%)	17	38
23	P	99/100 (99%)	98 (99%)	1 (1%)	73	82
24	Q	89/90 (99%)	87 (98%)	2 (2%)	47	65
25	R	84/84 (100%)	79 (94%)	5 (6%)	16	37
26	S	93/93 (100%)	88 (95%)	5 (5%)	18	40
27	T	80/84 (95%)	78 (98%)	2 (2%)	42	61
28	U	83/85 (98%)	81 (98%)	2 (2%)	44	62
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	56 (98%)	1 (2%)	54	71
31	X	67/68 (98%)	66 (98%)	1 (2%)	60	75
32	Y	55/55 (100%)	50 (91%)	5 (9%)	7	24
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	178 (99%)	2 (1%)	70	80
36	c	170/190 (90%)	168 (99%)	2 (1%)	67	79
37	d	172/173 (99%)	168 (98%)	4 (2%)	45	64
38	e	114/126 (90%)	113 (99%)	1 (1%)	75	83
39	f	87/116 (75%)	85 (98%)	2 (2%)	45	64
40	g	124/147 (84%)	121 (98%)	3 (2%)	44	62
41	h	104/105 (99%)	102 (98%)	2 (2%)	52	69
42	i	105/107 (98%)	100 (95%)	5 (5%)	21	43
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	86 (97%)	3 (3%)	32	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	l	103/104 (99%)	102 (99%)	1 (1%)	73 82
46	m	92/96 (96%)	90 (98%)	2 (2%)	47 65
47	n	79/84 (94%)	75 (95%)	4 (5%)	20 41
48	o	76/77 (99%)	75 (99%)	1 (1%)	65 77
49	p	65/65 (100%)	65 (100%)	0	100 100
50	q	74/78 (95%)	73 (99%)	1 (1%)	62 75
51	r	56/65 (86%)	55 (98%)	1 (2%)	54 71
52	s	72/79 (91%)	66 (92%)	6 (8%)	9 27
53	t	65/66 (98%)	65 (100%)	0	100 100
54	u	46/61 (75%)	44 (96%)	2 (4%)	25 46
57	y	1/1 (100%)	1 (100%)	0	100 100
All	All	4627/4830 (96%)	4516 (98%)	111 (2%)	45 62

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	S	104	THR
54	u	37	TYR
36	c	167	TYR
54	u	15	LEU
47	n	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
32	Y	45	GLN
41	h	75	GLN
35	b	17	HIS
39	f	3	HIS
44	k	80	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	575 (37%)	0
55	v	76/77 (98%)	30 (39%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	w	74/76 (97%)	32 (43%)	0
58	z	10/33 (30%)	6 (60%)	0
8	A	2897/2903 (99%)	1092 (37%)	86 (2%)
9	B	119/120 (99%)	46 (38%)	2 (1%)
All	All	4712/4751 (99%)	1781 (37%)	88 (1%)

5 of 1781 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	14	A
8	A	15	G
8	A	16	C
8	A	23	G

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1921	G
8	A	2405	G
8	A	2015	A
8	A	2192	U
8	A	2474	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	4SU	v	8	55	18,21,22	3.56	7 (38%)	26,30,33	2.08	6 (23%)
8	PSU	A	2604	8	18,21,22	1.06	2 (11%)	22,30,33	2.03	5 (22%)
56	4SU	w	8	56	18,21,22	3.57	8 (44%)	26,30,33	2.31	4 (15%)
8	6MZ	A	1618	8	18,25,26	4.09	8 (44%)	16,36,39	2.40	6 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	PSU	A	2504	8	18,21,22	1.10	3 (16%)	22,30,33	2.17	5 (22%)
55	H2U	v	20	55	18,21,22	2.95	5 (27%)	21,30,33	2.17	5 (23%)
56	5MU	w	54	56	19,22,23	1.45	6 (31%)	28,32,35	2.26	7 (25%)
8	PSU	A	2605	8	18,21,22	1.00	1 (5%)	22,30,33	2.05	4 (18%)
56	PSU	w	32	56	18,21,22	1.06	1 (5%)	22,30,33	1.65	5 (22%)
34	2MG	a	1516	34	18,26,27	2.46	7 (38%)	16,38,41	1.32	3 (18%)
8	2MG	A	1835	8	18,26,27	2.51	7 (38%)	16,38,41	1.49	3 (18%)
8	OMC	A	2498	8	19,22,23	0.95	1 (5%)	26,31,34	1.49	2 (7%)
34	G7M	a	527	34	20,26,27	2.29	7 (35%)	17,39,42	1.37	2 (11%)
8	2MA	A	2503	8	19,25,26	2.99	7 (36%)	21,37,40	1.84	4 (19%)
55	PSU	v	55	55	18,21,22	1.11	1 (5%)	22,30,33	1.80	4 (18%)
34	2MG	a	966	34	18,26,27	2.57	7 (38%)	16,38,41	1.49	3 (18%)
56	PSU	w	55	56	18,21,22	1.43	3 (16%)	22,30,33	1.89	7 (31%)
57	FME	y	101	57	8,9,10	0.90	0	7,9,11	1.14	0
8	OMG	A	2251	8,56	18,26,27	2.53	8 (44%)	19,38,41	1.60	4 (21%)
56	PSU	w	39	56	18,21,22	1.10	1 (5%)	22,30,33	1.74	3 (13%)
8	5MU	A	1939	8	19,22,23	4.76	7 (36%)	28,32,35	3.71	13 (46%)
8	PSU	A	955	8	18,21,22	1.05	1 (5%)	22,30,33	1.88	5 (22%)
56	G7M	w	46	56	20,26,27	2.31	7 (35%)	17,39,42	1.26	1 (5%)
34	MA6	a	1519	34	18,26,27	1.05	1 (5%)	19,38,41	2.66	2 (10%)
34	PSU	a	516	34	18,21,22	1.07	1 (5%)	22,30,33	1.62	3 (13%)
8	2MG	A	2445	8	18,26,27	2.45	7 (38%)	16,38,41	1.59	4 (25%)
34	UR3	a	1498	34	19,22,23	2.48	6 (31%)	26,32,35	1.27	1 (3%)
34	MA6	a	1518	34	18,26,27	1.11	1 (5%)	19,38,41	1.90	2 (10%)
56	MIA	w	37	56	24,31,32	2.44	4 (16%)	26,44,47	3.10	9 (34%)
8	PSU	A	2457	8	18,21,22	1.05	2 (11%)	22,30,33	1.99	5 (22%)
34	5MC	a	967	34	18,22,23	3.66	7 (38%)	26,32,35	1.18	3 (11%)
8	1MG	A	745	8	18,26,27	2.57	4 (22%)	19,39,42	1.42	3 (15%)
8	PSU	A	1911	8	18,21,22	1.07	2 (11%)	22,30,33	2.15	6 (27%)
8	5MC	A	1962	8	18,22,23	3.49	7 (38%)	26,32,35	1.34	4 (15%)
8	PSU	A	1917	8	18,21,22	0.97	1 (5%)	22,30,33	1.88	4 (18%)
34	5MC	a	1407	34	18,22,23	3.44	7 (38%)	26,32,35	1.18	3 (11%)
34	2MG	a	1207	34	18,26,27	2.40	7 (38%)	16,38,41	1.44	3 (18%)
34	4OC	a	1402	34	20,23,24	2.94	8 (40%)	26,32,35	1.24	5 (19%)
8	G7M	A	2069	8	20,26,27	2.25	8 (40%)	17,39,42	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	OMU	A	2552	8	19,22,23	2.90	7 (36%)	26,31,34	1.95	6 (23%)
55	5MU	v	54	55	19,22,23	4.80	7 (36%)	28,32,35	3.54	11 (39%)
8	PSU	A	746	8	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
8	PSU	A	2580	8	18,21,22	1.32	2 (11%)	22,30,33	2.23	7 (31%)
8	5MC	A	747	8	18,22,23	3.51	7 (38%)	26,32,35	1.50	2 (7%)
8	6MZ	A	2030	8	18,25,26	4.06	8 (44%)	16,36,39	2.60	4 (25%)

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
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
56	4SU	w	8	56	-	2/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	5/5/27/28	0/3/3/3
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
56	5MU	w	54	56	-	3/7/25/26	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	OMC	A	2498	8	-	3/9/27/28	0/2/2/2
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
8	2MA	A	2503	8	-	3/3/25/26	0/3/3/3
55	PSU	v	55	55	-	3/7/25/26	0/2/2/2
34	2MG	a	966	34	-	1/5/27/28	0/3/3/3
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2
57	FME	y	101	57	-	6/7/9/11	-
8	OMG	A	2251	8,56	-	3/5/27/28	0/3/3/3
56	PSU	w	39	56	-	5/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	1/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
56	G7M	w	46	56	-	3/3/25/26	0/3/3/3
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
34	PSU	a	516	34	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	4/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	3/7/29/30	0/3/3/3
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
34	5MC	a	967	34	-	1/7/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
8	PSU	A	1911	8	-	1/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	4/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	4OC	a	1402	34	-	3/9/29/30	0/2/2/2
8	G7M	A	2069	8	-	2/3/25/26	0/3/3/3
8	OMU	A	2552	8	-	6/9/27/28	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
8	PSU	A	746	8	-	1/7/25/26	0/2/2/2
8	PSU	A	2580	8	-	2/7/25/26	0/2/2/2
8	5MC	A	747	8	-	2/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3

The worst 5 of 210 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	54	5MU	C2-N1	11.24	1.56	1.38
8	A	1939	5MU	C2-N1	11.04	1.56	1.38
55	v	54	5MU	C6-N1	10.29	1.55	1.38
8	A	1939	5MU	C6-N1	10.01	1.55	1.38
55	v	54	5MU	C4-C5	9.91	1.61	1.44

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1939	5MU	C5-C4-N3	11.77	125.36	115.31
55	v	54	5MU	C5-C4-N3	11.06	124.75	115.31
8	A	1939	5MU	C5-C6-N1	-10.15	112.89	123.34
34	a	1519	MA6	N1-C6-N6	-9.77	106.78	117.06
55	v	54	5MU	C5-C6-N1	-9.01	114.07	123.34

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	20	H2U	O4'-C1'-N1-C6
55	v	20	H2U	C2'-C1'-N1-C2
55	v	20	H2U	C2'-C1'-N1-C6
8	A	747	5MC	C3'-C4'-C5'-O5'
8	A	1618	6MZ	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
60	AM2	a	2001	-	40,40,40	1.66	10 (25%)	53,60,60	1.71	11 (20%)

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
60	AM2	a	2001	-	-	8/12/84/84	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	a	2001	AM2	OA4-CA1	4.04	1.52	1.41
60	a	2001	AM2	CB3-CB4	-3.69	1.48	1.53
60	a	2001	AM2	OA5-CA8	3.20	1.50	1.41
60	a	2001	AM2	OA5-CA4	3.08	1.51	1.44
60	a	2001	AM2	OB1-CB1	2.89	1.49	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	a	2001	AM2	CA1-OA1-CC1	-5.36	104.71	117.96
60	a	2001	AM2	CA8-CA7-NA7	-3.99	103.86	111.00
60	a	2001	AM2	CB1-OA8-CA8	-3.84	107.56	114.42
60	a	2001	AM2	CA9-NA7-CA7	-3.31	109.57	114.38
60	a	2001	AM2	OA1-CA1-CA2	3.21	113.61	108.23

There are no chirality outliers.

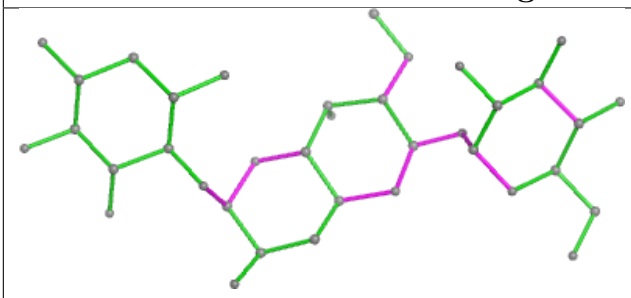
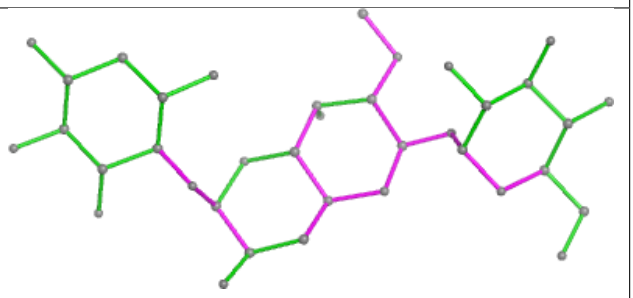
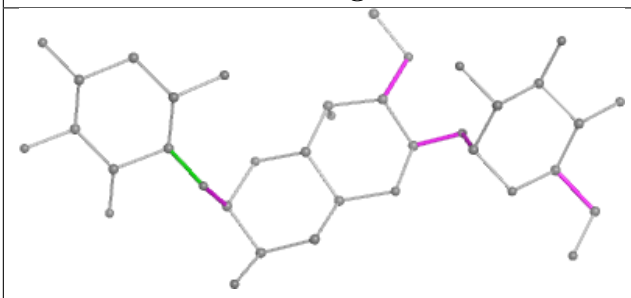
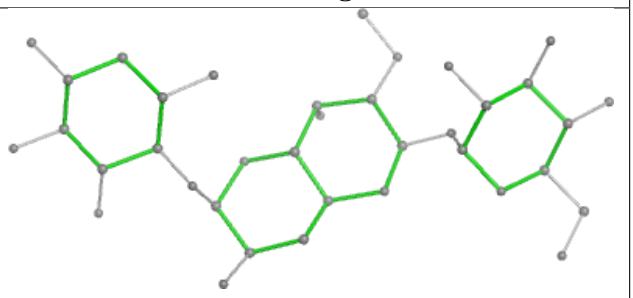
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	a	2001	AM2	CA7-CA8-OA8-CB1
60	a	2001	AM2	OA5-CA8-OA8-CB1
60	a	2001	AM2	OB1-CB5-CB6-OB6
60	a	2001	AM2	CB4-CB5-CB6-OB6
60	a	2001	AM2	OB1-CB1-OA8-CA8

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AM2 a 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.