wwPDB EM Validation Summary Report (i)

Mar 6, 2025 – 03:00 pm GMT

PDB ID	:	8RCL
EMDB ID	:	EMD-19054
Title	:	Escherichia coli paused disome complex (Non-rotated disome interface class 1)
Authors	:	Fluegel, T.; Schacherl, M.
Deposited on	:	2023-12-06
Resolution	:	3.49 Å(reported)
Based on initial model	:	7N1P

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 (i)) were used in the production of this report:

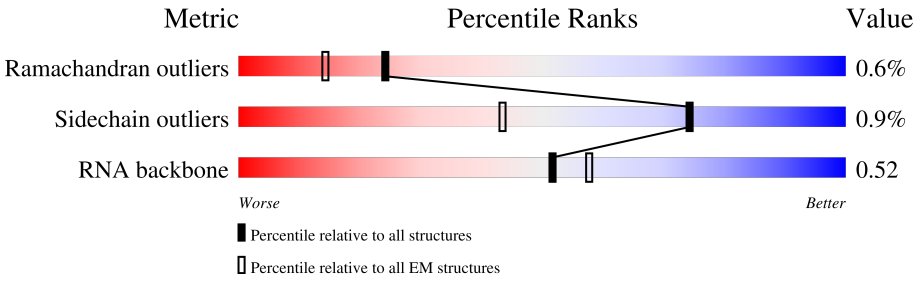
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 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	12	78	96%
2	32	59	95%
3	4	70	83% 13%
4	62	65	98%
5	71	2904	99%
5	72	2904	83% 17%
6	82	120	78% 21%
7	A1	1542	70% 30%
7	A2	1542	73% 26%

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Mol	Chain	Length	Quality of chain
8	B	241	95%
8	B2	241	93% 6%
9	C1	233	90% 9%
9	C2	233	91% 9%
10	D1	206	97%
10	D2	206	99%
11	E1	167	95% 5%
11	E2	167	95% 5%
12	F1	135	79% 21%
12	F2	135	77% 21%
13	G1	179	87% 13%
13	G2	179	82% 14%
14	H1	130	99%
14	H2	130	99%
15	I1	130	98%
15	I2	130	98%
16	J1	103	98%
16	J2	103	91% 6%
17	K1	129	87% 11%
17	K2	129	90% 9%
18	L1	124	98%
18	L2	124	99%
19	M1	118	97%
19	M2	118	99%
20	N1	101	97%

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Mol	Chain	Length	Quality of chain
20	N2	101	99%
21	O1	89	99%
21	O2	89	98%
22	P1	82	99%
23	Q1	84	95% 5%
23	Q2	84	94% 5%
24	R1	75	96%
24	R2	75	93% 5%
25	S1	92	89% 10%
25	S2	92	90% 10%
26	T1	87	92% 7%
27	U1	71	96%
27	U2	71	96%
28	V2	64	31% 67%
29	W	76	59% 32% 9%
30	W1	76	29% 17% 53%
31	X2	77	58% 35% 6%
32	Y1	76	38% 8% 53%
33	Y2	76	64% 32%
34	Z1	557	98%
35	a2	234	57% 43%
36	b2	273	99%
37	e2	179	98%
38	g2	55	95% 5%
39	h2	136	100%

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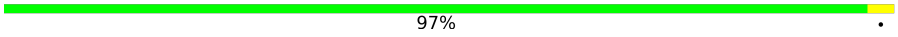
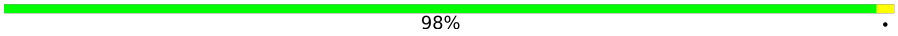
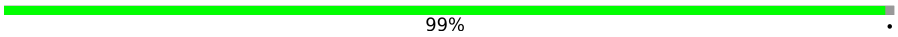
Mol	Chain	Length	Quality of chain
40	i2	149	
41	l2	46	
42	o2	144	
43	p	10	
44	r2	117	
45	z2	85	

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 188653 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 L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	12	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	32	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	62	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	71	30	Total	C	N	O	P	0	0
			644	288	119	207	30		
5	72	2904	Total	C	N	O	P	0	0
			62355	27824	11468	20159	2904		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	82	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A1	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		
7	A2	1537	Total	C	N	O	P	0	0
			32990	14721	6049	10683	1537		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	233	Total	C	N	O	S	0	0
			1815	1145	325	337	8		
8	B2	227	Total	C	N	O	S	0	0
			1776	1123	318	327	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C1	213	Total	C	N	O	S	0	0
			1665	1054	312	295	4		
9	C2	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D1	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		
10	D2	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E1	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		
11	E2	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		
12	F2	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G1	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		
13	G2	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
14	H2	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
15	I2	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J1	102	Total	C	N	O	S	0	0
			817	509	157	150	1		
16	J2	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K1	115	Total	C	N	O	S	0	0
			857	528	168	158	3		
17	K2	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L1	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
18	L2	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M1	115	Total	C	N	O	S	0	0
			891	552	179	157	3		
19	M2	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		
20	N2	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
21	O2	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q1	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
23	Q2	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R1	74	Total	C	N	O	S	0	0
			624	395	122	105	2		
24	R2	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S1	83	Total	C	N	O	S	0	0
			663	424	126	111	2		
25	S2	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U1	70	Total	C	N	O	S	0	0
			590	366	125	98	1		
27	U2	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	64	Total	C	N	O	P	0	0
			1382	619	267	432	64		

- Molecule 29 is a RNA chain called tRNA-Trp (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	W	76	Total	C	N	O	P	S	0	0
			1630	730	286	536	76	2		

- Molecule 30 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	W1	36	Total	C	N	O	P	S	0	0
			781	352	143	248	36	2		

- Molecule 31 is a RNA chain called tRNA-Arg (E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	X2	77	Total	C	N	O	P	S	0	0
			1654	740	297	538	77	2		

- Molecule 32 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y1	36	Total	C	N	O	P	0	0
			778	348	142	252	36		

- Molecule 33 is a RNA chain called tRNA-Ala (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y2	76	Total	C	N	O	P	0	0
			1628	726	293	533	76		

- Molecule 34 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Z1	9	Total	C	N	O	0	0
			75	49	10	16		

- Molecule 35 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a2	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 37 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e2	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 38 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	g2	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h2	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i2	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 41 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 42 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o2	51	Total	C	N	O	S	0	0
			377	231	83	62	1		

- Molecule 43 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	p	10	Total	C	N	O	0	0
			76	47	18	11		

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	r2	116	Total	C	N	O	0	0
			891	552	178	161		

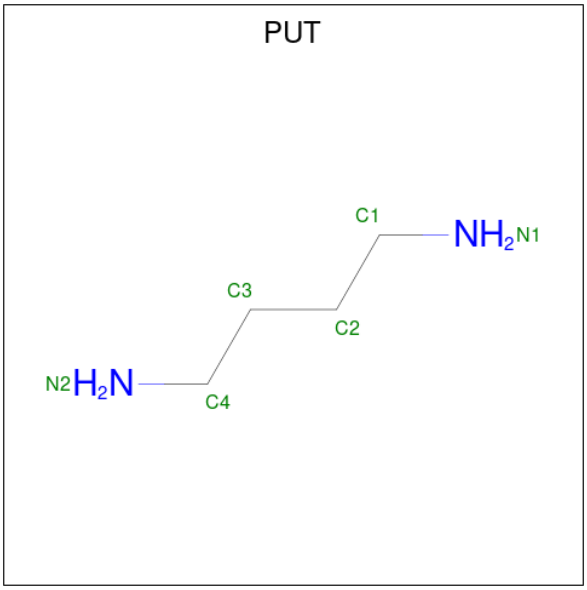
- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z2	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

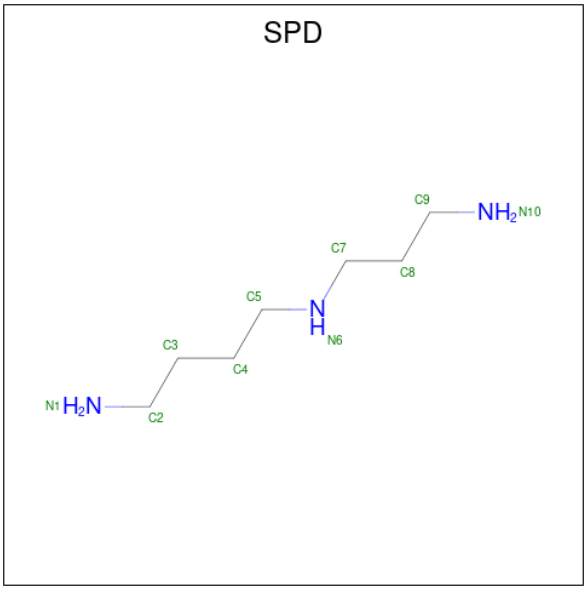
Mol	Chain	Residues	Atoms		AltConf
46	4	1	Total	Zn	0
			1	1	
46	B	1	Total	Zn	0
			1	1	

- Molecule 47 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	AltConf
47	72	1	Total C N 6 4 2	0
47	72	1	Total C N 6 4 2	0

- Molecule 48 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
48	72	1	Total C N 10 7 3	0

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
49	72	189	Total Mg 189 189	0
49	82	1	Total Mg 1 1	0
49	A1	59	Total Mg 59 59	0
49	A2	42	Total Mg 42 42	0
49	V2	1	Total Mg 1 1	0
49	W	1	Total Mg 1 1	0
49	Y2	1	Total Mg 1 1	0

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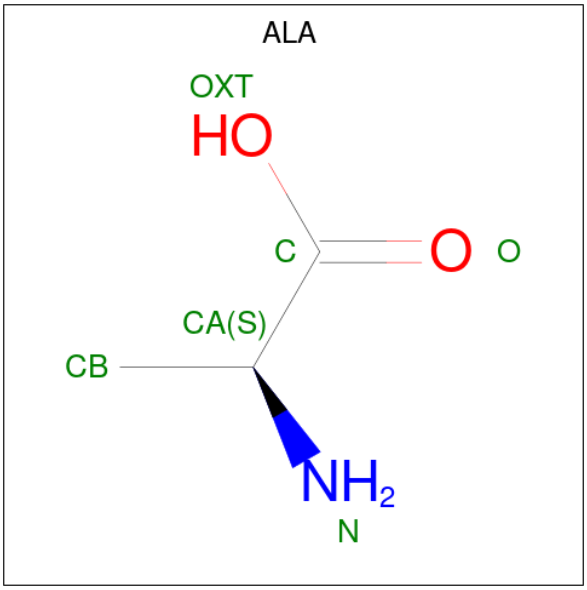
Mol	Chain	Residues	Atoms	AltConf
49	b2	1	Total Mg 1 1	0
49	o2	1	Total Mg 1 1	0

- Molecule 50 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



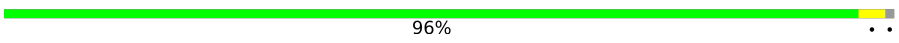
Mol	Chain	Residues	Atoms	AltConf
50	Y2	1	Total C N O 5 3 1 1	0

3 Residue-property plots (i)

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

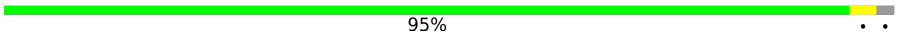
• Molecule 1: 50S ribosomal protein L28

Chain 12:



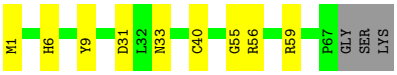
• Molecule 2: 50S ribosomal protein L30

Chain 32:



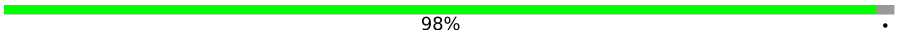
• Molecule 3: Large ribosomal subunit protein bL31

Chain 4:



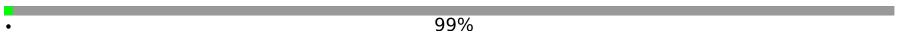
• Molecule 4: 50S ribosomal protein L35

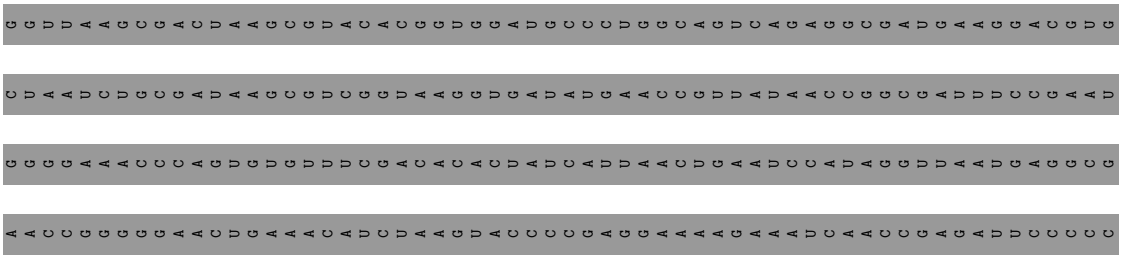
Chain 62:

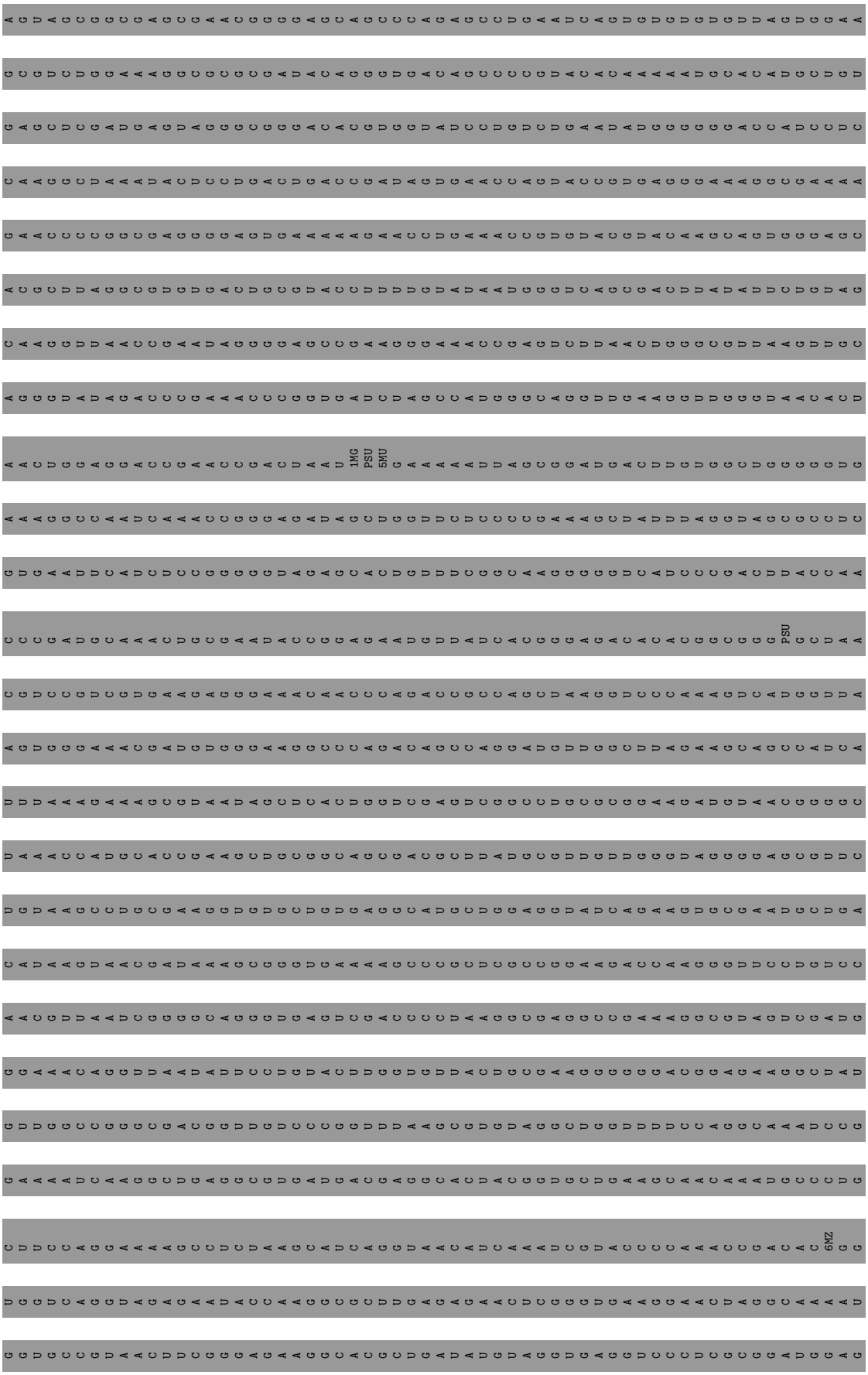


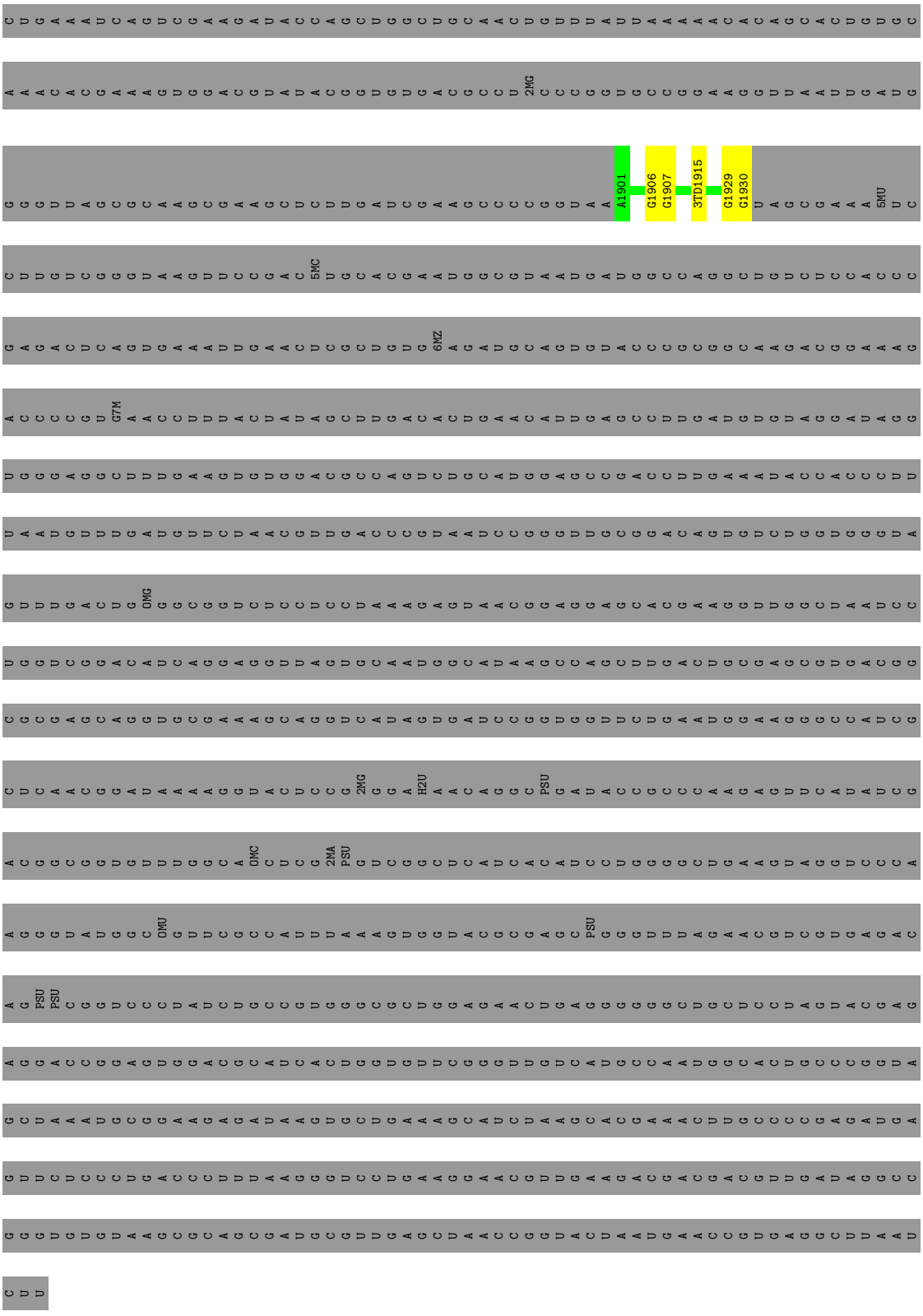
• Molecule 5: 23S ribosomal RNA

Chain 71:



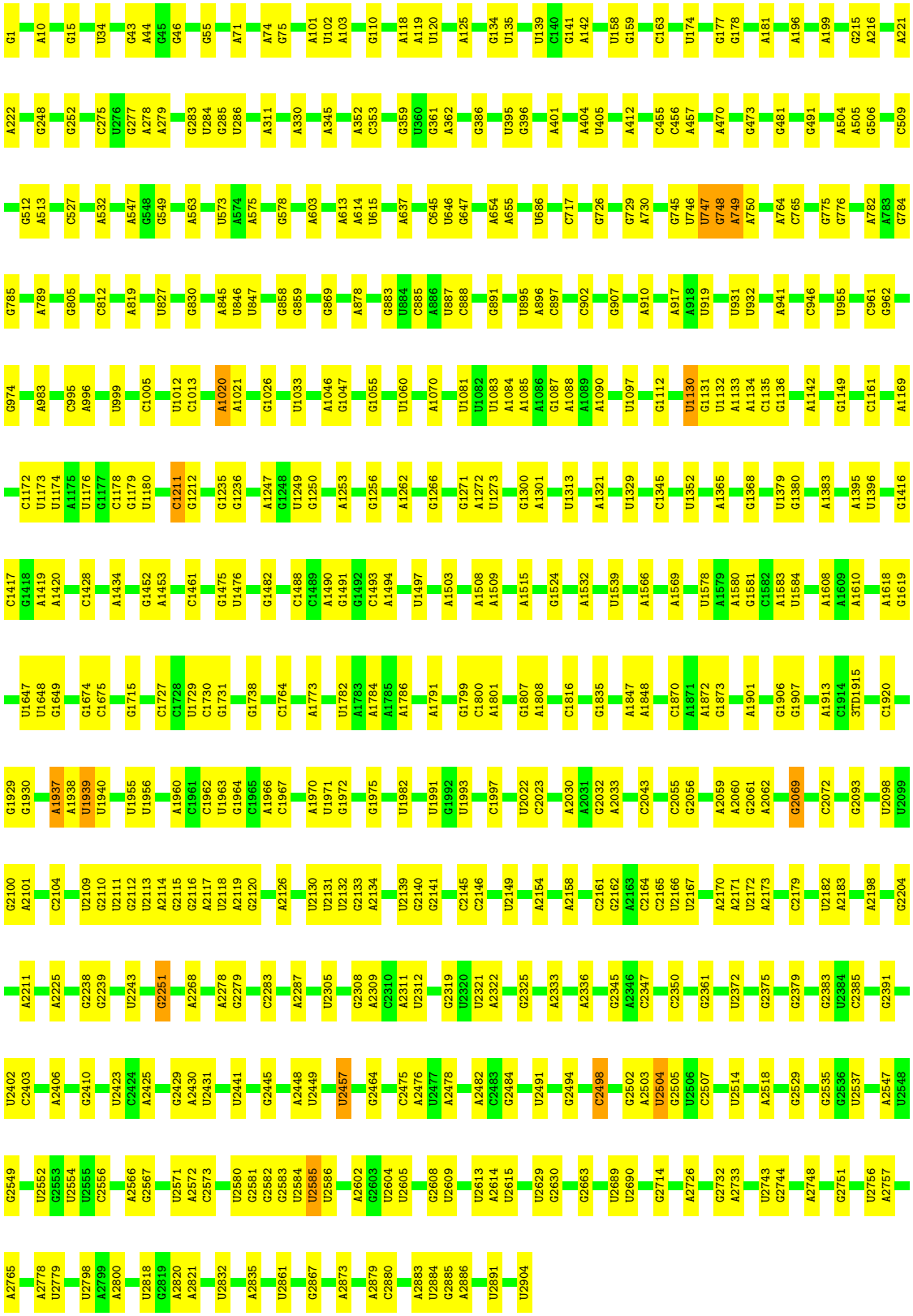



1MG
PSU
5MU
PSU
6MZ



• Molecule 5: 23S ribosomal RNA

Chain 72:

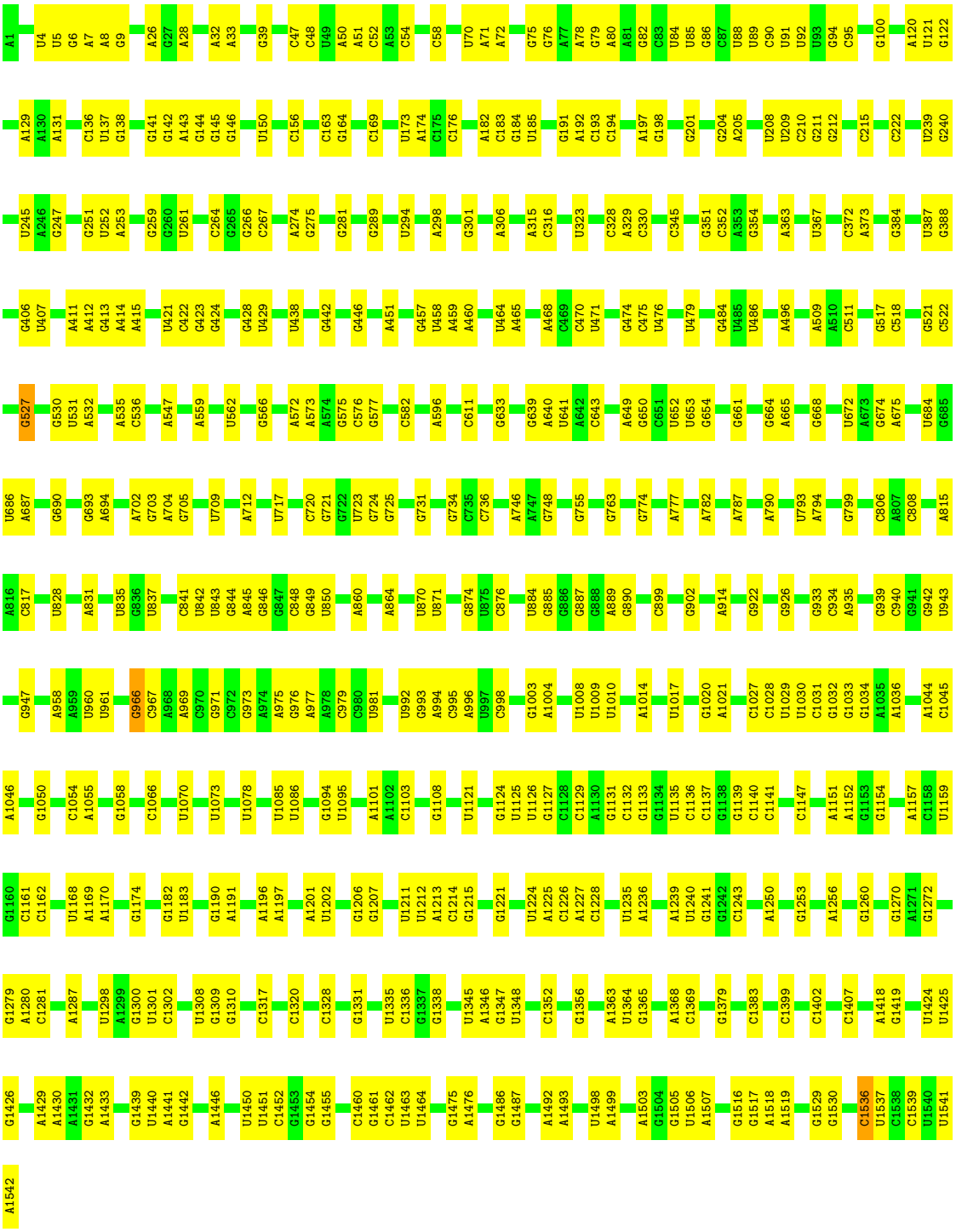


• Molecule 6: 5S ribosomal RNA

Chain 82: 78% 21%

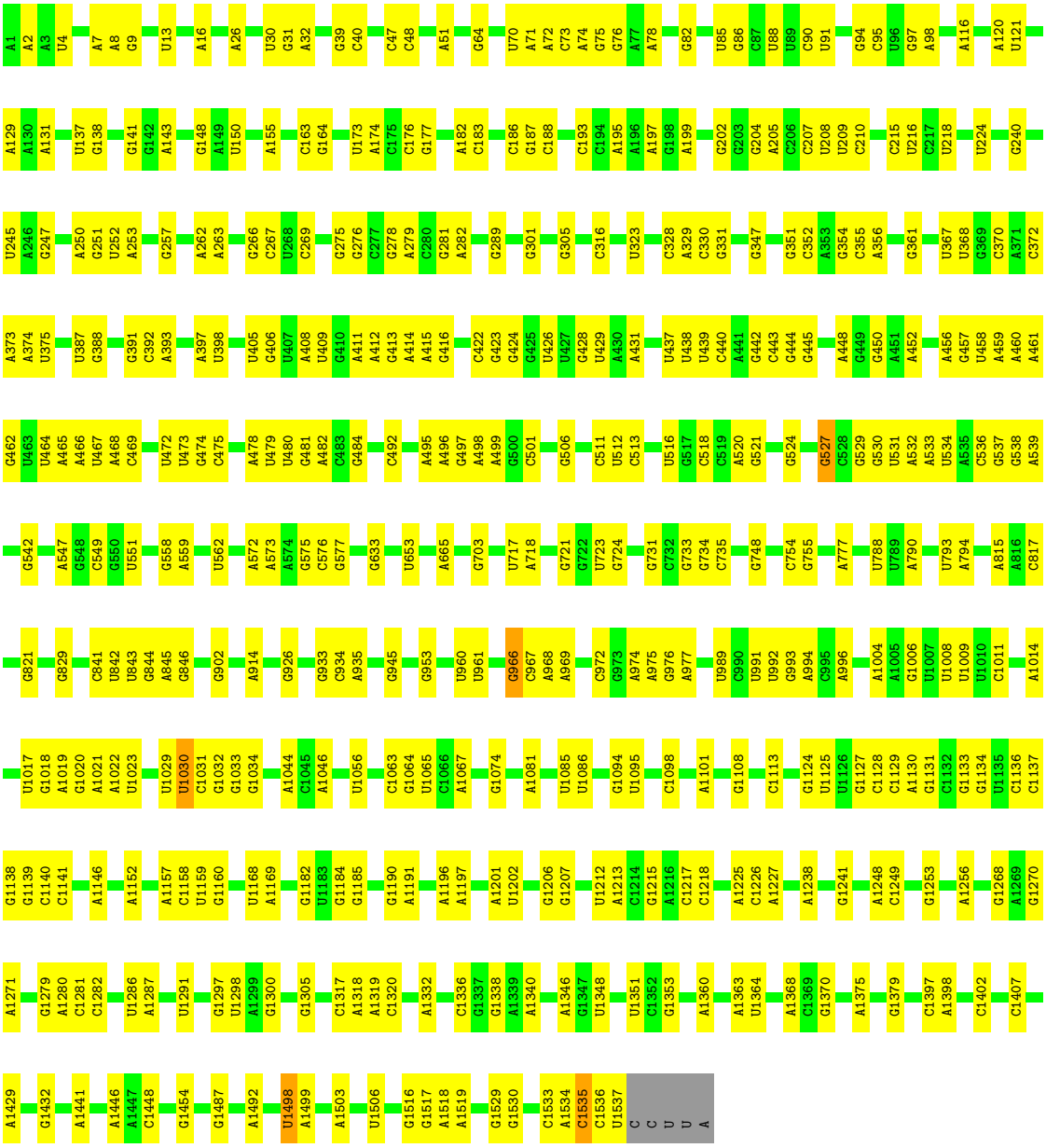
• Molecule 7: 16S ribosomal RNA

Chain A1:



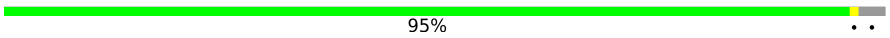
• Molecule 7: 16S ribosomal RNA

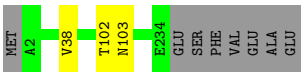
Chain A2:



• Molecule 8: Small ribosomal subunit protein uS2

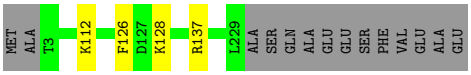
Chain B:





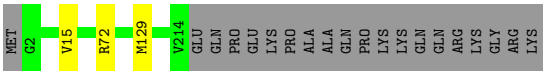
• Molecule 8: Small ribosomal subunit protein uS2

Chain B2:



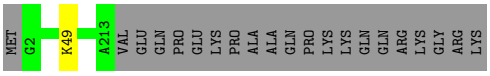
• Molecule 9: Small ribosomal subunit protein uS3

Chain C1:



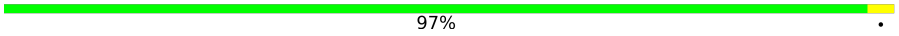
• Molecule 9: Small ribosomal subunit protein uS3

Chain C2:



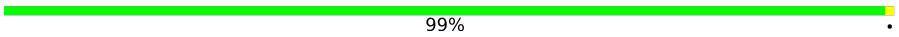
• Molecule 10: Small ribosomal subunit protein uS4

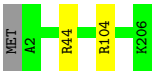
Chain D1:



• Molecule 10: Small ribosomal subunit protein uS4

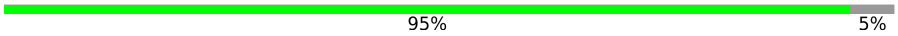
Chain D2:





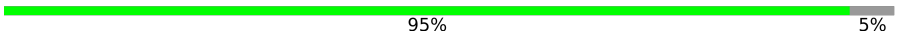
• Molecule 11: Small ribosomal subunit protein uS5

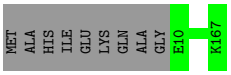
Chain E1:



• Molecule 11: Small ribosomal subunit protein uS5

Chain E2:





• Molecule 12: 30S ribosomal protein S6

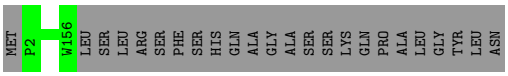
Chain F1:

• Molecule 12: 30S ribosomal protein S6

Chain F2: 

• Molecule 13: 30S ribosomal protein S7

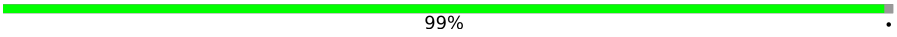
Chain G1: 



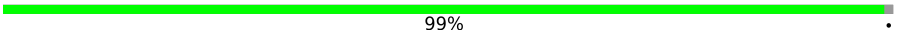
• Molecule 13: 30S ribosomal protein S7

Chain G2: 

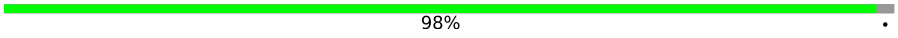
• Molecule 14: Small ribosomal subunit protein uS8

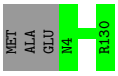
Chain H1: 

• Molecule 14: Small ribosomal subunit protein uS8

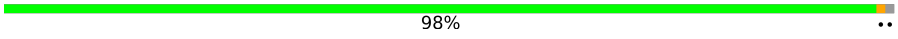
Chain H2: 

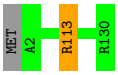
• Molecule 15: Small ribosomal subunit protein uS9

Chain I1: 



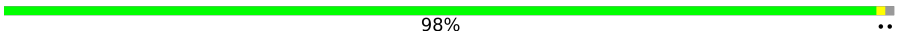
• Molecule 15: Small ribosomal subunit protein uS9

Chain I2: 



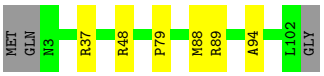
• Molecule 16: 30S ribosomal protein S10

Chain J1:



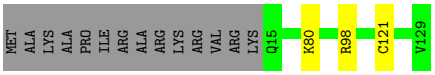
• Molecule 16: 30S ribosomal protein S10

Chain J2:



• Molecule 17: Small ribosomal subunit protein uS11

Chain K1:

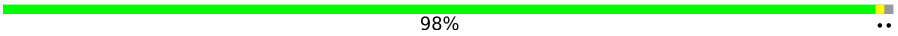


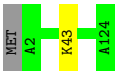
• Molecule 17: Small ribosomal subunit protein uS11

Chain K2:

• Molecule 18: Small ribosomal subunit protein uS12

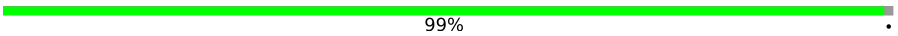
Chain L1:





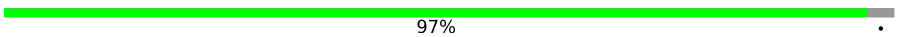
• Molecule 18: Small ribosomal subunit protein uS12

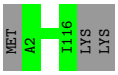
Chain L2:



• Molecule 19: Small ribosomal subunit protein uS13

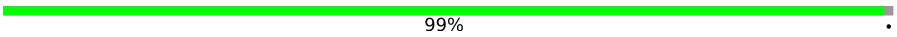
Chain M1:





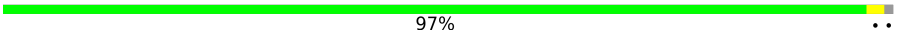
• Molecule 19: Small ribosomal subunit protein uS13

Chain M2:



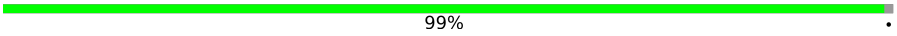
• Molecule 20: Small ribosomal subunit protein uS14

Chain N1:



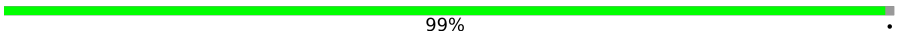
• Molecule 20: Small ribosomal subunit protein uS14

Chain N2:



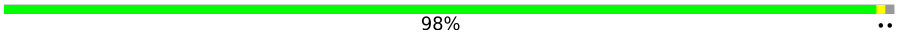
• Molecule 21: 30S ribosomal protein S15

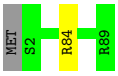
Chain O1:



• Molecule 21: 30S ribosomal protein S15

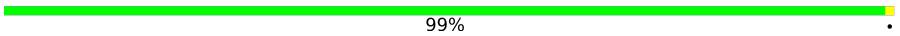
Chain O2:





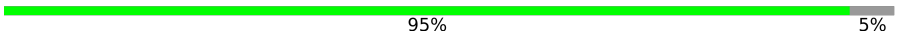
• Molecule 22: 30S ribosomal protein S16

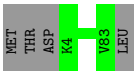
Chain P1:



• Molecule 23: Small ribosomal subunit protein uS17

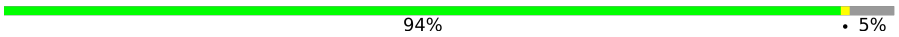
Chain Q1:

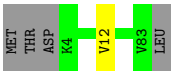




• Molecule 23: Small ribosomal subunit protein uS17

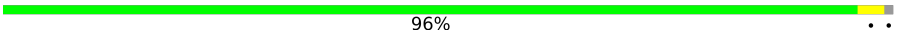
Chain Q2:

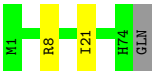




• Molecule 24: Small ribosomal subunit protein bS18

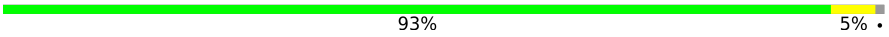
Chain R1:

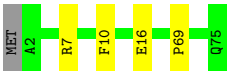




• Molecule 24: Small ribosomal subunit protein bS18

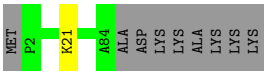
Chain R2:





• Molecule 25: Small ribosomal subunit protein uS19

Chain S1:



• Molecule 25: Small ribosomal subunit protein uS19

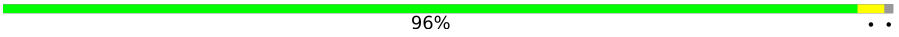
Chain S2:

• Molecule 26: Small ribosomal subunit protein bS20

Chain T1:

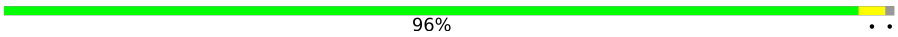
• Molecule 27: 30S ribosomal protein S21

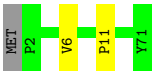
Chain U1:



• Molecule 27: 30S ribosomal protein S21

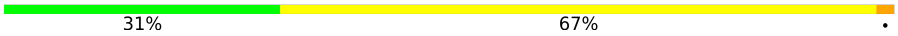
Chain U2:

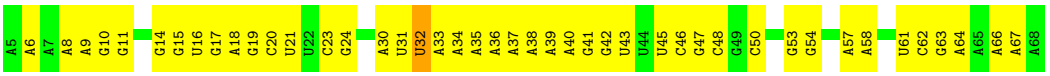




• Molecule 28: messenger RNA

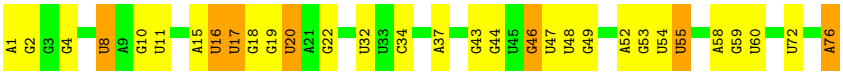
Chain V2:





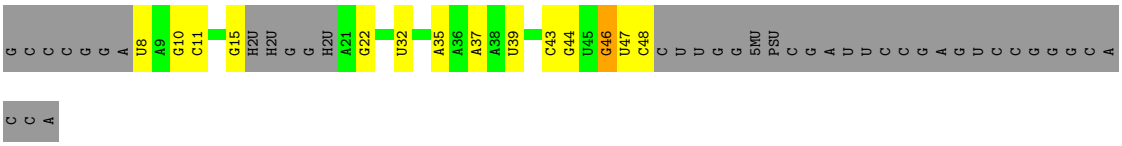
• Molecule 29: tRNA-Trp (P-site)

Chain W:



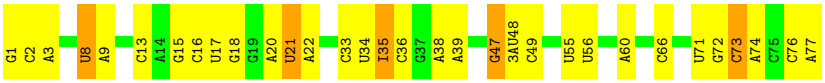
• Molecule 30: tRNA-Phe (P-site)

Chain W1:



• Molecule 31: tRNA-Arg (E-site)

Chain X2:

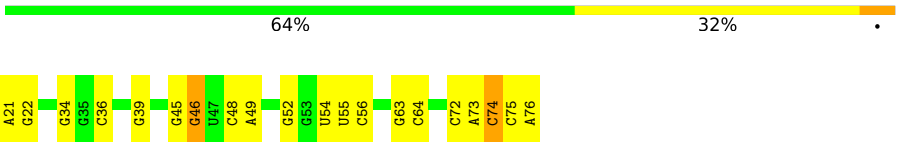


• Molecule 32: tRNA-Val (A-site)

Chain Y1:

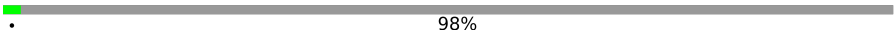
• Molecule 33: tRNA-Ala (A-site)

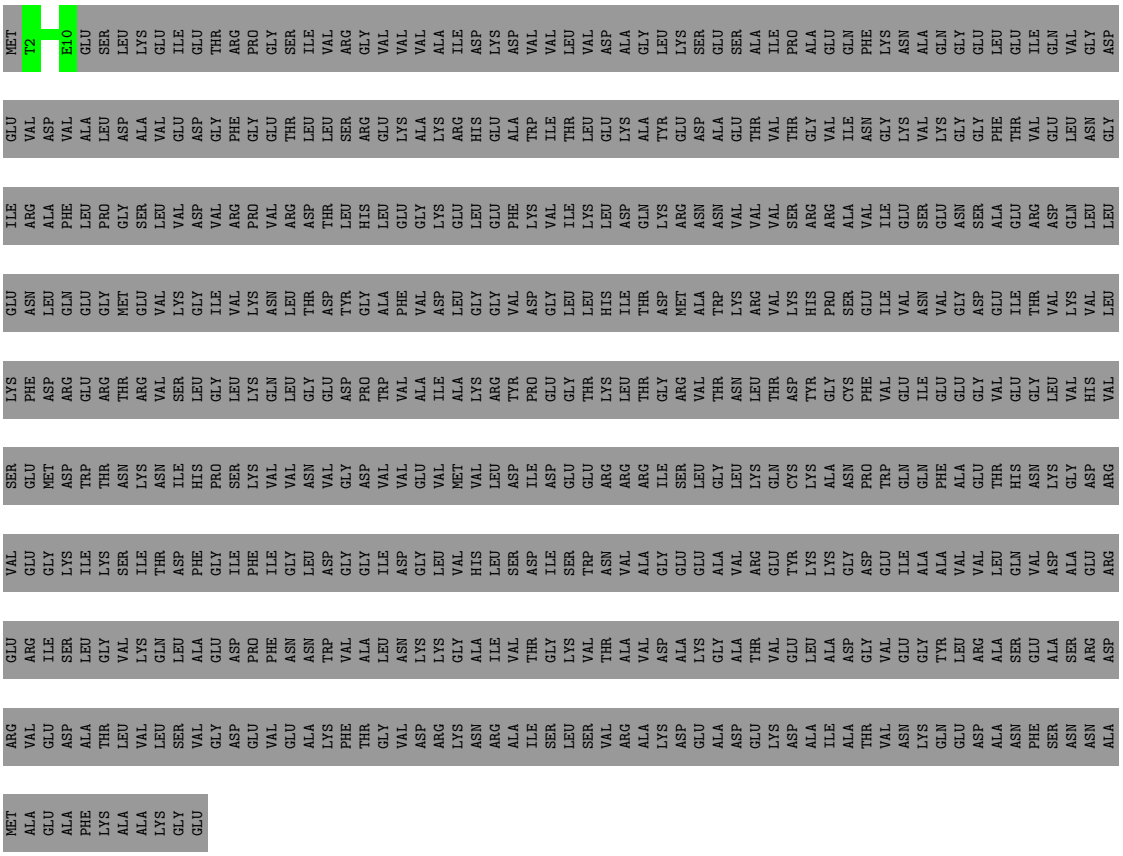
Chain Y2:



• Molecule 34: 30S ribosomal protein S1

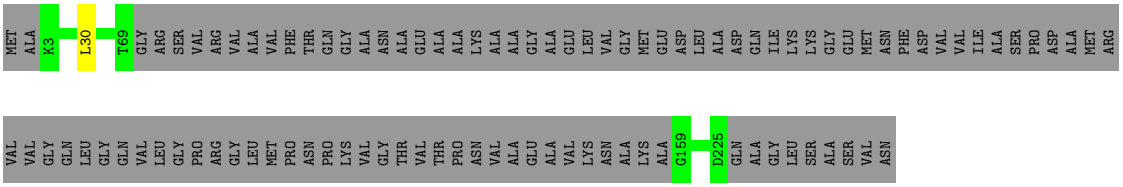
Chain Z1:





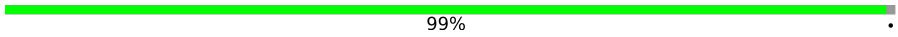
• Molecule 35: Large ribosomal subunit protein uL1

Chain a2:



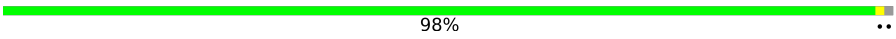
• Molecule 36: 50S ribosomal protein L2

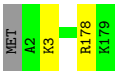
Chain b2:



• Molecule 37: 50S ribosomal protein L5

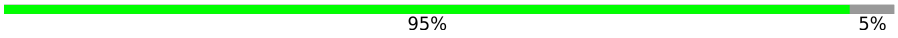
Chain e2:

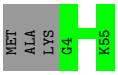




• Molecule 38: Large ribosomal subunit protein bL33

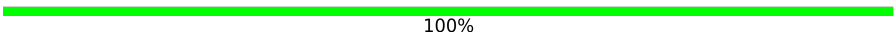
Chain g2:





• Molecule 39: 50S ribosomal protein L16

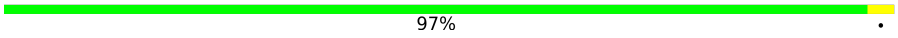
Chain h2:

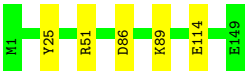


There are no outlier residues recorded for this chain.

• Molecule 40: 50S ribosomal protein L9

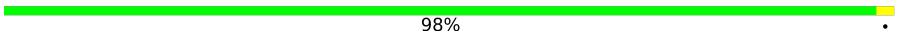
Chain i2:





• Molecule 41: 50S ribosomal protein L34

Chain l2:



• Molecule 42: 50S ribosomal protein L15

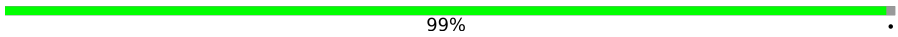
Chain o2:

• Molecule 43: Nascent chain

Chain p:

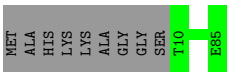
• Molecule 44: 50S ribosomal protein L18

Chain r2:



• Molecule 45: 50S ribosomal protein L27

Chain z2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39441	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RSP, PUT, 2MG, 3TD, PSU, 5MU, 4OC, 7MG, MG, MA6, ZN, G7M, SPD, CM0, OMG, 1MG, 6MZ, 2MA, 4SU, 3AU, OMC, UR3, MIA, OMU, 5MC, H2U

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	12	0.24	0/635	0.60	0/848
2	32	0.23	0/453	0.52	0/605
3	4	0.63	0/539	0.63	0/721
4	62	0.24	0/513	0.56	0/676
5	71	0.18	0/696	0.70	0/1081
5	72	0.20	1/69306 (0.0%)	0.70	20/108116 (0.0%)
6	82	0.22	1/2872 (0.0%)	0.75	2/4478 (0.0%)
7	A1	0.25	0/36794	0.77	1/57392 (0.0%)
7	A2	0.25	0/36681	0.75	7/57217 (0.0%)
8	B	0.24	0/1846	0.52	0/2488
8	B2	0.25	0/1807	0.49	0/2435
9	C1	0.25	0/1692	0.54	0/2280
9	C2	0.26	0/1685	0.56	0/2270
10	D1	0.25	0/1665	0.54	0/2227
10	D2	0.25	0/1665	0.55	0/2227
11	E1	0.27	0/1179	0.52	0/1584
11	E2	0.27	0/1179	0.53	0/1584
12	F1	0.24	0/881	0.51	0/1189
12	F2	0.25	0/881	0.50	0/1189
13	G1	0.25	0/1246	0.53	0/1672
13	G2	0.25	0/1230	0.56	0/1649
14	H1	0.26	0/989	0.54	0/1326
14	H2	0.26	0/989	0.54	0/1326
15	I1	0.25	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.28	0/827	0.59	0/1117
16	J2	0.26	0/813	0.63	0/1100
17	K1	0.25	0/873	0.55	0/1180
17	K2	0.26	0/900	0.56	0/1215
18	L1	0.27	0/969	0.61	0/1300
18	L2	0.27	0/969	0.61	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	M1	0.24	0/900	0.57	0/1204
19	M2	0.24	0/919	0.58	0/1226
20	N1	0.26	0/817	0.57	0/1088
20	N2	0.25	0/817	0.59	0/1088
21	O1	0.24	0/722	0.57	0/964
21	O2	0.24	0/722	0.59	0/964
22	P1	0.26	0/659	0.60	0/884
23	Q1	0.27	0/657	0.58	0/881
23	Q2	0.25	0/657	0.56	0/881
24	R1	0.25	0/635	0.57	0/849
24	R2	0.25	0/637	0.59	0/851
25	S1	0.25	0/680	0.51	0/915
25	S2	0.26	0/680	0.53	0/915
26	T1	0.25	0/676	0.52	0/895
27	U1	0.26	0/598	0.62	0/792
27	U2	0.25	0/592	0.58	0/785
28	V2	0.31	0/1552	0.88	3/2419 (0.1%)
29	W	0.41	1/1604 (0.1%)	0.81	1/2496 (0.0%)
30	W1	0.18	0/747	0.73	0/1161
31	X2	0.49	3/1628 (0.2%)	0.81	1/2526 (0.0%)
32	Y1	0.20	0/786	0.75	0/1216
33	Y2	0.38	1/1725 (0.1%)	0.82	2/2687 (0.1%)
34	Z1	0.27	0/76	0.34	0/101
35	a2	0.24	0/1033	0.47	0/1387
36	b2	0.26	0/2121	0.59	0/2852
37	e2	0.25	0/1444	0.52	0/1937
38	g2	0.25	0/434	0.51	0/576
39	h2	0.25	0/1104	0.57	0/1474
40	i2	0.25	0/1122	0.51	0/1515
41	l2	0.24	0/380	0.63	0/498
42	o2	0.27	0/383	0.69	0/501
43	p	0.58	0/77	0.86	0/104
44	r2	0.25	0/901	0.60	0/1209
45	z2	0.26	0/589	0.55	0/779
All	All	0.25	7/203930 (0.0%)	0.70	37/307181 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	D1	0	2
10	D2	0	1
15	I2	0	1
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
43	p	0	1
All	All	0	13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	1	A	OP3-P	-10.60	1.48	1.61
5	72	1	G	OP3-P	-10.59	1.48	1.61
31	X2	1	G	OP3-P	-10.57	1.48	1.61
33	Y2	1	G	OP3-P	-10.57	1.48	1.61
31	X2	35	I	C5-C6	7.33	1.54	1.39

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	72	2584	U	P-O3'-C3'	-13.29	103.75	119.70
5	72	2585	U	P-O3'-C3'	-12.31	104.93	119.70
5	72	1939	5MU	P-O3'-C3'	-11.85	105.48	119.70
5	72	747	5MU	P-O3'-C3'	-11.14	106.33	119.70
5	72	749	A	P-O3'-C3'	-10.63	106.94	119.70

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	56	ARG	Sidechain
3	4	59	ARG	Sidechain
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide
10	D2	104	ARG	Sidechain

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	12	75/78 (96%)	73 (97%)	2 (3%)	0	100 100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7 35
3	4	65/70 (93%)	54 (83%)	10 (15%)	1 (2%)	8 39
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100 100
8	B	231/241 (96%)	193 (84%)	35 (15%)	3 (1%)	10 41
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100 100
9	C1	211/233 (91%)	186 (88%)	23 (11%)	2 (1%)	14 49
9	C2	210/233 (90%)	184 (88%)	26 (12%)	0	100 100
10	D1	203/206 (98%)	181 (89%)	21 (10%)	1 (0%)	25 59
10	D2	203/206 (98%)	199 (98%)	4 (2%)	0	100 100
11	E1	156/167 (93%)	152 (97%)	4 (3%)	0	100 100
11	E2	156/167 (93%)	152 (97%)	4 (3%)	0	100 100
12	F1	104/135 (77%)	104 (100%)	0	0	100 100
12	F2	104/135 (77%)	79 (76%)	23 (22%)	2 (2%)	6 34
13	G1	153/179 (86%)	151 (99%)	2 (1%)	0	100 100
13	G2	152/179 (85%)	122 (80%)	24 (16%)	6 (4%)	2 21
14	H1	127/130 (98%)	127 (100%)	0	0	100 100
14	H2	127/130 (98%)	127 (100%)	0	0	100 100
15	I1	125/130 (96%)	103 (82%)	22 (18%)	0	100 100
15	I2	127/130 (98%)	116 (91%)	11 (9%)	0	100 100
16	J1	100/103 (97%)	92 (92%)	8 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	J2	98/103 (95%)	86 (88%)	8 (8%)	4 (4%)	2 20
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	14 49
17	K2	116/129 (90%)	100 (86%)	15 (13%)	1 (1%)	14 49
18	L1	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	16 51
18	L2	121/124 (98%)	116 (96%)	5 (4%)	0	100 100
19	M1	113/118 (96%)	109 (96%)	4 (4%)	0	100 100
19	M2	115/118 (98%)	108 (94%)	7 (6%)	0	100 100
20	N1	98/101 (97%)	85 (87%)	13 (13%)	0	100 100
20	N2	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
21	O1	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
21	O2	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
22	P1	80/82 (98%)	74 (92%)	6 (8%)	0	100 100
23	Q1	78/84 (93%)	77 (99%)	1 (1%)	0	100 100
23	Q2	78/84 (93%)	75 (96%)	2 (3%)	1 (1%)	10 41
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9 40
24	R2	72/75 (96%)	53 (74%)	18 (25%)	1 (1%)	9 40
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100 100
25	S2	81/92 (88%)	80 (99%)	1 (1%)	0	100 100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	5 30
27	U1	68/71 (96%)	57 (84%)	11 (16%)	0	100 100
27	U2	68/71 (96%)	59 (87%)	7 (10%)	2 (3%)	3 27
34	Z1	7/557 (1%)	7 (100%)	0	0	100 100
35	a2	130/234 (56%)	123 (95%)	7 (5%)	0	100 100
36	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100 100
37	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100 100
38	g2	50/55 (91%)	50 (100%)	0	0	100 100
39	h2	135/136 (99%)	135 (100%)	0	0	100 100
40	i2	147/149 (99%)	116 (79%)	29 (20%)	2 (1%)	9 40
41	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
42	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100 100
43	p	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
44	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100 100
45	z2	74/85 (87%)	73 (99%)	1 (1%)	0	100 100
All	All	6102/7240 (84%)	5611 (92%)	457 (8%)	34 (1%)	24 56

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
13	G2	18	PHE
13	G2	35	LYS
13	G2	54	SER
13	G2	146	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	12	67/68 (98%)	65 (97%)	2 (3%)	36 63
2	32	48/49 (98%)	47 (98%)	1 (2%)	48 71
3	4	60/62 (97%)	54 (90%)	6 (10%)	6 26
4	62	51/52 (98%)	51 (100%)	0	100 100
8	B	192/199 (96%)	192 (100%)	0	100 100
8	B2	189/199 (95%)	185 (98%)	4 (2%)	48 71
9	C1	173/190 (91%)	172 (99%)	1 (1%)	84 91
9	C2	172/190 (90%)	171 (99%)	1 (1%)	84 91
10	D1	172/173 (99%)	169 (98%)	3 (2%)	56 75
10	D2	172/173 (99%)	171 (99%)	1 (1%)	84 91
11	E1	120/126 (95%)	120 (100%)	0	100 100
11	E2	120/126 (95%)	120 (100%)	0	100 100
12	F1	92/116 (79%)	92 (100%)	0	100 100
12	F2	92/116 (79%)	92 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	G1	128/147 (87%)	128 (100%)	0	100 100
13	G2	127/147 (86%)	126 (99%)	1 (1%)	79 88
14	H1	104/105 (99%)	104 (100%)	0	100 100
14	H2	104/105 (99%)	104 (100%)	0	100 100
15	I1	105/107 (98%)	105 (100%)	0	100 100
15	I2	106/107 (99%)	105 (99%)	1 (1%)	75 86
16	J1	89/90 (99%)	88 (99%)	1 (1%)	70 83
16	J2	88/90 (98%)	88 (100%)	0	100 100
17	K1	88/99 (89%)	87 (99%)	1 (1%)	70 83
17	K2	91/99 (92%)	91 (100%)	0	100 100
18	L1	103/104 (99%)	103 (100%)	0	100 100
18	L2	103/104 (99%)	103 (100%)	0	100 100
19	M1	93/96 (97%)	93 (100%)	0	100 100
19	M2	95/96 (99%)	95 (100%)	0	100 100
20	N1	83/84 (99%)	81 (98%)	2 (2%)	44 68
20	N2	83/84 (99%)	83 (100%)	0	100 100
21	O1	76/77 (99%)	76 (100%)	0	100 100
21	O2	76/77 (99%)	76 (100%)	0	100 100
22	P1	65/65 (100%)	65 (100%)	0	100 100
23	Q1	74/78 (95%)	74 (100%)	0	100 100
23	Q2	74/78 (95%)	74 (100%)	0	100 100
24	R1	64/65 (98%)	63 (98%)	1 (2%)	58 76
24	R2	64/65 (98%)	61 (95%)	3 (5%)	22 51
25	S1	72/79 (91%)	71 (99%)	1 (1%)	62 79
25	S2	72/79 (91%)	72 (100%)	0	100 100
26	T1	65/66 (98%)	61 (94%)	4 (6%)	15 42
27	U1	60/61 (98%)	58 (97%)	2 (3%)	33 61
27	U2	59/61 (97%)	59 (100%)	0	100 100
34	Z1	8/461 (2%)	8 (100%)	0	100 100
35	a2	110/181 (61%)	109 (99%)	1 (1%)	75 86
36	b2	216/218 (99%)	216 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	e2	149/150 (99%)	147 (99%)	2 (1%)	65 81
38	g2	47/49 (96%)	47 (100%)	0	100 100
39	h2	110/109 (101%)	110 (100%)	0	100 100
40	i2	114/114 (100%)	111 (97%)	3 (3%)	41 66
41	l2	38/38 (100%)	37 (97%)	1 (3%)	41 66
42	o2	35/103 (34%)	35 (100%)	0	100 100
43	p	5/5 (100%)	4 (80%)	1 (20%)	1 6
44	r2	86/87 (99%)	86 (100%)	0	100 100
45	z2	58/63 (92%)	58 (100%)	0	100 100
All	All	5107/5932 (86%)	5063 (99%)	44 (1%)	74 86

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	R2	16	GLU
27	U1	66	ARG
25	S1	21	LYS
26	T1	71	LYS
37	e2	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
8	B2	177	ASN
9	C2	190	HIS
45	z2	50	ASN
16	J2	35	GLN
18	L2	29	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	63/64 (98%)	42 (66%)	8 (12%)
29	W	74/76 (97%)	26 (35%)	4 (5%)
30	W1	33/76 (43%)	8 (24%)	2 (6%)
31	X2	73/77 (94%)	26 (35%)	5 (6%)
32	Y1	32/76 (42%)	4 (12%)	2 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	Y2	75/76 (98%)	23 (30%)	2 (2%)
5	71	28/2904 (0%)	4 (14%)	0
5	72	2899/2904 (99%)	460 (15%)	33 (1%)
6	82	119/120 (99%)	21 (17%)	4 (3%)
7	A1	1538/1542 (99%)	449 (29%)	36 (2%)
7	A2	1533/1542 (99%)	397 (25%)	33 (2%)
All	All	6467/9457 (68%)	1460 (22%)	129 (1%)

5 of 1460 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1906	G
5	71	1907	G
5	71	1929	G
5	71	1930	G
5	72	10	A

5 of 129 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	W	18	G
30	W1	43	C
7	A1	412	A
7	A1	372	C
31	X2	22	A

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

73 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	$\#\|Z\| > 2$
7	2MG	A1	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.34	3 (18%)
7	5MC	A1	967	7	18,22,23	4.03	7 (38%)	26,32,35	1.01	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	H2U	X2	17	31	18,21,22	3.09	5 (27%)	21,30,33	1.95	5 (23%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
30	4SU	W1	8	30	18,21,22	3.80	7 (38%)	26,30,33	2.21	4 (15%)
7	2MG	A1	1516	7	18,26,27	2.84	7 (38%)	16,38,41	1.36	3 (18%)
5	5MU	72	747	5	19,22,23	0.34	0	28,32,35	0.58	0
7	MA6	A2	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.41	3 (15%)
5	2MG	72	1835	5	18,26,27	2.80	7 (38%)	16,38,41	1.41	4 (25%)
32	CM0	Y1	34	32	23,26,27	3.73	6 (26%)	27,37,40	1.52	2 (7%)
5	6MZ	72	2030	5	18,25,26	2.07	3 (16%)	16,36,39	2.31	3 (18%)
31	G7M	X2	47	31	20,26,27	2.81	7 (35%)	17,39,42	1.21	1 (5%)
31	5MU	X2	55	31	19,22,23	0.25	0	28,32,35	0.18	0
5	G7M	72	2069	5	20,26,27	2.77	7 (35%)	17,39,42	1.04	1 (5%)
5	PSU	72	746	5	18,21,22	0.99	2 (11%)	22,30,33	0.95	1 (4%)
33	5MU	Y2	54	33	19,22,23	0.24	0	28,32,35	0.24	0
5	PSU	72	2605	5	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
29	PSU	W	32	29	18,21,22	4.63	8 (44%)	22,30,33	1.88	5 (22%)
7	2MG	A2	1516	7	18,26,27	2.81	7 (38%)	16,38,41	1.36	3 (18%)
5	H2U	72	2449	49,5	18,21,22	3.04	5 (27%)	21,30,33	2.03	5 (23%)
5	3TD	71	1915	5	19,22,23	4.09	7 (36%)	21,32,35	1.70	2 (9%)
7	4OC	A1	1402	7	20,23,24	3.22	8 (40%)	26,32,35	0.93	1 (3%)
7	UR3	A2	1498	7	19,22,23	2.73	8 (42%)	26,32,35	1.29	2 (7%)
5	2MG	72	2445	5	18,26,27	2.82	7 (38%)	16,38,41	1.41	4 (25%)
31	3AU	X2	48	31	24,28,29	2.84	7 (29%)	33,40,43	1.29	3 (9%)
31	H2U	X2	21	31	18,21,22	3.07	5 (27%)	21,30,33	2.04	5 (23%)
30	PSU	W1	32	30	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
29	G7M	W	46	29	20,26,27	2.79	7 (35%)	17,39,42	1.12	1 (5%)
5	OMC	72	2498	49,5	19,22,23	3.29	8 (42%)	26,31,34	0.76	0
5	1MG	72	745	5	18,26,27	2.75	6 (33%)	19,39,42	1.43	3 (15%)
29	5MU	W	54	29	19,22,23	0.25	0	28,32,35	0.39	0
5	6MZ	72	1618	5	18,25,26	2.03	2 (11%)	16,36,39	2.20	4 (25%)
7	2MG	A2	1207	7	18,26,27	2.86	7 (38%)	16,38,41	1.37	3 (18%)
7	UR3	A1	1498	7	19,22,23	2.75	8 (42%)	26,32,35	1.29	3 (11%)
5	2MA	72	2503	5	19,25,26	3.58	6 (31%)	21,37,40	3.66	4 (19%)
31	4SU	X2	8	31	18,21,22	3.79	7 (38%)	26,30,33	2.27	4 (15%)
31	PSU	X2	56	31	18,21,22	0.87	1 (5%)	22,30,33	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	H2U	Y2	17	33	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
33	PSU	Y2	55	33	18,21,22	0.88	1 (5%)	22,30,33	0.64	0
5	OMG	72	2251	29,5	18,26,27	2.82	7 (38%)	19,38,41	1.55	4 (21%)
29	H2U	W	16	29	18,21,22	3.05	5 (27%)	21,30,33	1.98	5 (23%)
5	PSU	72	2504	49,5	18,21,22	4.67	8 (44%)	22,30,33	1.92	5 (22%)
30	MIA	W1	37	30	24,31,32	2.34	3 (12%)	26,44,47	2.67	7 (26%)
5	PSU	72	2604	5	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
30	PSU	W1	39	30	18,21,22	4.64	8 (44%)	22,30,33	1.84	5 (22%)
31	RSP	X2	33	31	17,21,22	4.13	7 (41%)	22,30,33	0.78	0
29	4SU	W	8	29	18,21,22	3.77	7 (38%)	26,30,33	2.26	5 (19%)
7	G7M	A1	527	7	20,26,27	2.79	8 (40%)	17,39,42	1.04	1 (5%)
29	MIA	W	37	29	24,31,32	2.32	3 (12%)	26,44,47	2.53	7 (26%)
7	5MC	A1	1407	7	18,22,23	4.03	7 (38%)	26,32,35	0.99	2 (7%)
7	5MC	A2	1407	7	18,22,23	4.00	7 (38%)	26,32,35	0.97	2 (7%)
32	6MZ	Y1	37	32	18,25,26	2.06	3 (16%)	16,36,39	2.35	4 (25%)
29	H2U	W	17	29	18,21,22	3.08	5 (27%)	21,30,33	2.01	5 (23%)
33	G7M	Y2	46	33	20,26,27	2.81	8 (40%)	17,39,42	1.09	1 (5%)
5	PSU	72	955	5	18,21,22	4.67	8 (44%)	22,30,33	1.87	5 (22%)
29	PSU	W	55	29	18,21,22	0.85	1 (5%)	22,30,33	0.79	1 (4%)
7	MA6	A1	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.38	3 (15%)
31	2MA	X2	38	31	19,25,26	3.64	6 (31%)	21,37,40	3.60	3 (14%)
29	H2U	W	20	29	18,21,22	3.04	5 (27%)	21,30,33	2.02	5 (23%)
5	3TD	72	1915	5	19,22,23	4.03	7 (36%)	21,32,35	1.78	3 (14%)
7	4OC	A2	1402	7	20,23,24	3.24	8 (40%)	26,32,35	0.90	1 (3%)
7	2MG	A1	966	7	18,26,27	2.85	7 (38%)	16,38,41	1.41	3 (18%)
7	G7M	A2	527	7	20,26,27	2.77	7 (35%)	17,39,42	1.02	1 (5%)
7	2MG	A2	966	7	18,26,27	2.85	7 (38%)	16,38,41	1.35	3 (18%)
5	5MU	72	1939	5	19,22,23	0.74	0	28,32,35	1.27	2 (7%)
5	PSU	72	2580	5	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
30	G7M	W1	46	30	20,26,27	2.81	7 (35%)	17,39,42	1.12	1 (5%)
7	MA6	A1	1519	7	18,26,27	1.08	2 (11%)	19,38,41	3.47	3 (15%)
5	5MC	72	1962	5	18,22,23	4.01	7 (38%)	26,32,35	1.06	2 (7%)
7	5MC	A2	967	7	18,22,23	4.01	7 (38%)	26,32,35	1.00	2 (7%)
32	7MG	Y1	46	32	22,26,27	3.89	10 (45%)	29,39,42	2.07	9 (31%)
7	MA6	A2	1519	7	18,26,27	1.08	2 (11%)	19,38,41	3.42	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PSU	72	2457	5	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)

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
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
7	5MC	A1	967	7	-	0/7/25/26	0/2/2/2
31	H2U	X2	17	31	-	6/7/38/39	0/2/2/2
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
5	5MU	72	747	5	-	0/7/25/26	0/2/2/2
7	MA6	A2	1518	7	-	0/7/29/30	0/3/3/3
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3
32	CM0	Y1	34	32	-	2/12/30/31	0/2/2/2
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
31	G7M	X2	47	31	-	3/3/25/26	0/3/3/3
31	5MU	X2	55	31	-	2/7/25/26	0/2/2/2
5	G7M	72	2069	5	-	2/3/25/26	0/3/3/3
5	PSU	72	746	5	-	1/7/25/26	0/2/2/2
33	5MU	Y2	54	33	-	2/7/25/26	0/2/2/2
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
29	PSU	W	32	29	-	0/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3
5	H2U	72	2449	49,5	-	1/7/38/39	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
7	4OC	A1	1402	7	-	2/9/29/30	0/2/2/2
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
31	3AU	X2	48	31	-	6/16/34/35	0/2/2/2
31	H2U	X2	21	31	-	3/7/38/39	0/2/2/2
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
29	G7M	W	46	29	-	3/3/25/26	0/3/3/3
5	OMC	72	2498	49,5	-	2/9/27/28	0/2/2/2
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
5	2MA	72	2503	5	-	0/3/25/26	0/3/3/3
31	4SU	X2	8	31	-	2/7/25/26	0/2/2/2
31	PSU	X2	56	31	-	2/7/25/26	0/2/2/2
33	H2U	Y2	17	33	-	7/7/38/39	0/2/2/2
33	PSU	Y2	55	33	-	0/7/25/26	0/2/2/2
5	OMG	72	2251	29,5	-	3/5/27/28	0/3/3/3
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
5	PSU	72	2504	49,5	-	1/7/25/26	0/2/2/2
30	MIA	W1	37	30	-	6/11/33/34	0/3/3/3
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
31	RSP	X2	33	31	-	1/7/25/26	0/2/2/2
29	4SU	W	8	29	-	2/7/25/26	0/2/2/2
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3
29	MIA	W	37	29	-	1/11/33/34	0/3/3/3
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
29	H2U	W	17	29	-	1/7/38/39	0/2/2/2
33	G7M	Y2	46	33	-	2/3/25/26	0/3/3/3
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
29	PSU	W	55	29	-	3/7/25/26	0/2/2/2
7	MA6	A1	1518	7	-	3/7/29/30	0/3/3/3
31	2MA	X2	38	31	-	3/3/25/26	0/3/3/3
29	H2U	W	20	29	-	1/7/38/39	0/2/2/2
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
7	2MG	A1	966	7	-	0/5/27/28	0/3/3/3
7	G7M	A2	527	7	-	3/3/25/26	0/3/3/3
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
5	5MU	72	1939	5	-	2/7/25/26	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
30	G7M	W1	46	30	-	3/3/25/26	0/3/3/3
7	MA6	A1	1519	7	-	6/7/29/30	0/3/3/3
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
7	MA6	A2	1519	7	-	2/7/29/30	0/3/3/3
5	PSU	72	2457	5	-	2/7/25/26	0/2/2/2

The worst 5 of 414 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y1	34	CM0	C6-C5	12.87	1.48	1.34
5	71	1915	3TD	C6-C5	12.74	1.50	1.35
5	72	1915	3TD	C6-C5	12.52	1.49	1.35
5	72	2504	PSU	C6-C5	12.20	1.49	1.35
5	72	955	PSU	C6-C5	12.17	1.49	1.35

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	72	2503	2MA	C1'-N9-C4	14.94	152.89	126.64
31	X2	38	2MA	C1'-N9-C4	14.60	152.28	126.64
7	A2	1519	MA6	N1-C6-N6	-12.56	103.84	117.06
7	A1	1519	MA6	N1-C6-N6	-12.55	103.85	117.06
7	A2	1518	MA6	N1-C6-N6	-12.40	104.00	117.06

There are no chirality outliers.

5 of 117 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	1402	4OC	C1'-C2'-O2'-CM2
7	A1	1518	MA6	C5-C6-N6-C9
7	A1	1518	MA6	C5-C6-N6-C10
7	A1	1519	MA6	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C5-C6-N6-C10

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 302 ligands modelled in this entry, 298 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
48	SPD	72	3003	-	9,9,9	0.32	0	8,8,8	0.87	0
47	PUT	72	3002	-	5,5,5	0.24	0	4,4,4	0.56	0
50	ALA	Y2	102	33	3,4,5	0.48	0	2,4,6	2.56	2 (100%)
47	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SPD	72	3003	-	-	0/7/7/7	-
47	PUT	72	3002	-	-	0/3/3/3	-
50	ALA	Y2	102	33	-	0/0/2/4	-
47	PUT	72	3001	-	-	1/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	Y2	102	ALA	CB-CA-N	-3.01	100.32	109.85
50	Y2	102	ALA	O-C-CA	-2.02	117.88	124.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.