wwPDB EM Validation Summary Report

Apr 16, 2024 – 03:41 am BST

PDB ID	:	8RCS
EMDB ID	:	EMD-19058
Title	:	Escherichia coli paused disome complex (Rotated disome interface class 1)
Authors	:	Fluegel, T.; Schacherl, M.
Deposited on	:	2023-12-07
Resolution	:	4.46 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 ⓘ symbol.

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

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

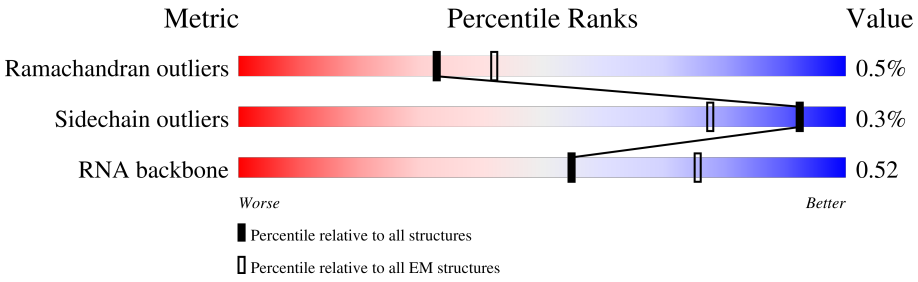
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	12	78	96%
2	32	59	97%
3	4	70	91% 6%
3	41	70	20% 80%
4	62	65	98%
5	71	2904	99%
5	72	2904	83% 17%
6	82	120	80% 19%
7	A1	1542	70% 30%

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Mol	Chain	Length	Quality of chain
7	A2	1542	73% 26%
8	B	241	95%
8	B2	241	94% 6%
9	C1	233	90% 9%
9	C2	233	91% 9%
10	D1	206	98%
10	D2	206	98%
11	E1	167	95% 5%
11	E2	167	95% 5%
12	F1	135	79% 21%
12	F2	135	78% 21%
13	G1	179	87% 13%
13	G2	179	81% 5% 14%
14	H1	130	99%
14	H2	130	99%
15	I1	130	98%
15	I2	130	99%
16	J1	103	99%
16	J2	103	92% 5%
17	K1	129	88% 11%
17	K2	129	90% 9%
18	L1	124	98%
18	L2	124	99%
19	M1	118	97%
19	M2	118	99%

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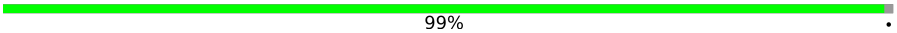
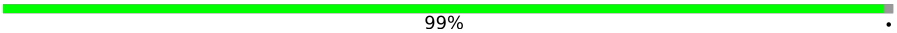
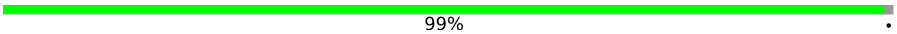
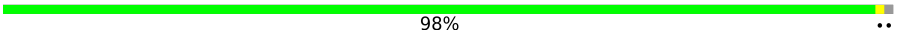
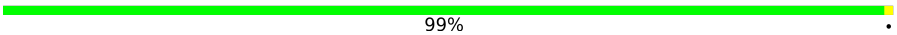
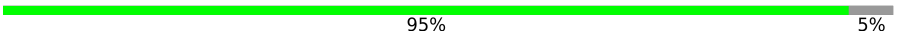
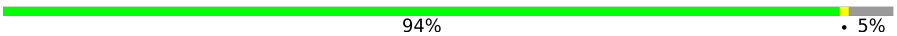
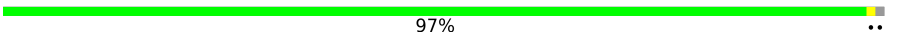
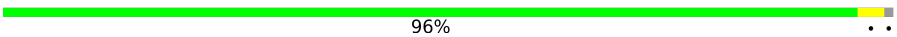
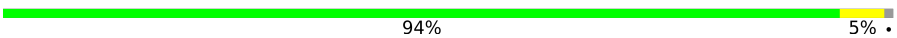
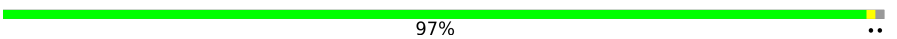
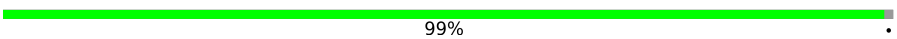
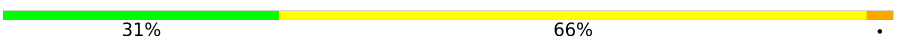
Mol	Chain	Length	Quality of chain
20	N1	101	
20	N2	101	
21	O1	89	
21	O2	89	
22	P1	82	
23	Q1	84	
23	Q2	84	
24	R1	75	
24	R2	75	
25	S1	92	
25	S2	92	
26	T1	87	
27	U1	71	
27	U2	71	
28	V2	59	
29	W	76	
30	W1	76	
31	Y	76	
32	Y1	76	
33	Z1	557	
34	a2	234	
35	b2	273	
36	e2	179	
37	g2	55	
38	h2	136	

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Mol	Chain	Length	Quality of chain
39	i2	149	98%
40	l2	46	98%
41	o2	144	35% 65%
42	p	10	70% 30%
43	r2	117	99%
44	z2	85	89% 11%

2 Entry composition (i)

There are 48 unique types of molecules in this entry. The entry contains 187319 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
			Total	C	N	O	S		
1	12	77	625	388	129	106	2	0	0

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

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

- Molecule 3 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	68	533	330	101	96	6	0	0
			Total	C	N	O			
3	41	14	118	74	26	18		0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	71	19	406	182	73	132	19	0	0
			Total	C	N	O	P		
5	72	2904	62355	27824	11468	20159	2904	0	0

- 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 857	C 528	N 168	O 158	S 3	0	0
17	K2	118	Total 884	C 545	N 175	O 161	S 3	0	0

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

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

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

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

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

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

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

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

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

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

- 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
			590	366	125	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	59	Total	C	N	O	P	0	0
			1272	569	242	402	59		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	W1	33	Total	C	N	O	P	S	0	0
			718	324	133	226	33	2		

- Molecule 31 is a RNA chain called tRNA-Ala (A/P-site).

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y1	34	CM0	U	variant	GB 1847302804

- Molecule 33 is a protein called 30S ribosomal protein S1.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a2	223	Total	C	N	O	S	0	0
			1661	1039	302	314	6		

- Molecule 35 is a protein called 50S ribosomal protein L2.

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L33.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L9.

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

- Molecule 40 is a protein called 50S ribosomal protein L34.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called Nascent chain.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

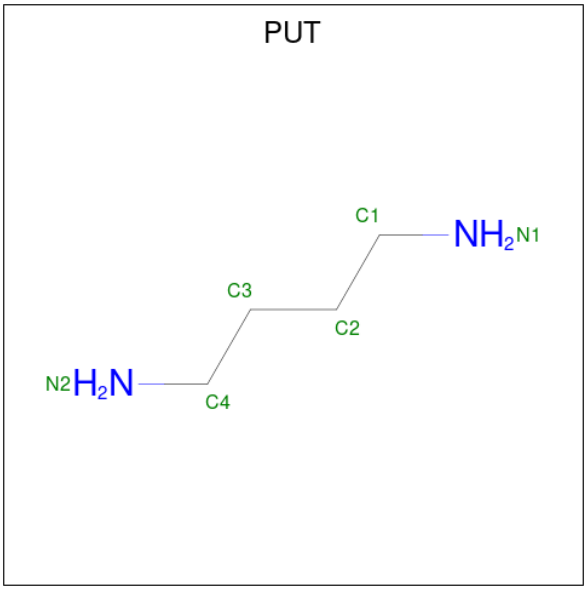
- Molecule 44 is a protein called 50S ribosomal protein L27.

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

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

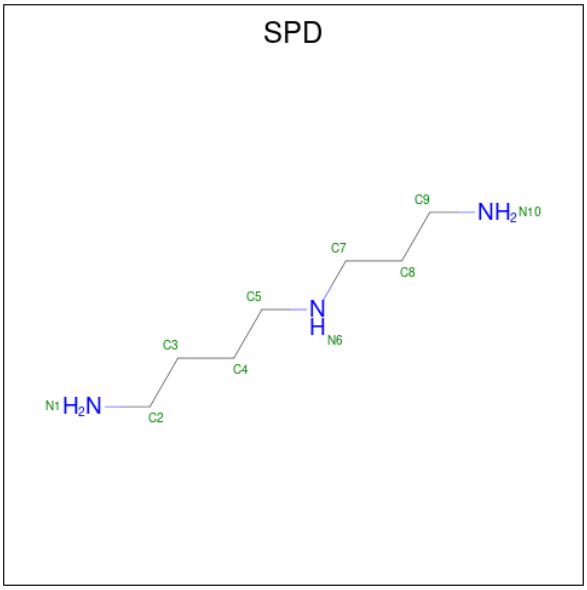
Mol	Chain	Residues	Atoms		AltConf
45	4	1	Total 1	Zn 1	0
45	B	1	Total 1	Zn 1	0

- Molecule 46 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	AltConf
46	72	1	Total C N 6 4 2	0
46	72	1	Total C N 6 4 2	0

- Molecule 47 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
47	72	1	Total C N 10 7 3	0

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

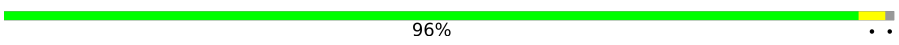
Mol	Chain	Residues	Atoms	AltConf
48	72	165	Total Mg 165 165	0
48	A1	60	Total Mg 60 60	0
48	A2	41	Total Mg 41 41	0
48	N2	1	Total Mg 1 1	0
48	Y	1	Total Mg 1 1	0
48	o2	1	Total Mg 1 1	0

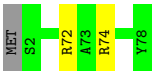
3 Residue-property plots (i)

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

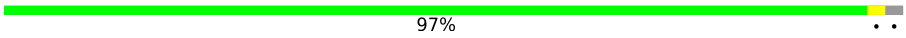
Chain 12:





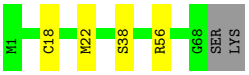
- Molecule 2: 50S ribosomal protein L30

Chain 32:



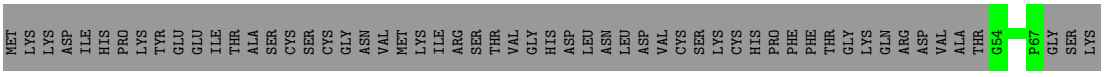
- Molecule 3: Large ribosomal subunit protein bL31A

Chain 4:



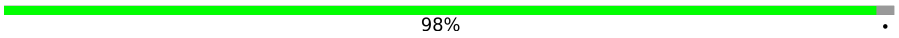
- Molecule 3: Large ribosomal subunit protein bL31A

Chain 41:



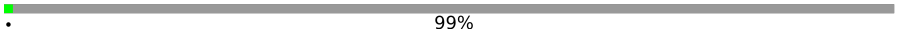
- Molecule 4: 50S ribosomal protein L35

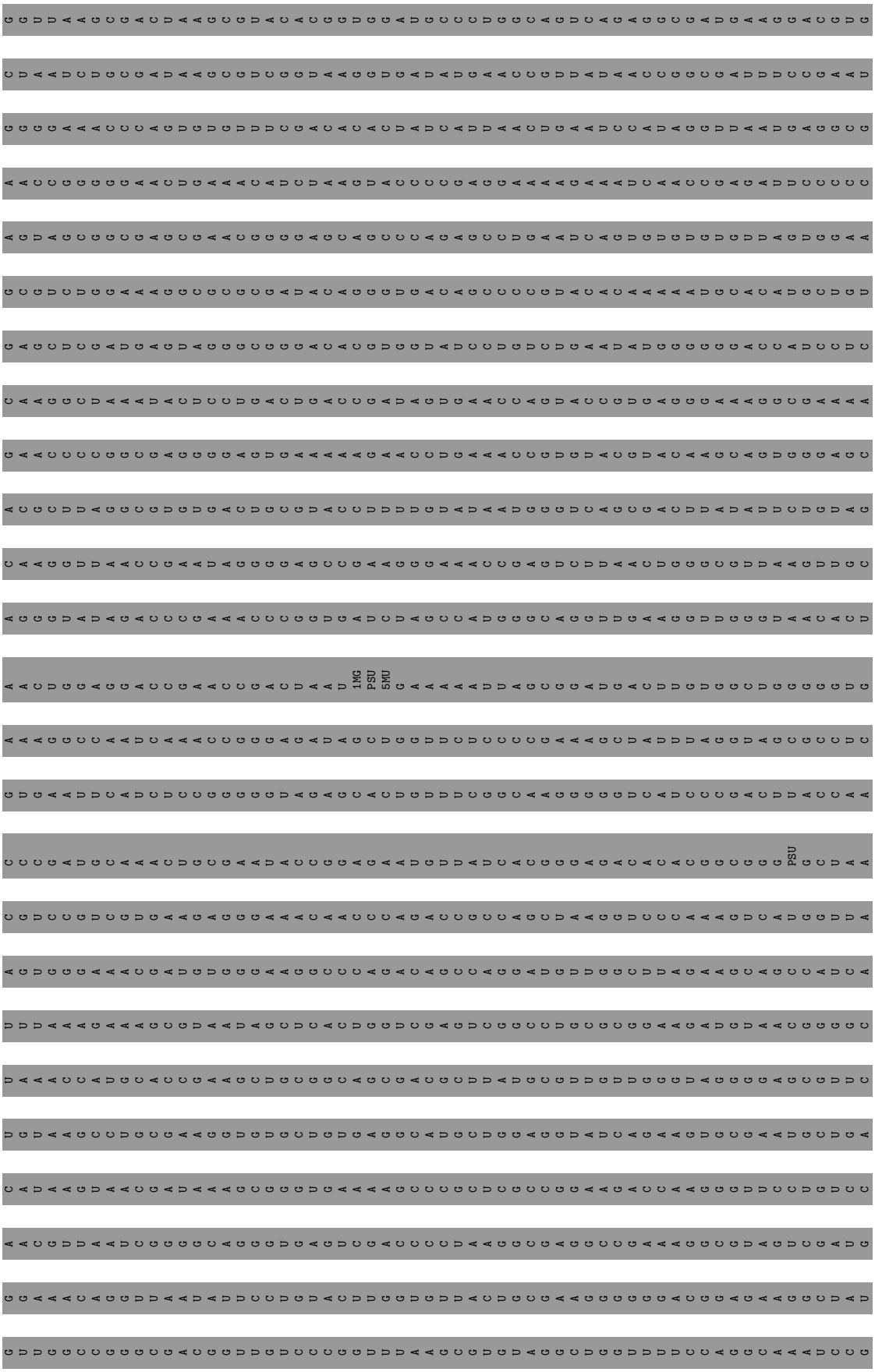
Chain 62:

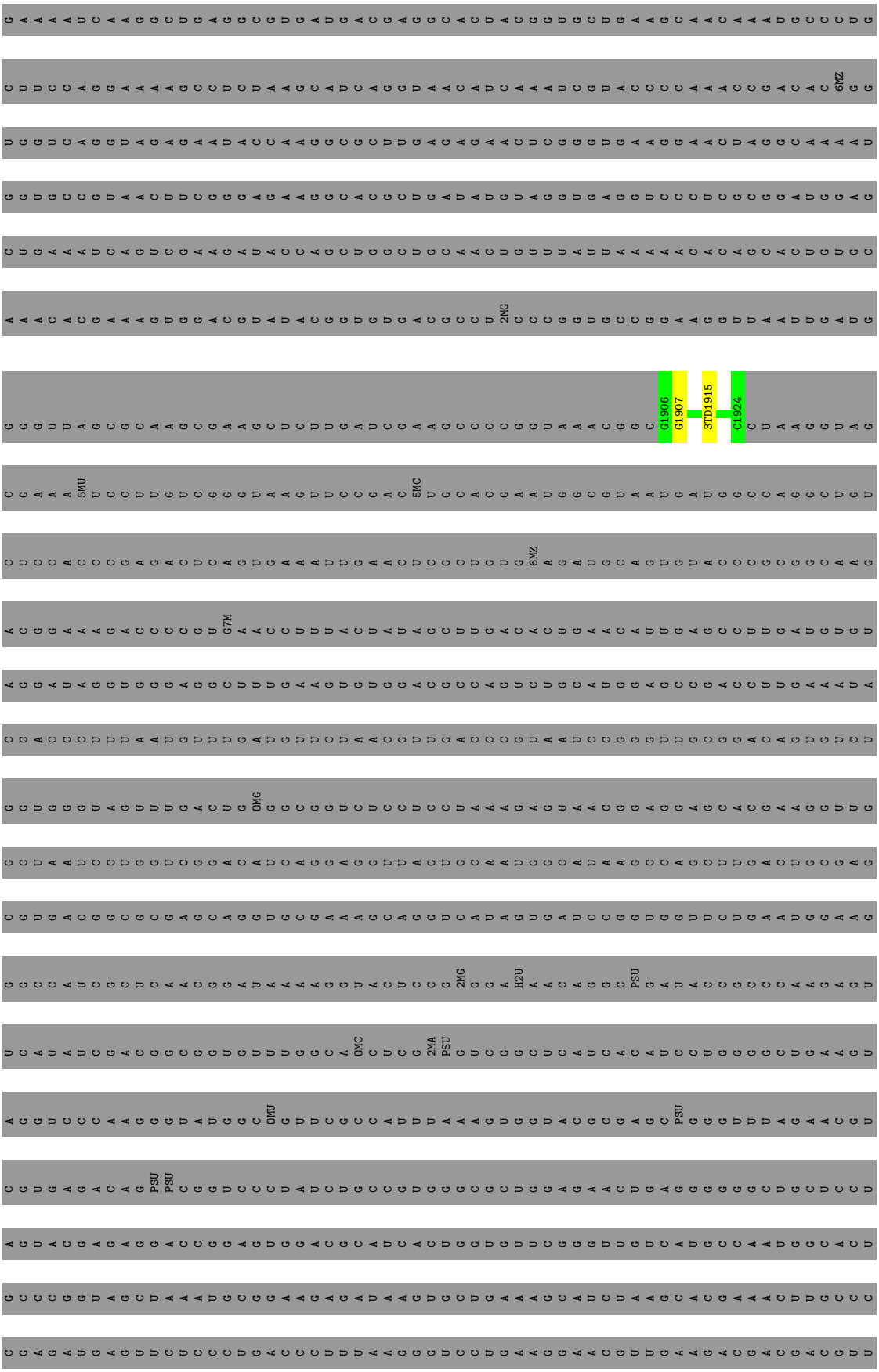


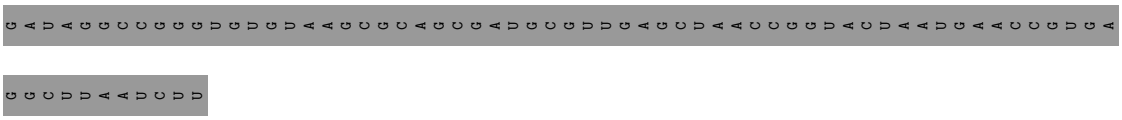
- Molecule 5: 23S ribosomal RNA

Chain 71:



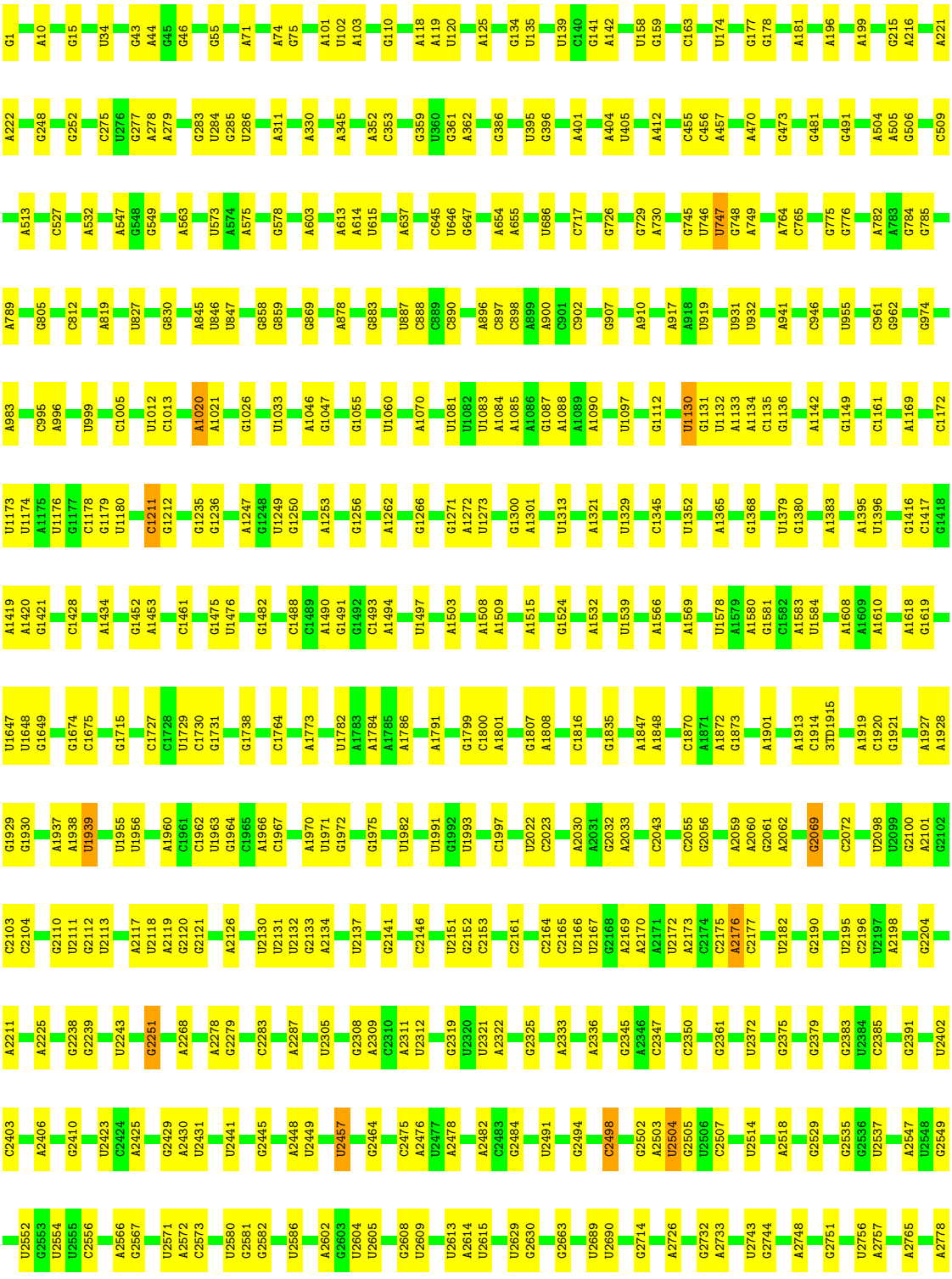

1MG
PSU
5MU
PSU

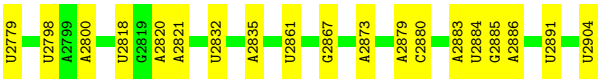

6MZ
2MG
G1906
G1907
3TD1915
C1924
5MU
5MC
6MZ
G7M
OMG
2MG
H2U
PSU
OMC
2MA
PSU
OMU
PSU
PSU



• Molecule 5: 23S ribosomal RNA

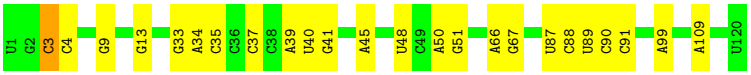
Chain 72:





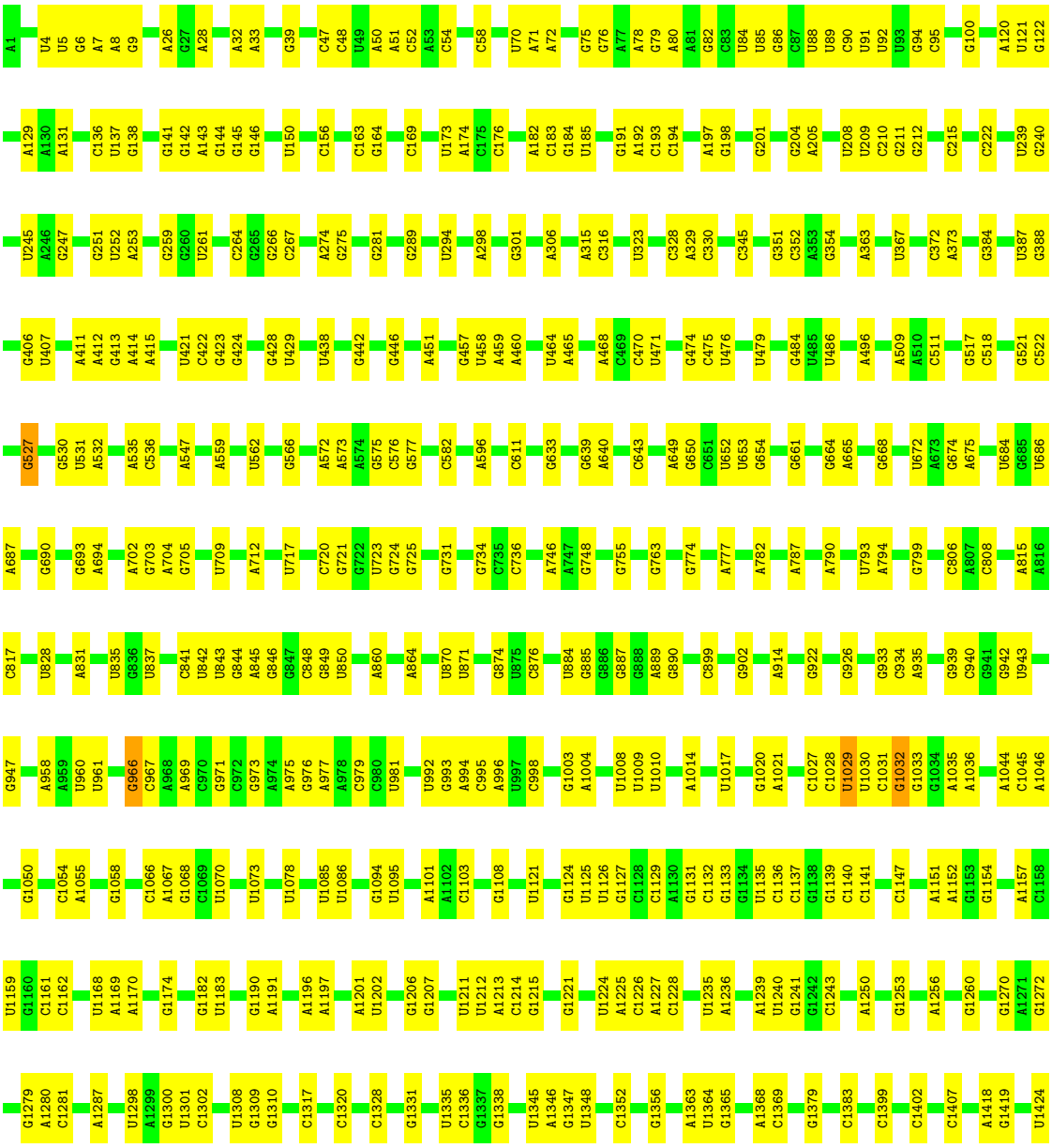
• Molecule 6: 5S ribosomal RNA

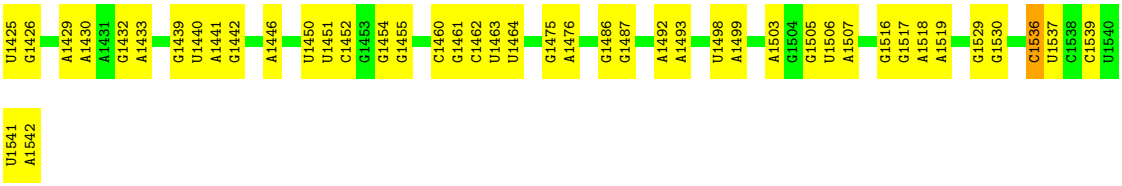
Chain 82:



• Molecule 7: 16S ribosomal RNA

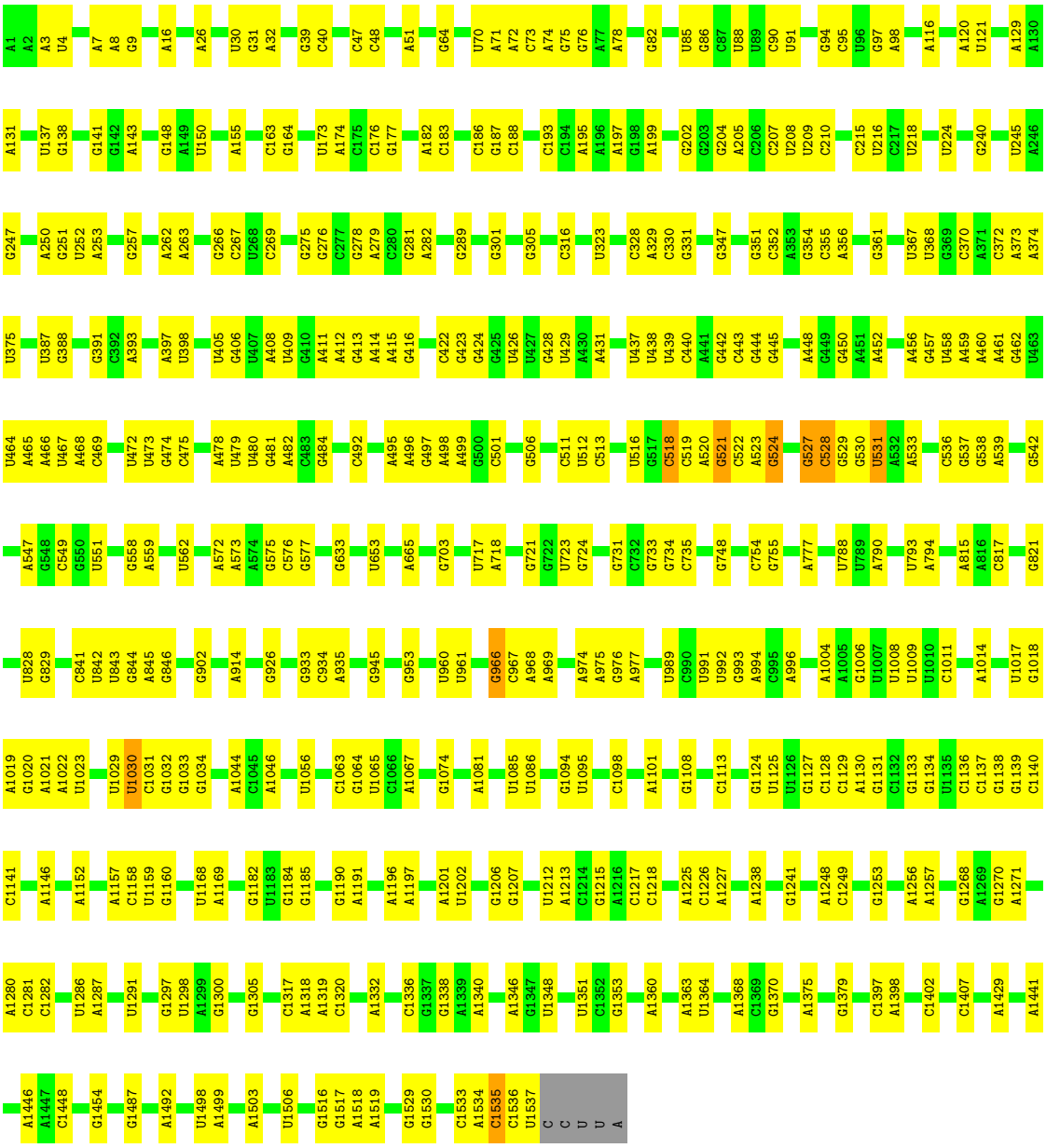
Chain A1:





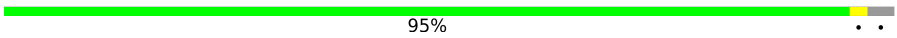
• Molecule 7: 16S ribosomal RNA

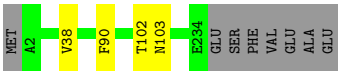
Chain A2:



• Molecule 8: Small ribosomal subunit protein uS2

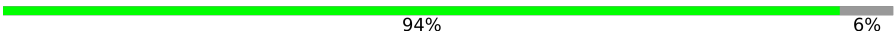
Chain B:

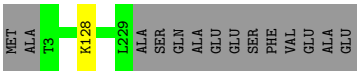




• Molecule 8: Small ribosomal subunit protein uS2

Chain B2:





• Molecule 9: Small ribosomal subunit protein uS3

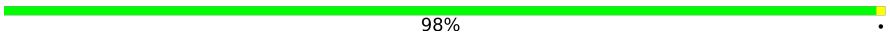
Chain C1:

• Molecule 9: Small ribosomal subunit protein uS3

Chain C2:

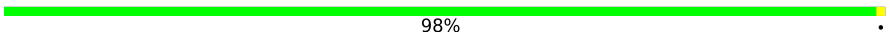
• Molecule 10: Small ribosomal subunit protein uS4

Chain D1:



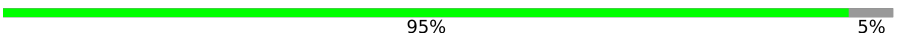
• Molecule 10: Small ribosomal subunit protein uS4

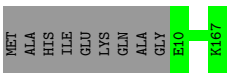
Chain D2:



• Molecule 11: Small ribosomal subunit protein uS5

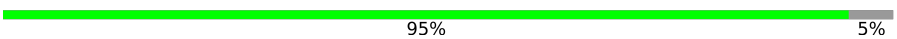
Chain E1:

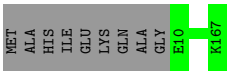




• Molecule 11: Small ribosomal subunit protein uS5

Chain E2:





• Molecule 12: 30S ribosomal protein S6

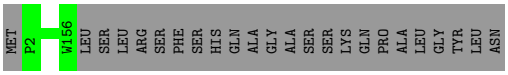
Chain F1:

• Molecule 12: 30S ribosomal protein S6

Chain F2:

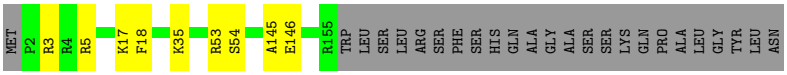
• Molecule 13: 30S ribosomal protein S7

Chain G1:



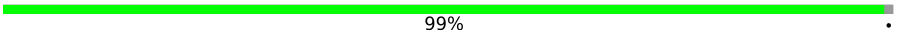
• Molecule 13: 30S ribosomal protein S7

Chain G2:



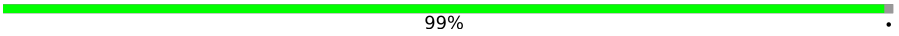
• Molecule 14: Small ribosomal subunit protein uS8

Chain H1:



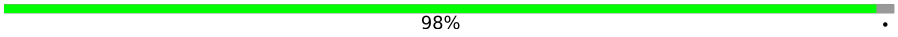
• Molecule 14: Small ribosomal subunit protein uS8

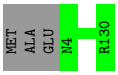
Chain H2:



• Molecule 15: Small ribosomal subunit protein uS9

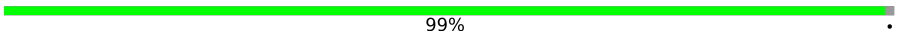
Chain I1:





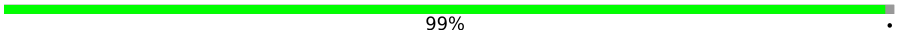
• Molecule 15: Small ribosomal subunit protein uS9

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

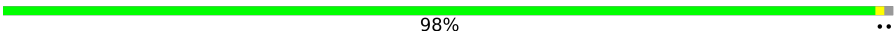
Chain K1:

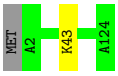
• Molecule 17: Small ribosomal subunit protein uS11

Chain K2:

• Molecule 18: Small ribosomal subunit protein uS12

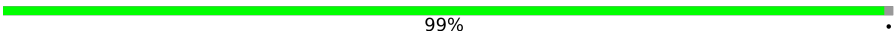
Chain L1:





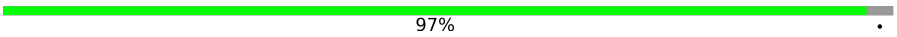
• Molecule 18: Small ribosomal subunit protein uS12

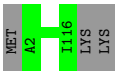
Chain L2:



• Molecule 19: Small ribosomal subunit protein uS13

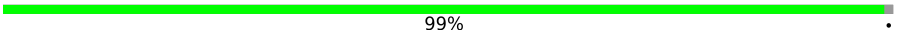
Chain M1:





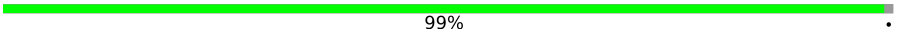
• Molecule 19: Small ribosomal subunit protein uS13

Chain M2:



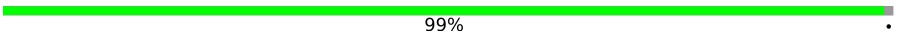
• Molecule 20: Small ribosomal subunit protein uS14

Chain N1:



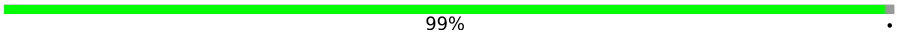
• Molecule 20: Small ribosomal subunit protein uS14

Chain N2:



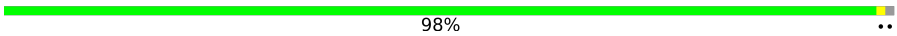
• Molecule 21: 30S ribosomal protein S15

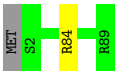
Chain O1:



• Molecule 21: 30S ribosomal protein S15

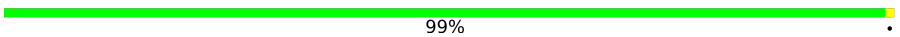
Chain O2:





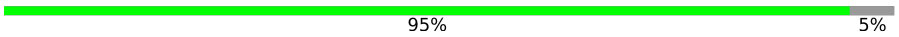
• Molecule 22: 30S ribosomal protein S16

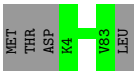
Chain P1:



• Molecule 23: Small ribosomal subunit protein uS17

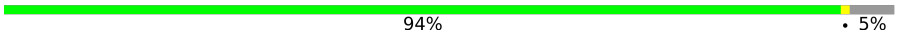
Chain Q1:

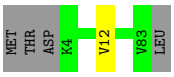




• Molecule 23: Small ribosomal subunit protein uS17

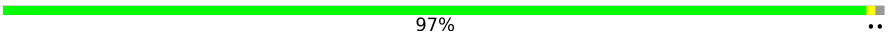
Chain Q2:

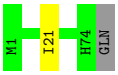




• Molecule 24: Small ribosomal subunit protein bS18

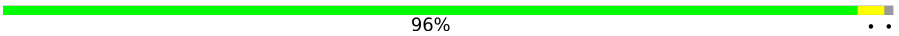
Chain R1:

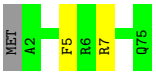




• Molecule 24: Small ribosomal subunit protein bS18

Chain R2:





• Molecule 25: Small ribosomal subunit protein uS19

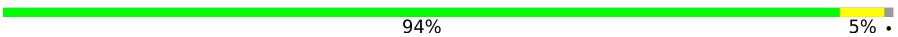
Chain S1:

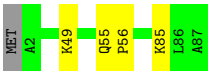
• Molecule 25: Small ribosomal subunit protein uS19

Chain S2:

• Molecule 26: Small ribosomal subunit protein bS20

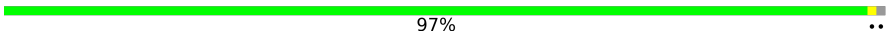
Chain T1:

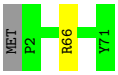




• Molecule 27: 30S ribosomal protein S21

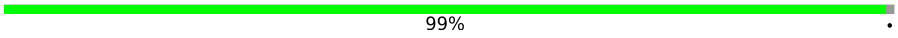
Chain U1:





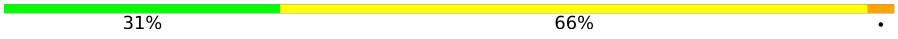
• Molecule 27: 30S ribosomal protein S21

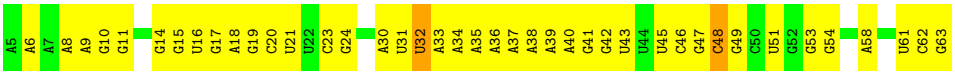
Chain U2:



• Molecule 28: messenger RNA

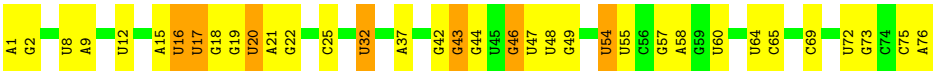
Chain V2:





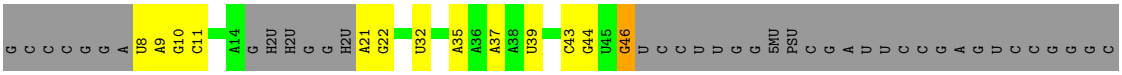
• Molecule 29: tRNA-Trp (P/E-site)

Chain W:



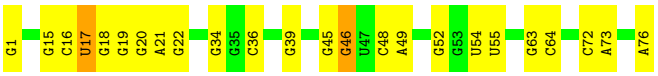
• Molecule 30: tRNA-Phe (P/E-site)

Chain W1:



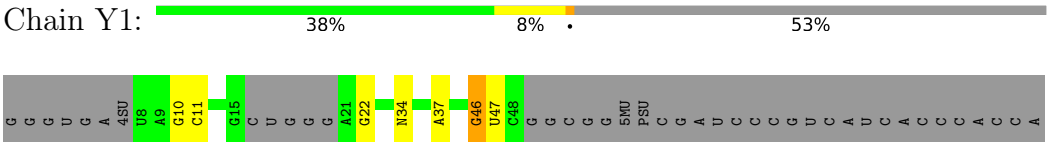
• Molecule 31: tRNA-Ala (A/P-site)

Chain Y:



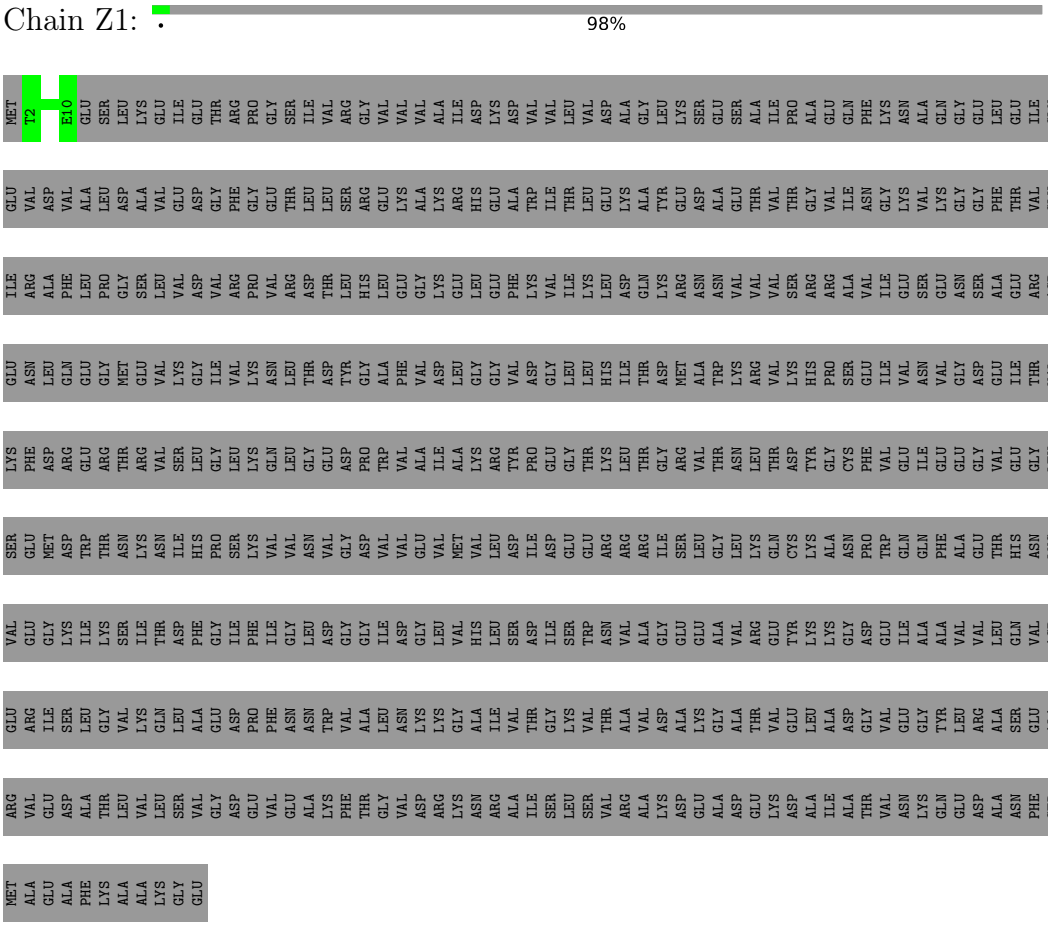
• Molecule 32: tRNA-Val (A/P-site)

Chain Y1:



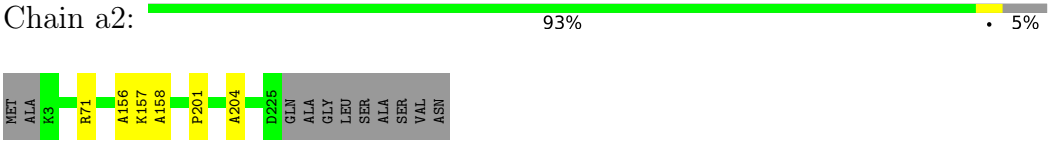
• Molecule 33: 30S ribosomal protein S1

Chain Z1:



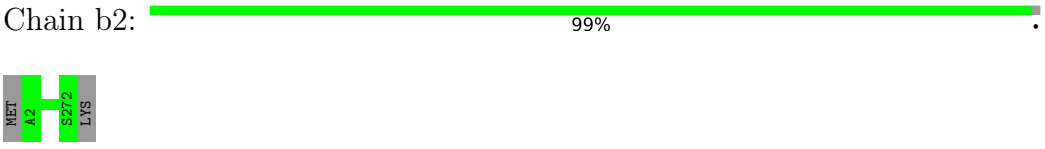
• Molecule 34: Large ribosomal subunit protein uL1

Chain a2:



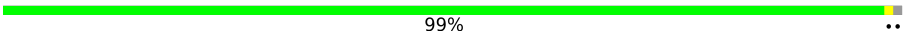
• Molecule 35: 50S ribosomal protein L2

Chain b2:



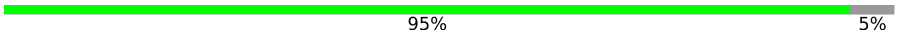
• Molecule 36: 50S ribosomal protein L5

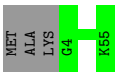
Chain e2:



• Molecule 37: 50S ribosomal protein L33

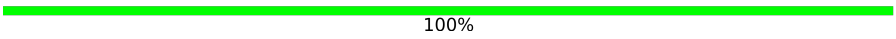
Chain g2:





• Molecule 38: 50S ribosomal protein L16

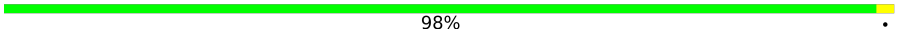
Chain h2:

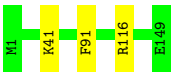


There are no outlier residues recorded for this chain.

• Molecule 39: 50S ribosomal protein L9

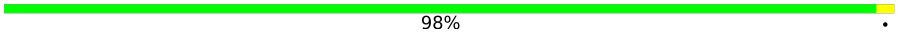
Chain i2:

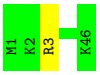




• Molecule 40: 50S ribosomal protein L34

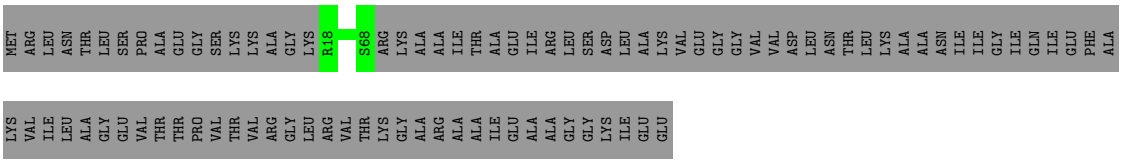
Chain l2:





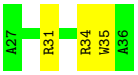
• Molecule 41: 50S ribosomal protein L15

Chain o2:



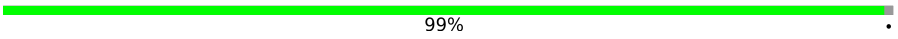
• Molecule 42: Nascent chain

Chain p:



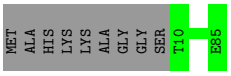
• Molecule 43: 50S ribosomal protein L18

Chain r2:



• Molecule 44: 50S ribosomal protein L27

Chain z2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10748	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: 6MZ, OMG, CM0, MG, 4SU, 3TD, 2MA, 1MG, H2U, OMU, MA6, MIA, PSU, PUT, SPD, UR3, 2MG, OMC, 4OC, ZN, G7M, 5MU, 5MC, 7MG

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	0.25	0/635	0.63	0/848
2	32	0.22	0/453	0.52	0/605
3	4	0.37	0/543	0.65	1/726 (0.1%)
3	41	0.25	0/120	0.60	0/158
4	62	0.24	0/513	0.56	0/676
5	71	0.16	0/429	0.69	0/664
5	72	0.18	1/69306 (0.0%)	0.70	12/108116 (0.0%)
6	82	0.18	0/2872	0.73	2/4478 (0.0%)
7	A1	0.24	0/36794	0.77	7/57392 (0.0%)
7	A2	0.24	0/36681	0.76	16/57217 (0.0%)
8	B	0.24	0/1846	0.53	0/2488
8	B2	0.25	0/1807	0.50	0/2435
9	C1	0.26	0/1692	0.55	0/2280
9	C2	0.29	0/1685	0.61	0/2270
10	D1	0.25	0/1665	0.53	0/2227
10	D2	0.25	0/1665	0.54	0/2227
11	E1	0.26	0/1179	0.52	0/1584
11	E2	0.26	0/1179	0.52	0/1584
12	F1	0.24	0/881	0.51	0/1189
12	F2	0.25	0/881	0.51	0/1189
13	G1	0.24	0/1246	0.53	0/1672
13	G2	0.28	0/1230	0.58	0/1649
14	H1	0.25	0/989	0.53	0/1326
14	H2	0.25	0/989	0.53	0/1326
15	I1	0.25	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.25	0/827	0.61	0/1117
16	J2	0.25	0/813	0.63	0/1100
17	K1	0.26	0/873	0.56	0/1180
17	K2	0.28	0/900	0.57	0/1215
18	L1	0.26	0/969	0.60	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
18	L2	0.26	0/969	0.61	0/1300
19	M1	0.25	0/900	0.57	0/1204
19	M2	0.24	0/919	0.58	0/1226
20	N1	0.26	0/817	0.60	0/1088
20	N2	0.25	0/817	0.57	0/1088
21	O1	0.23	0/722	0.55	0/964
21	O2	0.23	0/722	0.57	0/964
22	P1	0.25	0/659	0.60	0/884
23	Q1	0.27	0/657	0.58	0/881
23	Q2	0.25	0/657	0.58	0/881
24	R1	0.24	0/635	0.57	0/849
24	R2	0.25	0/637	0.62	0/851
25	S1	0.25	0/680	0.52	0/915
25	S2	0.26	0/680	0.53	0/915
26	T1	0.25	0/676	0.53	0/895
27	U1	0.26	0/598	0.61	0/792
27	U2	0.25	0/598	0.58	0/792
28	V2	0.32	0/1427	0.92	6/2224 (0.3%)
29	W	0.40	1/1604 (0.1%)	1.29	5/2496 (0.2%)
30	W1	0.28	0/677	0.89	0/1052
31	Y	0.35	1/1725 (0.1%)	0.79	2/2687 (0.1%)
32	Y1	0.20	0/786	0.79	0/1216
33	Z1	0.26	0/76	0.35	0/101
34	a2	0.24	0/1676	0.49	0/2259
35	b2	0.26	0/2121	0.59	0/2852
36	e2	0.25	0/1444	0.52	0/1937
37	g2	0.25	0/434	0.51	0/576
38	h2	0.25	0/1104	0.57	0/1474
39	i2	0.26	0/1122	0.55	0/1515
40	l2	0.24	0/380	0.63	0/498
41	o2	0.26	0/383	0.67	0/501
42	p	0.72	0/77	0.64	0/104
43	r2	0.25	0/901	0.59	0/1209
44	z2	0.26	0/589	0.54	0/779
All	All	0.23	3/202613 (0.0%)	0.71	51/304976 (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
1	12	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	1
9	C2	0	1
10	D1	0	2
10	D2	0	1
13	G2	0	3
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
34	a2	0	1
39	i2	0	1
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	1	G	OP3-P	-10.65	1.48	1.61
31	Y	1	G	OP3-P	-10.59	1.48	1.61
29	W	1	A	OP3-P	-10.58	1.48	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	W	43	G	O5'-P-OP2	-28.03	77.06	110.70
29	W	43	G	OP1-P-OP2	-27.59	78.22	119.60
29	W	43	G	O5'-P-OP1	15.97	129.86	110.70
29	W	42	G	OP1-P-O3'	-14.70	72.86	105.20
29	W	42	G	OP2-P-O3'	14.49	137.08	105.20

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	12	74	ARG	Sidechain
3	4	56	ARG	Sidechain
9	C2	42	TYR	Mainchain
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide

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%)	72 (96%)	3 (4%)	0	100 100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	8 42
3	4	66/70 (94%)	55 (83%)	11 (17%)	0	100 100
3	41	12/70 (17%)	10 (83%)	2 (17%)	0	100 100
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100 100
8	B	231/241 (96%)	193 (84%)	34 (15%)	4 (2%)	9 43
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100 100
9	C1	211/233 (91%)	185 (88%)	24 (11%)	2 (1%)	17 56
9	C2	210/233 (90%)	185 (88%)	25 (12%)	0	100 100
10	D1	203/206 (98%)	183 (90%)	19 (9%)	1 (0%)	29 68
10	D2	203/206 (98%)	200 (98%)	3 (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%)	80 (77%)	23 (22%)	1 (1%)	15 54
13	G1	153/179 (86%)	151 (99%)	2 (1%)	0	100 100
13	G2	152/179 (85%)	122 (80%)	24 (16%)	6 (4%)	3 26
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%)	117 (92%)	10 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J1	100/103 (97%)	92 (92%)	8 (8%)	0	100	100
16	J2	98/103 (95%)	86 (88%)	9 (9%)	3 (3%)	4	31
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	17	56
17	K2	116/129 (90%)	100 (86%)	15 (13%)	1 (1%)	17	56
18	L1	121/124 (98%)	115 (95%)	5 (4%)	1 (1%)	19	60
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%)	86 (88%)	12 (12%)	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%)	75 (94%)	5 (6%)	0	100	100
23	Q1	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
23	Q2	78/84 (93%)	75 (96%)	2 (3%)	1 (1%)	12	48
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	11	47
24	R2	72/75 (96%)	53 (74%)	18 (25%)	1 (1%)	11	47
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
25	S2	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	6	36
27	U1	68/71 (96%)	58 (85%)	10 (15%)	0	100	100
27	U2	68/71 (96%)	60 (88%)	8 (12%)	0	100	100
33	Z1	7/557 (1%)	7 (100%)	0	0	100	100
34	a2	221/234 (94%)	201 (91%)	15 (7%)	5 (2%)	6	37
35	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
36	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
37	g2	50/55 (91%)	50 (100%)	0	0	100	100
38	h2	135/136 (99%)	135 (100%)	0	0	100	100
39	i2	147/149 (99%)	120 (82%)	25 (17%)	2 (1%)	11	47
40	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
41	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	p	8/10 (80%)	7 (88%)	1 (12%)	0	100 100
43	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100 100
44	z2	74/85 (87%)	74 (100%)	0	0	100 100
All	All	6206/7310 (85%)	5715 (92%)	458 (7%)	33 (0%)	32 68

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
13	G2	18	PHE
13	G2	35	LYS
13	G2	146	GLU
23	Q2	12	VAL

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%)	66 (98%)	1 (2%)	65 80
2	32	48/49 (98%)	48 (100%)	0	100 100
3	4	60/62 (97%)	58 (97%)	2 (3%)	38 61
3	41	12/62 (19%)	12 (100%)	0	100 100
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%)	188 (100%)	1 (0%)	88 93
9	C1	173/190 (91%)	171 (99%)	2 (1%)	71 84
9	C2	172/190 (90%)	172 (100%)	0	100 100
10	D1	172/173 (99%)	172 (100%)	0	100 100
10	D2	172/173 (99%)	170 (99%)	2 (1%)	71 84
11	E1	120/126 (95%)	120 (100%)	0	100 100
11	E2	120/126 (95%)	120 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	F1	92/116 (79%)	92 (100%)	0	100	100
12	F2	92/116 (79%)	92 (100%)	0	100	100
13	G1	128/147 (87%)	128 (100%)	0	100	100
13	G2	127/147 (86%)	127 (100%)	0	100	100
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%)	106 (100%)	0	100	100
16	J1	89/90 (99%)	89 (100%)	0	100	100
16	J2	88/90 (98%)	88 (100%)	0	100	100
17	K1	88/99 (89%)	88 (100%)	0	100	100
17	K2	91/99 (92%)	90 (99%)	1 (1%)	73	85
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%)	83 (100%)	0	100	100
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%)	64 (100%)	0	100	100
24	R2	64/65 (98%)	63 (98%)	1 (2%)	62	79
25	S1	72/79 (91%)	72 (100%)	0	100	100
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	63 (97%)	2 (3%)	40	63
27	U1	60/61 (98%)	59 (98%)	1 (2%)	60	78
27	U2	60/61 (98%)	60 (100%)	0	100	100
33	Z1	8/461 (2%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	a2	174/181 (96%)	174 (100%)	0	100 100
35	b2	216/218 (99%)	216 (100%)	0	100 100
36	e2	149/150 (99%)	148 (99%)	1 (1%)	84 90
37	g2	47/49 (96%)	47 (100%)	0	100 100
38	h2	110/109 (101%)	110 (100%)	0	100 100
39	i2	114/114 (100%)	114 (100%)	0	100 100
40	l2	38/38 (100%)	37 (97%)	1 (3%)	46 67
41	o2	35/103 (34%)	35 (100%)	0	100 100
42	p	5/5 (100%)	2 (40%)	3 (60%)	0 0
43	r2	86/87 (99%)	86 (100%)	0	100 100
44	z2	58/63 (92%)	58 (100%)	0	100 100
All	All	5184/5994 (86%)	5166 (100%)	18 (0%)	92 95

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	l2	3	ARG
42	p	35	TRP
42	p	34	ARG
17	K2	13	ARG
36	e2	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
18	L2	29	GLN
35	b2	243	HIS
15	I1	75	GLN
15	I2	75	GLN
17	K1	40	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	58/59 (98%)	39 (67%)	8 (13%)
29	W	74/76 (97%)	28 (37%)	3 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	W1	31/76 (40%)	7 (22%)	2 (6%)
31	Y	75/76 (98%)	19 (25%)	2 (2%)
32	Y1	32/76 (42%)	5 (15%)	2 (6%)
5	71	17/2904 (0%)	1 (5%)	0
5	72	2899/2904 (99%)	458 (15%)	36 (1%)
6	82	119/120 (99%)	21 (17%)	3 (2%)
7	A1	1538/1542 (99%)	445 (28%)	36 (2%)
7	A2	1533/1542 (99%)	392 (25%)	30 (1%)
All	All	6376/9375 (68%)	1415 (22%)	122 (1%)

5 of 1415 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1907	G
5	72	10	A
5	72	15	G
5	72	34	U
5	72	44	A

5 of 122 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A1	686	U
28	V2	39	A
7	A1	1440	U
28	V2	37	A
31	Y	17	H2U

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

64 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PSU	72	955	5	18,21,22	4.68	8 (44%)	22,30,33	1.87	5 (22%)
29	4SU	W	8	29	18,21,22	3.81	7 (38%)	26,30,33	2.28	4 (15%)
31	H2U	Y	17	31	18,21,22	3.09	5 (27%)	21,30,33	2.02	5 (23%)
31	PSU	Y	55	31	18,21,22	5.79	14 (77%)	22,30,33	1.98	5 (22%)
5	5MU	72	747	5	19,22,23	0.27	0	28,32,35	0.58	0
5	5MC	72	1962	5	18,22,23	4.04	7 (38%)	26,32,35	1.05	2 (7%)
5	2MG	72	2445	5	18,26,27	2.85	7 (38%)	16,38,41	1.37	3 (18%)
29	G7M	W	46	29	20,26,27	2.81	7 (35%)	17,39,42	1.11	1 (5%)
31	5MU	Y	54	31	19,22,23	4.12	14 (73%)	28,32,35	3.97	12 (42%)
7	G7M	A2	527	7	20,26,27	6.09	12 (60%)	17,39,42	1.54	4 (23%)
7	2MG	A1	966	7	18,26,27	2.84	7 (38%)	16,38,41	1.41	4 (25%)
5	OMG	72	2251	31,5	18,26,27	2.84	7 (38%)	19,38,41	1.53	4 (21%)
5	OMC	72	2498	48,5	19,22,23	3.29	8 (42%)	26,31,34	0.75	0
5	PSU	72	2605	5	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
5	2MA	72	2503	48,5	17,25,26	2.65	5 (29%)	17,37,40	1.33	2 (11%)
5	G7M	72	2069	5	20,26,27	2.79	8 (40%)	17,39,42	1.03	1 (5%)
5	2MG	72	1835	5	18,26,27	2.84	7 (38%)	16,38,41	1.45	4 (25%)
32	6MZ	Y1	37	32	18,25,26	2.05	4 (22%)	16,36,39	2.44	4 (25%)
7	2MG	A1	1516	7	18,26,27	2.86	7 (38%)	16,38,41	1.35	3 (18%)
7	5MC	A1	1407	7	18,22,23	4.04	7 (38%)	26,32,35	0.96	2 (7%)
5	6MZ	72	1618	5	18,25,26	2.04	2 (11%)	16,36,39	2.27	4 (25%)
7	5MC	A2	1407	7	18,22,23	4.04	7 (38%)	26,32,35	0.96	2 (7%)
7	2MG	A2	966	7	18,26,27	2.84	7 (38%)	16,38,41	1.35	3 (18%)
29	5MU	W	54	29	19,22,23	4.11	14 (73%)	28,32,35	3.89	14 (50%)
30	PSU	W1	32	30	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
7	2MG	A2	1516	7	18,26,27	2.85	7 (38%)	16,38,41	1.36	3 (18%)
30	4SU	W1	8	30	18,21,22	3.80	7 (38%)	26,30,33	2.24	5 (19%)
29	MIA	W	37	29	24,31,32	2.28	3 (12%)	26,44,47	3.01	8 (30%)
7	2MG	A2	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.38	3 (18%)
5	5MU	72	1939	5	19,22,23	4.16	15 (78%)	28,32,35	4.12	12 (42%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
29	PSU	W	55	29	18,21,22	5.78	13 (72%)	22,30,33	2.12	5 (22%)
29	H2U	W	16	29	18,21,22	3.04	5 (27%)	21,30,33	1.99	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	5MC	A2	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.00	2 (7%)
5	PSU	72	2604	5	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)
7	5MC	A1	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.02	2 (7%)
31	G7M	Y	46	31	20,26,27	2.82	8 (40%)	17,39,42	1.10	1 (5%)
5	6MZ	72	2030	5	18,25,26	2.07	4 (22%)	16,36,39	2.33	3 (18%)
30	PSU	W1	39	30	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
7	UR3	A1	1498	7	19,22,23	2.77	8 (42%)	26,32,35	1.28	1 (3%)
7	MA6	A1	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.39	3 (15%)
7	MA6	A1	1519	7	18,26,27	1.07	2 (11%)	19,38,41	3.40	3 (15%)
30	G7M	W1	46	30	20,26,27	2.82	7 (35%)	17,39,42	1.13	1 (5%)
7	MA6	A2	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.37	3 (15%)
7	G7M	A1	527	7	20,26,27	2.80	8 (40%)	17,39,42	1.02	1 (5%)
32	CM0	Y1	34	32	23,26,27	3.74	6 (26%)	27,37,40	1.60	3 (11%)
5	3TD	72	1915	5	19,22,23	0.83	1 (5%)	21,32,35	0.70	0
5	3TD	71	1915	5	19,22,23	4.07	7 (36%)	21,32,35	1.75	3 (14%)
29	H2U	W	20	29	18,21,22	3.06	5 (27%)	21,30,33	2.03	5 (23%)
7	2MG	A1	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.32	3 (18%)
30	MIA	W1	37	30	24,31,32	2.34	3 (12%)	26,44,47	2.74	7 (26%)
5	H2U	72	2449	48,5	18,21,22	3.05	5 (27%)	21,30,33	2.05	5 (23%)
5	PSU	72	746	5	18,21,22	0.91	1 (5%)	22,30,33	0.61	0
32	7MG	Y1	46	32	22,26,27	3.89	10 (45%)	29,39,42	2.03	9 (31%)
7	MA6	A2	1519	7	18,26,27	1.06	2 (11%)	19,38,41	3.38	3 (15%)
7	4OC	A1	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.89	1 (3%)
7	UR3	A2	1498	7	19,22,23	2.78	8 (42%)	26,32,35	1.33	3 (11%)
5	1MG	72	745	5	18,26,27	2.74	6 (33%)	19,39,42	1.45	3 (15%)
5	PSU	72	2504	48,5	18,21,22	4.69	8 (44%)	22,30,33	1.85	5 (22%)
5	PSU	72	2580	5	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
29	PSU	W	32	29	18,21,22	4.66	8 (44%)	22,30,33	1.88	5 (22%)
5	PSU	72	2457	5	18,21,22	4.65	8 (44%)	22,30,33	1.89	5 (22%)
7	4OC	A2	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.91	1 (3%)
29	H2U	W	17	29	18,21,22	3.06	5 (27%)	21,30,33	2.02	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
29	4SU	W	8	29	-	0/7/25/26	0/2/2/2
31	H2U	Y	17	31	-	7/7/38/39	0/2/2/2
31	PSU	Y	55	31	-	2/7/25/26	0/2/2/2
5	5MU	72	747	5	-	1/7/25/26	0/2/2/2
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
29	G7M	W	46	29	-	1/3/25/26	0/3/3/3
31	5MU	Y	54	31	-	0/7/25/26	0/2/2/2
7	G7M	A2	527	7	-	2/3/25/26	0/3/3/3
7	2MG	A1	966	7	-	0/5/27/28	0/3/3/3
5	OMG	72	2251	31,5	-	3/5/27/28	0/3/3/3
5	OMC	72	2498	48,5	-	2/9/27/28	0/2/2/2
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
5	2MA	72	2503	48,5	-	0/3/25/26	0/3/3/3
5	G7M	72	2069	5	-	2/3/25/26	0/3/3/3
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
29	MIA	W	37	29	-	6/11/33/34	0/3/3/3
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
5	5MU	72	1939	5	-	2/7/25/26	0/2/2/2
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
29	PSU	W	55	29	-	1/7/25/26	0/2/2/2
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
7	5MC	A1	967	7	-	0/7/25/26	0/2/2/2
31	G7M	Y	46	31	-	2/3/25/26	0/3/3/3
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MA6	A1	1518	7	-	3/7/29/30	0/3/3/3
7	MA6	A1	1519	7	-	4/7/29/30	0/3/3/3
30	G7M	W1	46	30	-	2/3/25/26	0/3/3/3
7	MA6	A2	1518	7	-	0/7/29/30	0/3/3/3
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3
32	CM0	Y1	34	32	-	4/12/30/31	0/2/2/2
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
29	H2U	W	20	29	-	3/7/38/39	0/2/2/2
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
30	MIA	W1	37	30	-	6/11/33/34	0/3/3/3
5	H2U	72	2449	48,5	-	0/7/38/39	0/2/2/2
5	PSU	72	746	5	-	4/7/25/26	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
7	4OC	A1	1402	7	-	1/9/29/30	0/2/2/2
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
5	PSU	72	2504	48,5	-	0/7/25/26	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
29	PSU	W	32	29	-	3/7/25/26	0/2/2/2
5	PSU	72	2457	5	-	0/7/25/26	0/2/2/2
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
29	H2U	W	17	29	-	2/7/38/39	0/2/2/2

The worst 5 of 437 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	527	G7M	C2'-C1'	-18.04	1.26	1.53
32	Y1	34	CM0	C6-C5	12.73	1.48	1.34
5	71	1915	3TD	C6-C5	12.65	1.50	1.35
5	72	955	PSU	C6-C5	12.25	1.49	1.35
5	72	2504	PSU	C6-C5	12.20	1.49	1.35

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A1	1519	MA6	N1-C6-N6	-12.36	104.05	117.06
7	A2	1519	MA6	N1-C6-N6	-12.35	104.06	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A1	1518	MA6	N1-C6-N6	-12.22	104.19	117.06
7	A2	1518	MA6	N1-C6-N6	-12.12	104.30	117.06
29	W	37	MIA	C11-S10-C2	11.00	110.48	102.27

There are no chirality outliers.

5 of 91 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	A2	527	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 274 ligands modelled in this entry, 271 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
46	PUT	72	3002	-	5,5,5	0.25	0	4,4,4	0.54	0
47	SPD	72	3003	-	9,9,9	0.33	0	8,8,8	0.88	0
46	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
46	PUT	72	3002	-	-	0/3/3/3	-
47	SPD	72	3003	-	-	0/7/7/7	-
46	PUT	72	3001	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19058. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.