



Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 11:23 AM JST

PDB ID : 8Y38
EMDB ID : EMD-38875
Title : Cryo-EM structure of Staphylococcus aureus 70S ribosome (strain 15B196) in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 2.58 Å(reported)

This is a Full wwPDB EM Validation 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

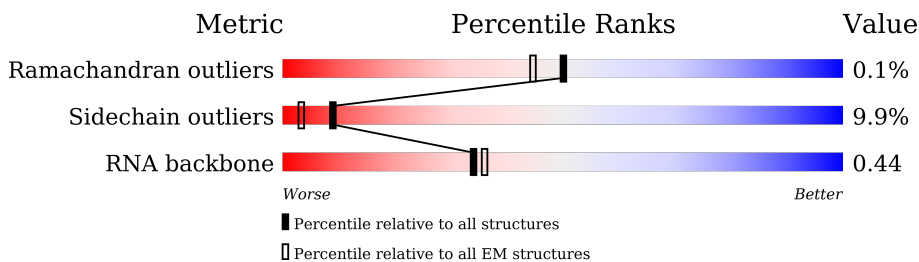
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 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.















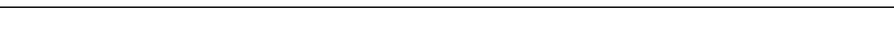

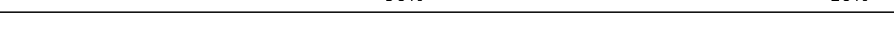

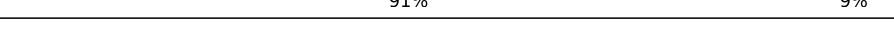



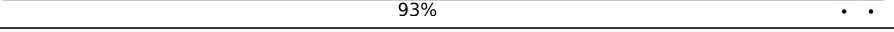
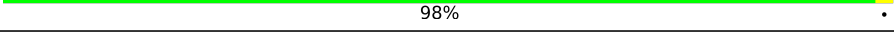



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	47	
2	2	43	
3	3	64	
4	4	37	
5	A	2921	
6	B	115	
7	C	274	
8	D	215	
9	E	206	




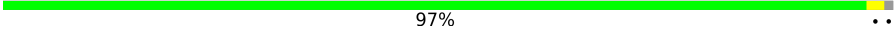





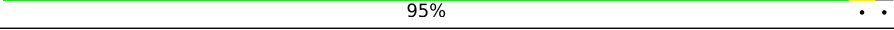
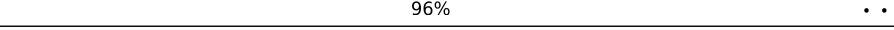
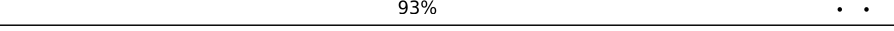

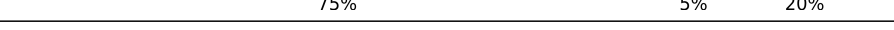

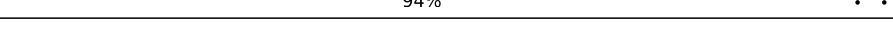
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Mol	Chain	Length	Quality of chain
10	F	175	
11	G	175	
12	H	145	
13	I	122	
14	J	146	
15	K	137	
16	L	120	
17	M	119	
18	N	114	
19	O	116	
20	P	102	
21	Q	117	
22	R	89	
23	S	103	
24	T	94	
25	U	82	
26	V	58	
27	W	67	
28	X	58	
29	Y	59	
30	Z	48	
31	a	1548	
32	b	232	
33	c	217	
34	d	200	

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Mol	Chain	Length	Quality of chain
35	e	166	 91% . 6%
36	f	98	 90% 7% .
37	g	156	 90% 10% .
38	h	132	 97% ..
39	i	130	 95% ..
40	j	102	 89% 6% 5%
41	k	129	 84% . 12%
42	l	149	 85% 5% . 9%
43	m	121	 90% 6% .
44	n	61	 95% ..
45	o	89	 96% ..
46	p	91	 93% . .
47	q	87	 83% 9% 8%
48	r	80	 75% 5% 20%
49	s	108	 70% 6% 24%
50	t	83	 94% . .

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 138224 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 Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2885	Total	C	N	O	P	0	0
			61861	27621	11312	20043	2885		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	274	Total	C	N	O	S	0	0
			2090	1301	415	369	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1317	835	223	253	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	175	Total	C	N	O	S	0	0
			1259	788	239	229	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			891	557	174	159	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O		0	0
			889	563	175	151			

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	112	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total	C	N	O		0	0
			711	456	127	128			

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	82	Total	C	N	O		0	0
			615	380	121	114			

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	58	Total	C	N	O		0	0
			445	277	96	72			

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	67	Total	C	N	O		0	0
			541	333	102	106			

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 29 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Y	57	Total	C	N	O	0	0
			353	214	65	74		

- Molecule 30 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	48	Total	C	N	O	S	0	0
			361	222	77	59	3		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1479	Total	C	N	O	P	0	0
			31706	14154	5809	10264	1479		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1032	N	C	conflict	GB 1747281577

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	224	Total	C	N	O	S	0	0
			1802	1149	314	332	7		

- Molecule 33 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	199	Total	C	N	O	S	0	0
			1616	1020	302	292	2		

- Molecule 35 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	156	Total	C	N	O	S	0	0
			1160	731	212	215	2		

- Molecule 36 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			789	498	138	150	3		

- Molecule 37 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	155	Total	C	N	O	S	0	0
			1242	775	239	224	4		

- Molecule 38 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1031	652	183	192	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O	S	0	0
			1007	624	201	181	1		

- Molecule 40 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	97	Total	C	N	O	S	0	0
			773	488	141	143	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	114	Total	C	N	O	S	0	0
			844	520	160	161	3		

- Molecule 42 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 43 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	116	Total	C	N	O	S	0	0
			922	566	183	172	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 45 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	87	Total	C	N	O	S	0	0
			726	448	149	128	1		

- Molecule 46 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	87	Total	C	N	O	S	0	0
			688	433	127	127	1		

- Molecule 47 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			657	416	117	123	1		

- Molecule 48 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	64	Total	C	N	O	S	0	0
			525	336	98	88	3		

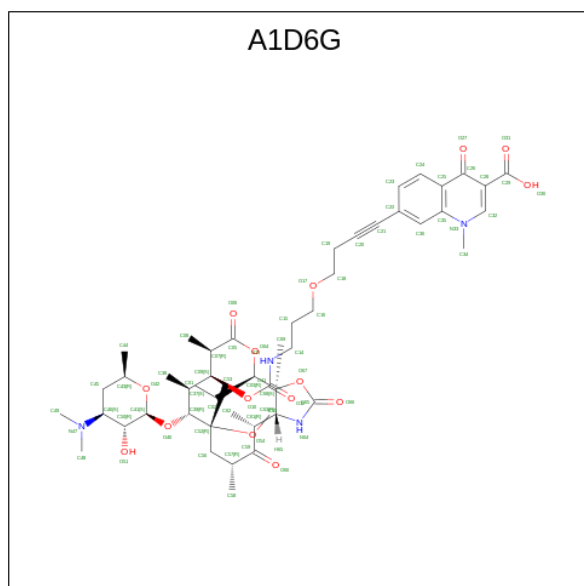
- Molecule 49 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			665	427	121	115	2		

- Molecule 50 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total	C	N	O	S	0	0
			611	370	120	119	2		

- Molecule 51 is 7-[4-[3-[(1 {S},2 {R},5 {R},6 {S},7 {S},8 {R},9 {R},11 {R},13 {R},14 {R})-8-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-9-methoxy-1,5,7,9,11,13-hexamethyl-4,12,16-tris(oxidanylidene)-3,17-dioxo-15-azabicyclo [12.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quinoline-3-carboxylic acid (three-letter code: A1D6G) (formula: C₅₀H₇₂N₄O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
51	A	1	Total	C	N	O	0
			69	50	4	15	

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	A	12	Total	Mg	0
			12	12	


- Molecule 53 is water.

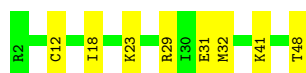
Mol	Chain	Residues	Atoms		AltConf
53	A	4	Total	O	0
			4	4	

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.

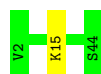
- Molecule 1: Large ribosomal subunit protein bL33B

Chain 1:  83% 17%



- Molecule 2: Large ribosomal subunit protein bL34

Chain 2:  98%




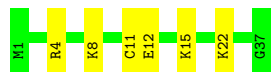
- Molecule 3: Large ribosomal subunit protein bL35

Chain 3:  89% 11%



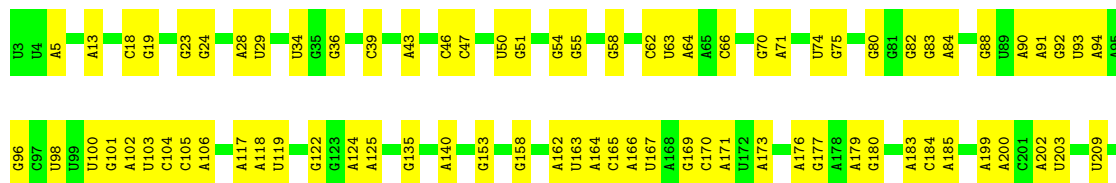
- Molecule 4: Large ribosomal subunit protein bL36

Chain 4:  84% 16%

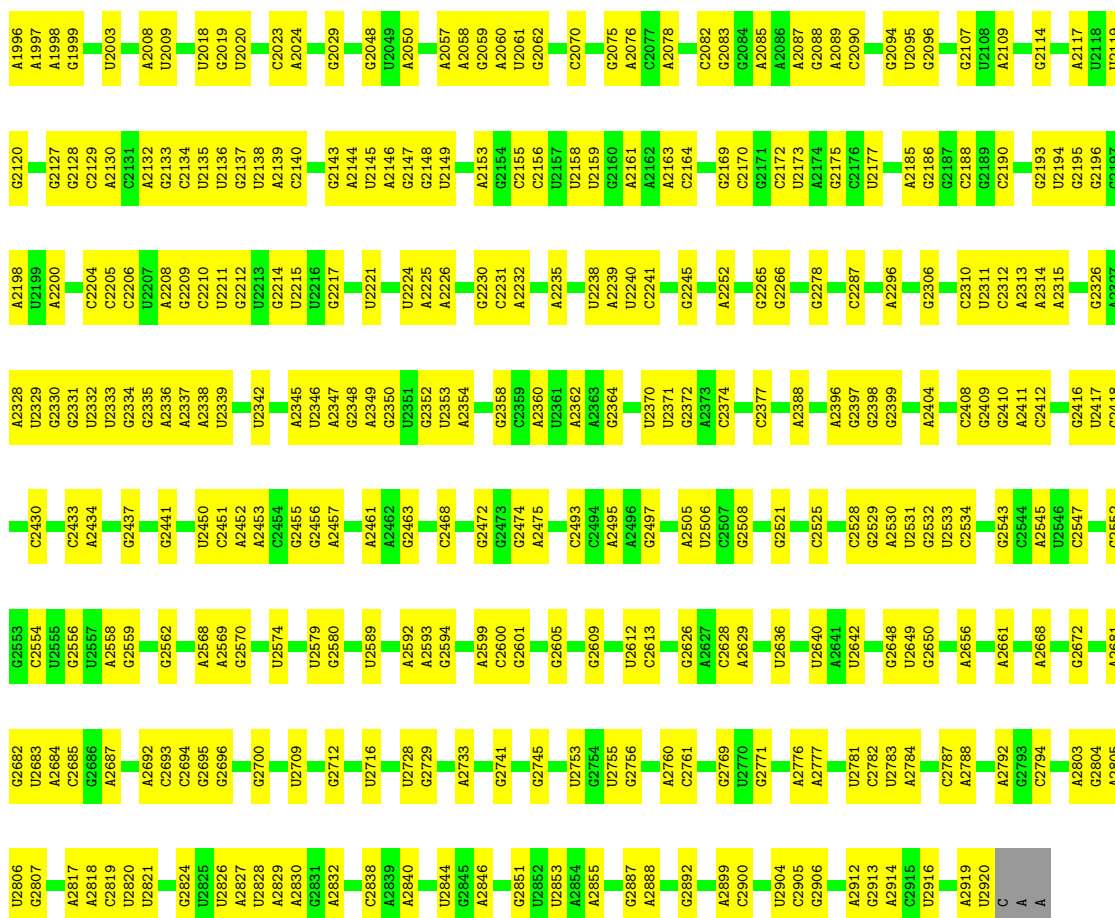


- Molecule 5: 23S ribosomal RNA

Chain A:  66% 33%

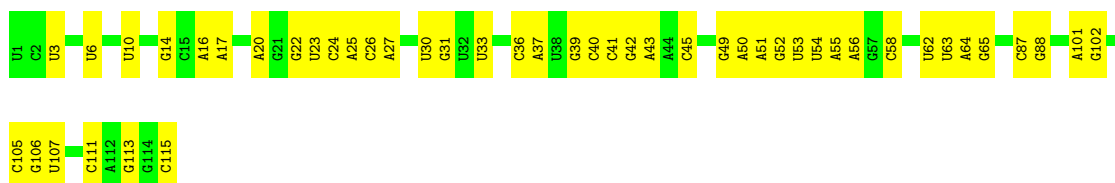






• Molecule 6: 5S ribosomal RNA

Chain B: 59% 41%



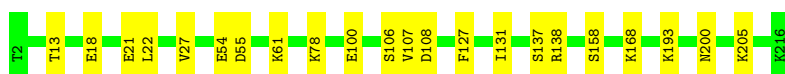
• Molecule 7: Large ribosomal subunit protein uL2

Chain C: 93% 7%



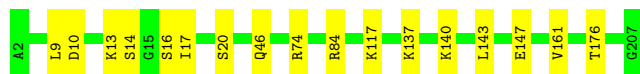
• Molecule 8: Large ribosomal subunit protein uL3

Chain D: 90% 10%




- Molecule 9: Large ribosomal subunit protein uL4

Chain E:  92% 8%




- Molecule 10: Large ribosomal subunit protein uL5

Chain F:  78% 22%



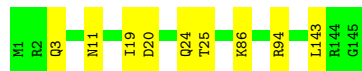
- Molecule 11: Large ribosomal subunit protein uL6

Chain G:  85% 15%




- Molecule 12: Large ribosomal subunit protein uL13

Chain H:  94% 6%



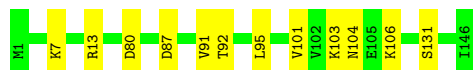
- Molecule 13: Large ribosomal subunit protein uL14

Chain I:  88% 11%




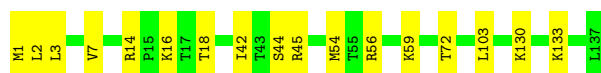
- Molecule 14: Large ribosomal subunit protein uL15

Chain J:  92% 8%



- Molecule 15: Large ribosomal subunit protein uL16

Chain K:  88% 12%



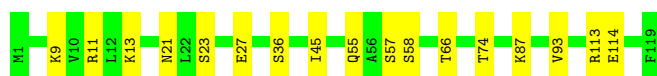
- Molecule 16: Large ribosomal subunit protein bL17

Chain L: 97%



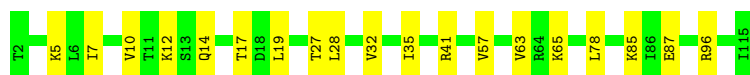
- Molecule 17: Large ribosomal subunit protein uL18

Chain M: 86%



- Molecule 18: Large ribosomal subunit protein bL19

Chain N: 83%



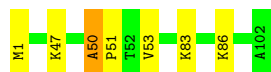
- Molecule 19: Large ribosomal subunit protein bL20

Chain O: 93%



- Molecule 20: Large ribosomal subunit protein bL21

Chain P: 93%



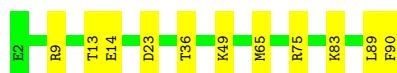
- Molecule 21: Large ribosomal subunit protein uL22

Chain Q: 88%

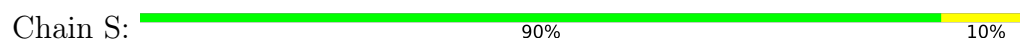


- Molecule 22: Large ribosomal subunit protein uL23

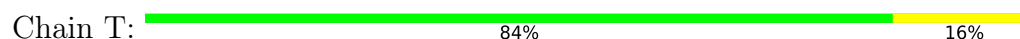
Chain R: 88%



- Molecule 23: Large ribosomal subunit protein uL24



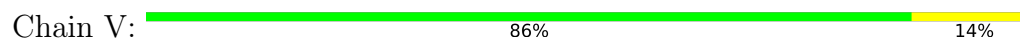
- Molecule 24: Large ribosomal subunit protein bL25



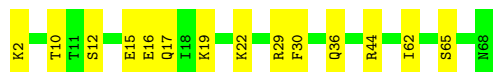
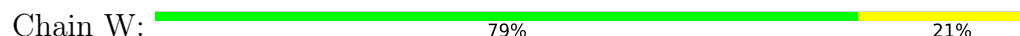
- Molecule 25: Large ribosomal subunit protein bL27



- Molecule 26: Large ribosomal subunit protein bL28



- Molecule 27: Large ribosomal subunit protein uL29

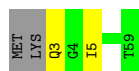


- Molecule 28: Large ribosomal subunit protein uL30



- Molecule 29: Large ribosomal subunit protein bL31B





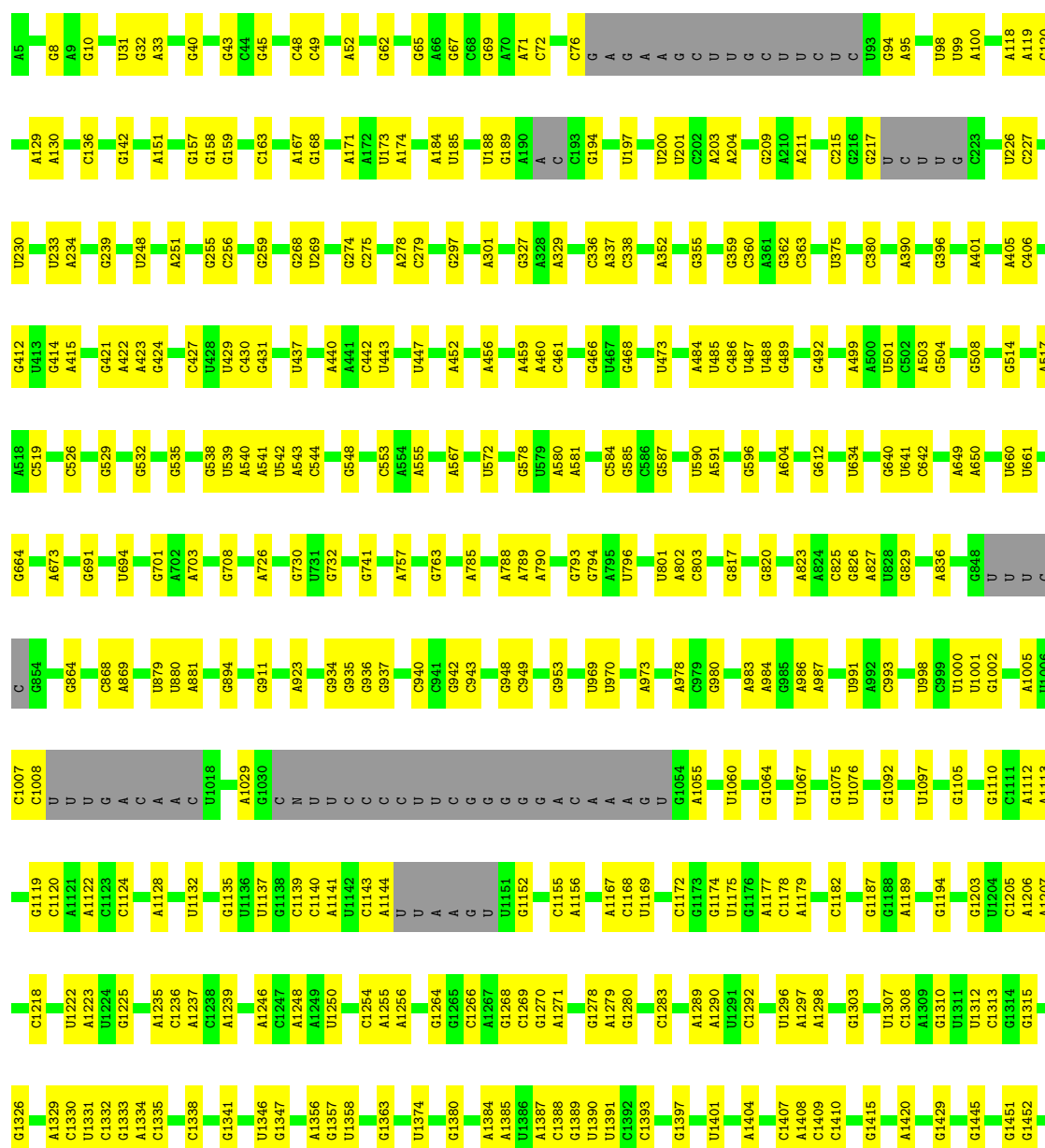
- Molecule 30: Large ribosomal subunit protein bL32

Chain Z: 98% .



- Molecule 31: 16S ribosomal RNA

Chain a: 71% 25% .





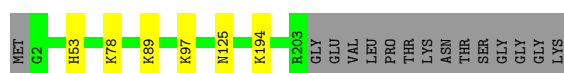
- Molecule 32: Small ribosomal subunit protein uS2

Chain b: 91% 5% .



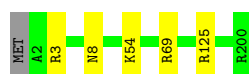
- Molecule 33: Small ribosomal subunit protein uS3

Chain c: 90% . 7%



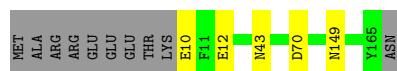
- Molecule 34: Small ribosomal subunit protein uS4

Chain d: 97% .



- Molecule 35: Small ribosomal subunit protein uS5

Chain e: 91% . 6%



- Molecule 36: Small ribosomal subunit protein bS6

Chain f: 90% 7% .



- Molecule 37: Small ribosomal subunit protein uS7

Chain g: 90% 10% .



- Molecule 38: Small ribosomal subunit protein uS8

Chain h: 97% ..



- Molecule 39: Small ribosomal subunit protein uS9

Chain i: 95% ..



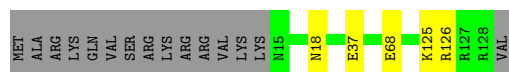
- Molecule 40: Small ribosomal subunit protein uS10

Chain j: 89% 6% 5%



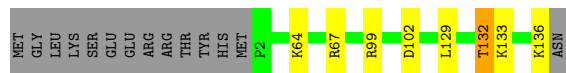
- Molecule 41: Small ribosomal subunit protein uS11

Chain k: 84% . 12%



- Molecule 42: Small ribosomal subunit protein uS12

Chain l: 85% 5% . 9%



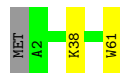
- Molecule 43: Small ribosomal subunit protein uS13

Chain m: 90% 6% .



- Molecule 44: Small ribosomal subunit protein uS14B

Chain n: 95% ..



- Molecule 45: Small ribosomal subunit protein uS15

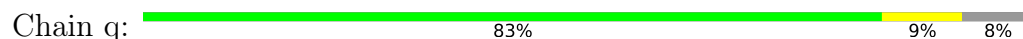
Chain o: 96% ..



- Molecule 46: Small ribosomal subunit protein bS16



- Molecule 47: Small ribosomal subunit protein uS17



- Molecule 48: Small ribosomal subunit protein bS18



- Molecule 49: Small ribosomal subunit protein uS19



- Molecule 50: Small ribosomal subunit protein bS20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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: 2MG, A1D6G, 5MU, MA6, 2MA, MG, OMG

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	1	0.60	0/395	0.85	0/530
2	2	0.44	0/371	0.71	0/484
3	3	0.61	0/526	0.81	0/690
4	4	0.73	0/299	0.91	0/393
5	A	0.52	0/69122	0.80	1/107793 (0.0%)
6	B	0.35	0/2733	0.71	0/4257
7	C	0.65	0/2125	0.87	0/2853
8	D	0.71	0/1651	0.83	0/2215
9	E	0.66	0/1595	0.76	0/2154
10	F	0.46	0/1332	0.79	0/1798
11	G	0.59	0/1277	0.78	0/1731
12	H	0.51	0/1165	0.71	0/1570
13	I	0.65	0/925	0.81	0/1242
14	J	0.46	0/1100	0.69	0/1467
15	K	0.64	0/1095	0.76	0/1472
16	L	0.46	0/936	0.69	0/1253
17	M	0.59	0/900	0.77	0/1205
18	N	0.59	0/901	0.76	0/1209
19	O	0.43	0/954	0.64	0/1264
20	P	0.51	0/800	0.72	1/1070 (0.1%)
21	Q	0.61	0/861	0.78	0/1161
22	R	0.53	0/723	0.71	0/966
23	S	0.48	0/779	0.73	0/1043
24	T	0.45	0/719	0.66	0/969
25	U	0.55	0/621	0.76	0/825
26	V	0.71	0/451	0.85	0/603
27	W	0.52	0/542	0.70	0/722
28	X	0.51	0/451	0.62	0/606
29	Y	0.37	0/361	0.67	0/500
30	Z	0.58	0/367	0.81	0/490
31	a	0.24	0/35498	0.83	0/55345
32	b	0.26	0/1829	0.53	0/2455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.23	0/1618	0.50	0/2173
34	d	0.25	0/1646	0.49	0/2211
35	e	0.28	0/1174	0.53	0/1584
36	f	0.27	0/800	0.57	0/1073
37	g	0.24	0/1262	0.51	0/1698
38	h	0.27	0/1043	0.50	0/1401
39	i	0.25	0/1023	0.59	0/1374
40	j	0.25	0/785	0.51	0/1060
41	k	0.29	0/859	0.57	0/1161
42	l	0.27	0/1075	0.57	0/1439
43	m	0.24	0/929	0.59	0/1246
44	n	0.25	0/511	0.53	0/678
45	o	0.23	0/735	0.52	0/982
46	p	0.27	0/699	0.53	0/942
47	q	0.29	0/665	0.57	0/889
48	r	0.29	0/534	0.63	0/715
49	s	0.26	0/683	0.55	0/916
50	t	0.23	0/611	0.46	0/817
All	All	0.45	0/150056	0.78	2/224694 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1555	G	C3'-C2'-C1'	-5.28	97.28	101.50
20	P	50	ALA	C-N-CD	5.13	139.18	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100
2	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
3	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
4	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
7	C	272/274 (99%)	245 (90%)	26 (10%)	1 (0%)	30	50
8	D	213/215 (99%)	200 (94%)	13 (6%)	0	100	100
9	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
10	F	173/175 (99%)	144 (83%)	28 (16%)	1 (1%)	22	41
11	G	173/175 (99%)	157 (91%)	16 (9%)	0	100	100
12	H	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
13	I	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	33
14	J	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
15	K	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	L	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
17	M	117/119 (98%)	107 (92%)	10 (8%)	0	100	100
18	N	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
19	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
20	P	100/102 (98%)	93 (93%)	5 (5%)	2 (2%)	6	11
21	Q	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
22	R	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
23	S	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
24	T	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
25	U	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
26	V	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
27	W	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
28	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
29	Y	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
30	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
32	b	222/232 (96%)	212 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	c	200/217 (92%)	190 (95%)	10 (5%)	0	100	100
34	d	197/200 (98%)	187 (95%)	10 (5%)	0	100	100
35	e	154/166 (93%)	149 (97%)	5 (3%)	0	100	100
36	f	93/98 (95%)	87 (94%)	6 (6%)	0	100	100
37	g	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	h	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
39	i	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
40	j	95/102 (93%)	89 (94%)	6 (6%)	0	100	100
41	k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
42	l	133/149 (89%)	122 (92%)	10 (8%)	1 (1%)	16	33
43	m	114/121 (94%)	105 (92%)	9 (8%)	0	100	100
44	n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	o	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
46	p	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
47	q	78/87 (90%)	74 (95%)	4 (5%)	0	100	100
48	r	62/80 (78%)	60 (97%)	2 (3%)	0	100	100
49	s	80/108 (74%)	73 (91%)	7 (9%)	0	100	100
50	t	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
All	All	5323/5563 (96%)	4979 (94%)	338 (6%)	6 (0%)	50	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	P	51	PRO
13	I	98	ILE
10	F	139	PRO
20	P	50	ALA
42	l	132	THR
7	C	271	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	44/45 (98%)	36 (82%)	8 (18%)	1	2
2	2	39/39 (100%)	38 (97%)	1 (3%)	41	65
3	3	55/55 (100%)	48 (87%)	7 (13%)	3	6
4	4	35/35 (100%)	29 (83%)	6 (17%)	1	2
7	C	220/221 (100%)	202 (92%)	18 (8%)	9	19
8	D	173/173 (100%)	151 (87%)	22 (13%)	3	6
9	E	168/168 (100%)	151 (90%)	17 (10%)	6	11
10	F	139/154 (90%)	102 (73%)	37 (27%)	0	0
11	G	123/153 (80%)	96 (78%)	27 (22%)	1	1
12	H	122/123 (99%)	113 (93%)	9 (7%)	11	23
13	I	100/100 (100%)	85 (85%)	15 (15%)	2	4
14	J	109/112 (97%)	97 (89%)	12 (11%)	5	9
15	K	108/114 (95%)	91 (84%)	17 (16%)	2	3
16	L	96/101 (95%)	92 (96%)	4 (4%)	25	48
17	M	86/95 (90%)	69 (80%)	17 (20%)	1	1
18	N	93/100 (93%)	74 (80%)	19 (20%)	1	1
19	O	96/96 (100%)	88 (92%)	8 (8%)	9	18
20	P	84/86 (98%)	79 (94%)	5 (6%)	16	33
21	Q	89/94 (95%)	80 (90%)	9 (10%)	6	11
22	R	78/80 (98%)	67 (86%)	11 (14%)	3	5
23	S	81/88 (92%)	71 (88%)	10 (12%)	4	7
24	T	75/82 (92%)	60 (80%)	15 (20%)	1	1
25	U	60/64 (94%)	53 (88%)	7 (12%)	4	8
26	V	44/49 (90%)	36 (82%)	8 (18%)	1	2
27	W	58/60 (97%)	44 (76%)	14 (24%)	0	1
28	X	52/52 (100%)	47 (90%)	5 (10%)	7	13
29	Y	21/56 (38%)	19 (90%)	2 (10%)	7	13
30	Z	36/44 (82%)	35 (97%)	1 (3%)	38	63
32	b	194/201 (96%)	182 (94%)	12 (6%)	15	31
33	c	164/175 (94%)	158 (96%)	6 (4%)	29	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	d	174/175 (99%)	169 (97%)	5 (3%)	37	62
35	e	122/131 (93%)	117 (96%)	5 (4%)	26	49
36	f	83/86 (96%)	76 (92%)	7 (8%)	9	18
37	g	131/132 (99%)	116 (88%)	15 (12%)	4	8
38	h	112/113 (99%)	109 (97%)	3 (3%)	40	64
39	i	105/107 (98%)	101 (96%)	4 (4%)	28	52
40	j	87/91 (96%)	81 (93%)	6 (7%)	13	26
41	k	90/104 (86%)	85 (94%)	5 (6%)	17	36
42	l	117/130 (90%)	109 (93%)	8 (7%)	13	27
43	m	100/104 (96%)	93 (93%)	7 (7%)	12	25
44	n	52/53 (98%)	50 (96%)	2 (4%)	28	52
45	o	79/81 (98%)	77 (98%)	2 (2%)	42	66
46	p	74/77 (96%)	72 (97%)	2 (3%)	40	64
47	q	75/82 (92%)	67 (89%)	8 (11%)	5	10
48	r	57/68 (84%)	53 (93%)	4 (7%)	12	25
49	s	71/91 (78%)	65 (92%)	6 (8%)	8	17
50	t	67/69 (97%)	64 (96%)	3 (4%)	23	45
All	All	4438/4709 (94%)	3997 (90%)	441 (10%)	9	12

All (441) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	12	CYS
1	1	18	ILE
1	1	23	LYS
1	1	29	ARG
1	1	31	GLU
1	1	32	MET
1	1	41	LYS
1	1	48	THR
2	2	15	LYS
3	3	31	HIS
3	3	52	LYS
3	3	53	SER
3	3	56	LYS
3	3	60	GLN

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Mol	Chain	Res	Type
3	3	62	LEU
3	3	65	LYS
4	4	4	ARG
4	4	8	LYS
4	4	11	CYS
4	4	12	GLU
4	4	15	LYS
4	4	22	LYS
7	C	3	ILE
7	C	4	LYS
7	C	65	ILE
7	C	68	LYS
7	C	71	LYS
7	C	75	ASN
7	C	87	ARG
7	C	115	ILE
7	C	116	VAL
7	C	123	ASP
7	C	125	LYS
7	C	134	ASN
7	C	136	PRO
7	C	243	ARG
7	C	245	SER
7	C	265	SER
7	C	267	ASP
7	C	272	ARG
8	D	13	THR
8	D	18	GLU
8	D	21	GLU
8	D	22	LEU
8	D	27	VAL
8	D	54	GLU
8	D	55	ASP
8	D	61	LYS
8	D	78	LYS
8	D	100	GLU
8	D	106	SER
8	D	107	VAL
8	D	108	ASP
8	D	127	PHE
8	D	131	ILE
8	D	137	SER

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Mol	Chain	Res	Type
8	D	138	ARG
8	D	158	SER
8	D	168	LYS
8	D	193	LYS
8	D	200	ASN
8	D	205	LYS
9	E	9	LEU
9	E	10	ASP
9	E	13	LYS
9	E	14	SER
9	E	16	SER
9	E	17	ILE
9	E	20	SER
9	E	46	GLN
9	E	74	ARG
9	E	84	ARG
9	E	117	LYS
9	E	137	LYS
9	E	140	LYS
9	E	143	LEU
9	E	147	GLU
9	E	161	VAL
9	E	176	THR
10	F	5	LYS
10	F	6	GLU
10	F	16	LEU
10	F	17	MET
10	F	23	SER
10	F	24	SER
10	F	25	VAL
10	F	27	GLU
10	F	38	MET
10	F	45	GLN
10	F	51	ASP
10	F	56	GLU
10	F	59	LEU
10	F	60	ILE
10	F	64	LYS
10	F	66	LEU
10	F	67	VAL
10	F	72	LYS
10	F	78	ARG

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Mol	Chain	Res	Type
10	F	85	ILE
10	F	88	LYS
10	F	95	ARG
10	F	110	ARG
10	F	120	LYS
10	F	128	TYR
10	F	133	LYS
10	F	135	GLN
10	F	136	LEU
10	F	138	PHE
10	F	143	TYR
10	F	148	LYS
10	F	149	VAL
10	F	150	ARG
10	F	152	MET
10	F	154	ILE
10	F	156	ILE
10	F	168	GLU
11	G	25	THR
11	G	35	ARG
11	G	39	GLU
11	G	42	THR
11	G	45	GLN
11	G	49	THR
11	G	53	VAL
11	G	54	ARG
11	G	57	ASP
11	G	58	SER
11	G	59	LYS
11	G	68	THR
11	G	69	ARG
11	G	77	GLN
11	G	79	VAL
11	G	81	GLN
11	G	84	VAL
11	G	85	LYS
11	G	97	GLN
11	G	98	MET
11	G	99	GLN
11	G	107	VAL
11	G	109	TYR
11	G	121	ILE

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Mol	Chain	Res	Type
11	G	122	THR
11	G	124	SER
11	G	175	LYS
12	H	3	GLN
12	H	11	ASN
12	H	19	ILE
12	H	20	ASP
12	H	24	GLN
12	H	25	THR
12	H	86	LYS
12	H	94	ARG
12	H	143	LEU
13	I	3	GLN
13	I	14	SER
13	I	34	ASN
13	I	64	ARG
13	I	66	LYS
13	I	67	SER
13	I	69	VAL
13	I	70	ARG
13	I	71	ARG
13	I	73	ASP
13	I	81	GLU
13	I	98	ILE
13	I	102	VAL
13	I	120	GLU
13	I	122	LEU
14	J	7	LYS
14	J	13	ARG
14	J	80	ASP
14	J	87	ASP
14	J	91	VAL
14	J	92	THR
14	J	95	LEU
14	J	101	VAL
14	J	103	LYS
14	J	104	ASN
14	J	106	LYS
14	J	131	SER
15	K	1	MET
15	K	2	LEU
15	K	3	LEU

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Mol	Chain	Res	Type
15	K	7	VAL
15	K	14	ARG
15	K	16	LYS
15	K	18	THR
15	K	42	ILE
15	K	44	SER
15	K	45	ARG
15	K	54	MET
15	K	56	ARG
15	K	59	LYS
15	K	72	THR
15	K	103	LEU
15	K	130	LYS
15	K	133	LYS
16	L	29	ARG
16	L	59	ARG
16	L	79	GLN
16	L	102	ARG
17	M	9	LYS
17	M	11	ARG
17	M	13	LYS
17	M	21	ASN
17	M	23	SER
17	M	27	GLU
17	M	36	SER
17	M	45	ILE
17	M	55	GLN
17	M	57	SER
17	M	58	SER
17	M	66	THR
17	M	74	THR
17	M	87	LYS
17	M	93	VAL
17	M	113	ARG
17	M	114	GLU
18	N	5	LYS
18	N	7	ILE
18	N	10	VAL
18	N	12	LYS
18	N	14	GLN
18	N	17	THR
18	N	19	LEU

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Mol	Chain	Res	Type
18	N	27	THR
18	N	28	LEU
18	N	32	VAL
18	N	35	ILE
18	N	41	ARG
18	N	57	VAL
18	N	63	VAL
18	N	65	LYS
18	N	78	LEU
18	N	85	LYS
18	N	87	GLU
18	N	96	ARG
19	O	8	THR
19	O	9	VAL
19	O	51	ARG
19	O	59	LYS
19	O	78	ARG
19	O	89	ASP
19	O	96	SER
19	O	117	LEU
20	P	1	MET
20	P	47	LYS
20	P	53	VAL
20	P	83	LYS
20	P	86	LYS
21	Q	9	THR
21	Q	38	LEU
21	Q	43	SER
21	Q	51	LEU
21	Q	52	MET
21	Q	65	ASN
21	Q	67	ASP
21	Q	81	THR
21	Q	86	ARG
22	R	9	ARG
22	R	13	THR
22	R	14	GLU
22	R	23	ASP
22	R	36	THR
22	R	49	LYS
22	R	65	MET
22	R	75	ARG

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Mol	Chain	Res	Type
22	R	83	LYS
22	R	89	LEU
22	R	90	PHE
23	S	4	LYS
23	S	7	ASP
23	S	29	LYS
23	S	30	LYS
23	S	31	ASP
23	S	34	VAL
23	S	38	VAL
23	S	74	LYS
23	S	77	GLU
23	S	100	GLU
24	T	3	SER
24	T	7	ILE
24	T	8	ILE
24	T	9	ARG
24	T	21	LEU
24	T	22	ARG
24	T	23	LYS
24	T	24	SER
24	T	27	VAL
24	T	38	ASN
24	T	50	LYS
24	T	53	ARG
24	T	58	ASN
24	T	77	TYR
24	T	90	ASP
25	U	12	LYS
25	U	45	LEU
25	U	53	ILE
25	U	75	VAL
25	U	82	ARG
25	U	83	ASP
25	U	84	LYS
26	V	3	LYS
26	V	7	VAL
26	V	11	LYS
26	V	27	ARG
26	V	40	VAL
26	V	50	SER
26	V	52	ARG

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Mol	Chain	Res	Type
26	V	58	LYS
27	W	2	LYS
27	W	10	THR
27	W	12	SER
27	W	15	GLU
27	W	16	GLU
27	W	17	GLN
27	W	19	LYS
27	W	22	LYS
27	W	29	ARG
27	W	30	PHE
27	W	36	GLN
27	W	44	ARG
27	W	62	ILE
27	W	65	SER
28	X	5	GLN
28	X	6	ILE
28	X	7	THR
28	X	10	ARG
28	X	18	THR
29	Y	3	GLN
29	Y	5	ILE
30	Z	39	SER
32	b	6	MET
32	b	10	LEU
32	b	43	LEU
32	b	44	GLN
32	b	86	ARG
32	b	93	ASN
32	b	119	LYS
32	b	122	GLU
32	b	126	PHE
32	b	141	TYR
32	b	154	MET
32	b	157	MET
33	c	53	HIS
33	c	78	LYS
33	c	89	LYS
33	c	97	LYS
33	c	125	ASN
33	c	194	LYS
34	d	3	ARG

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Mol	Chain	Res	Type
34	d	8	ASN
34	d	54	LYS
34	d	69	ARG
34	d	125	ARG
35	e	10	GLU
35	e	12	GLU
35	e	43	ASN
35	e	70	ASP
35	e	149	ASN
36	f	1	MET
36	f	25	ARG
36	f	43	TRP
36	f	71	LYS
36	f	75	GLU
36	f	81	LYS
36	f	83	SER
37	g	9	LYS
37	g	10	ARG
37	g	11	ASP
37	g	12	VAL
37	g	13	LEU
37	g	16	PRO
37	g	32	LEU
37	g	35	LYS
37	g	54	SER
37	g	66	ILE
37	g	72	VAL
37	g	73	LEU
37	g	78	ARG
37	g	153	HIS
37	g	155	ARG
38	h	54	ASP
38	h	60	LEU
38	h	121	ARG
39	i	9	ARG
39	i	60	LYS
39	i	96	TYR
39	i	102	ARG
40	j	10	LEU
40	j	23	GLU
40	j	30	LYS
40	j	31	ARG

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Mol	Chain	Res	Type
40	j	92	LEU
40	j	97	ASP
41	k	18	ASN
41	k	37	GLU
41	k	68	GLU
41	k	125	LYS
41	k	126	ARG
42	l	64	LYS
42	l	67	ARG
42	l	99	ARG
42	l	102	ASP
42	l	129	LEU
42	l	132	THR
42	l	133	LYS
42	l	136	LYS
43	m	27	THR
43	m	34	LEU
43	m	51	ASP
43	m	68	ASP
43	m	78	LYS
43	m	87	ARG
43	m	114	LYS
44	n	38	LYS
44	n	61	TRP
45	o	10	GLU
45	o	74	ASP
46	p	32	ARG
46	p	51	LYS
47	q	6	ASP
47	q	20	ASP
47	q	28	GLU
47	q	31	LYS
47	q	44	LYS
47	q	56	LYS
47	q	74	ARG
47	q	84	SER
48	r	17	TYR
48	r	25	HIS
48	r	39	SER
48	r	59	MET
49	s	12	ASP
49	s	16	MET

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Mol	Chain	Res	Type
49	s	34	TRP
49	s	55	ARG
49	s	69	HIS
49	s	77	THR
50	t	15	GLU
50	t	40	SER
50	t	72	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	7	GLN
14	J	83	ASN
16	L	106	GLN
21	Q	40	ASN
24	T	88	HIS
32	b	94	GLN
33	c	88	ASN
37	g	142	HIS
37	g	148	ASN
41	k	119	ASN
49	s	22	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1470/1548 (94%)	382 (25%)	0
5	A	2877/2921 (98%)	941 (32%)	78 (2%)
6	B	114/115 (99%)	46 (40%)	4 (3%)
All	All	4461/4584 (97%)	1369 (30%)	82 (1%)

All (1369) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	5	A
5	A	13	A
5	A	18	C
5	A	19	G
5	A	23	G
5	A	24	G

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Mol	Chain	Res	Type
5	A	28	A
5	A	29	U
5	A	34	U
5	A	36	G
5	A	39	C
5	A	43	A
5	A	46	C
5	A	47	C
5	A	50	U
5	A	51	G
5	A	54	G
5	A	55	G
5	A	58	G
5	A	62	C
5	A	63	U
5	A	64	A
5	A	66	C
5	A	70	G
5	A	71	A
5	A	74	U
5	A	75	G
5	A	80	G
5	A	83	G
5	A	84	A
5	A	88	G
5	A	90	A
5	A	91	A
5	A	92	G
5	A	93	U
5	A	94	A
5	A	96	G
5	A	100	U
5	A	101	G
5	A	102	A
5	A	103	U
5	A	104	C
5	A	105	C
5	A	106	A
5	A	117	A
5	A	118	A
5	A	119	U
5	A	122	G

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Mol	Chain	Res	Type
5	A	124	A
5	A	125	A
5	A	135	G
5	A	140	A
5	A	153	G
5	A	158	G
5	A	162	A
5	A	163	U
5	A	164	A
5	A	165	C
5	A	166	A
5	A	167	U
5	A	169	G
5	A	170	C
5	A	171	A
5	A	173	A
5	A	176	A
5	A	177	G
5	A	179	A
5	A	180	G
5	A	183	A
5	A	184	C
5	A	185	A
5	A	199	A
5	A	200	A
5	A	202	A
5	A	203	U
5	A	209	U
5	A	213	C
5	A	215	G
5	A	216	A
5	A	218	G
5	A	219	A
5	A	224	A
5	A	225	A
5	A	226	A
5	A	231	A
5	A	232	U
5	A	234	C
5	A	235	G
5	A	236	A
5	A	242	U

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Mol	Chain	Res	Type
5	A	244	A
5	A	248	G
5	A	251	G
5	A	255	G
5	A	268	A
5	A	269	G
5	A	272	C
5	A	275	A
5	A	278	A
5	A	280	C
5	A	281	A
5	A	282	A
5	A	284	C
5	A	286	U
5	A	287	G
5	A	288	C
5	A	289	U
5	A	290	U
5	A	292	U
5	A	293	U
5	A	294	G
5	A	299	U
5	A	300	G
5	A	301	U
5	A	302	A
5	A	303	G
5	A	305	A
5	A	309	U
5	A	310	C
5	A	311	U
5	A	312	A
5	A	318	A
5	A	321	U
5	A	324	A
5	A	326	A
5	A	327	G
5	A	328	G
5	A	329	A
5	A	333	C
5	A	335	U
5	A	336	U
5	A	353	A

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Mol	Chain	Res	Type
5	A	354	A
5	A	360	A
5	A	372	A
5	A	388	A
5	A	390	A
5	A	392	U
5	A	393	G
5	A	397	U
5	A	399	U
5	A	401	U
5	A	403	U
5	A	404	U
5	A	405	G
5	A	406	A
5	A	411	A
5	A	417	A
5	A	432	G
5	A	434	G
5	A	440	C
5	A	447	A
5	A	448	A
5	A	449	U
5	A	451	U
5	A	452	G
5	A	459	C
5	A	460	C
5	A	461	A
5	A	463	C
5	A	468	A
5	A	482	U
5	A	489	A
5	A	490	C
5	A	492	G
5	A	497	U
5	A	502	C
5	A	503	A
5	A	506	A
5	A	507	C
5	A	511	G
5	A	512	A
5	A	513	G
5	A	520	G

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Mol	Chain	Res	Type
5	A	521	U
5	A	523	A
5	A	525	A
5	A	527	G
5	A	529	A
5	A	530	C
5	A	537	A
5	A	540	G
5	A	549	U
5	A	550	A
5	A	553	A
5	A	554	C
5	A	565	G
5	A	566	U
5	A	567	G
5	A	572	C
5	A	574	A
5	A	575	G
5	A	576	U
5	A	577	A
5	A	578	G
5	A	581	A
5	A	583	A
5	A	591	A
5	A	592	A
5	A	606	G
5	A	608	C
5	A	616	G
5	A	617	A
5	A	618	A
5	A	619	U
5	A	621	A
5	A	623	C
5	A	629	A
5	A	630	G
5	A	644	C
5	A	645	A
5	A	646	A
5	A	647	G
5	A	659	A
5	A	661	U
5	A	666	A

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Mol	Chain	Res	Type
5	A	672	A
5	A	676	A
5	A	679	G
5	A	682	A
5	A	690	U
5	A	691	A
5	A	696	G
5	A	698	U
5	A	699	U
5	A	700	A
5	A	715	A
5	A	716	C
5	A	720	A
5	A	722	A
5	A	731	U
5	A	746	G
5	A	749	G
5	A	775	A
5	A	792	5MU
5	A	797	A
5	A	802	G
5	A	805	G
5	A	809	A
5	A	810	A
5	A	815	G
5	A	816	G
5	A	820	G
5	A	821	C
5	A	822	G
5	A	827	A
5	A	828	A
5	A	829	U
5	A	830	U
5	A	834	A
5	A	835	U
5	A	837	G
5	A	838	A
5	A	850	G
5	A	856	U
5	A	857	C
5	A	868	A
5	A	872	U

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Mol	Chain	Res	Type
5	A	873	U
5	A	891	A
5	A	899	U
5	A	904	G
5	A	911	A
5	A	917	U
5	A	922	G
5	A	925	G
5	A	926	G
5	A	927	G
5	A	928	C
5	A	938	G
5	A	939	U
5	A	940	U
5	A	942	C
5	A	943	C
5	A	944	G
5	A	945	A
5	A	951	G
5	A	952	A
5	A	955	A
5	A	957	C
5	A	960	C
5	A	964	U
5	A	965	G
5	A	970	U
5	A	971	U
5	A	973	A
5	A	975	U
5	A	977	A
5	A	985	A
5	A	989	A
5	A	990	G
5	A	992	A
5	A	993	C
5	A	1003	A
5	A	1005	G
5	A	1012	G
5	A	1018	A
5	A	1019	A
5	A	1024	A
5	A	1027	A

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Mol	Chain	Res	Type
5	A	1028	G
5	A	1029	C
5	A	1033	G
5	A	1034	A
5	A	1035	C
5	A	1037	A
5	A	1040	A
5	A	1043	U
5	A	1046	G
5	A	1047	G
5	A	1056	U
5	A	1057	A
5	A	1061	G
5	A	1063	U
5	A	1064	A
5	A	1066	G
5	A	1070	A
5	A	1071	A
5	A	1077	U
5	A	1083	G
5	A	1086	G
5	A	1089	C
5	A	1090	A
5	A	1091	G
5	A	1092	A
5	A	1093	C
5	A	1094	A
5	A	1095	A
5	A	1096	C
5	A	1097	U
5	A	1098	A
5	A	1100	G
5	A	1101	A
5	A	1105	U
5	A	1106	G
5	A	1109	U
5	A	1111	A
5	A	1113	A
5	A	1114	A
5	A	1115	G
5	A	1116	C
5	A	1117	A

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Mol	Chain	Res	Type
5	A	1118	G
5	A	1119	C
5	A	1120	C
5	A	1125	U
5	A	1126	U
5	A	1127	U
5	A	1130	A
5	A	1131	G
5	A	1132	A
5	A	1133	G
5	A	1135	G
5	A	1138	U
5	A	1143	G
5	A	1145	U
5	A	1147	A
5	A	1148	C
5	A	1149	U
5	A	1151	G
5	A	1153	C
5	A	1154	G
5	A	1155	A
5	A	1156	G
5	A	1157	U
5	A	1159	A
5	A	1160	C
5	A	1163	U
5	A	1166	G
5	A	1174	U
5	A	1175	G
5	A	1176	U
5	A	1177	A
5	A	1179	C
5	A	1180	G
5	A	1183	G
5	A	1185	U
5	A	1186	A
5	A	1192	A
5	A	1200	A
5	A	1201	G
5	A	1208	A
5	A	1215	U
5	A	1217	U

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Mol	Chain	Res	Type
5	A	1220	A
5	A	1225	G
5	A	1234	G
5	A	1245	G
5	A	1258	A
5	A	1265	G
5	A	1273	G
5	A	1274	G
5	A	1275	A
5	A	1276	G
5	A	1284	A
5	A	1286	G
5	A	1287	U
5	A	1290	G
5	A	1291	A
5	A	1294	G
5	A	1304	G
5	A	1309	G
5	A	1310	A
5	A	1312	A
5	A	1337	A
5	A	1338	U
5	A	1339	U
5	A	1340	G
5	A	1341	A
5	A	1342	C
5	A	1344	A
5	A	1348	U
5	A	1349	U
5	A	1357	G
5	A	1360	G
5	A	1361	G
5	A	1362	C
5	A	1366	U
5	A	1370	C
5	A	1378	U
5	A	1384	G
5	A	1387	C
5	A	1396	A
5	A	1397	G
5	A	1402	A
5	A	1405	G

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Mol	Chain	Res	Type
5	A	1415	A
5	A	1416	U
5	A	1421	A
5	A	1422	A
5	A	1432	A
5	A	1433	U
5	A	1434	U
5	A	1440	A
5	A	1443	A
5	A	1450	A
5	A	1451	U
5	A	1454	U
5	A	1455	U
5	A	1457	U
5	A	1458	A
5	A	1459	A
5	A	1460	U
5	A	1462	G
5	A	1463	A
5	A	1464	U
5	A	1465	G
5	A	1471	A
5	A	1472	C
5	A	1476	G
5	A	1477	U
5	A	1478	A
5	A	1479	G
5	A	1481	A
5	A	1482	U
5	A	1484	G
5	A	1487	G
5	A	1488	A
5	A	1489	A
5	A	1490	G
5	A	1493	U
5	A	1494	G
5	A	1497	A
5	A	1498	U
5	A	1499	U
5	A	1500	G
5	A	1504	U
5	A	1505	G

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Mol	Chain	Res	Type
5	A	1506	C
5	A	1507	A
5	A	1508	C
5	A	1509	G
5	A	1511	C
5	A	1512	U
5	A	1513	A
5	A	1517	A
5	A	1522	G
5	A	1523	G
5	A	1524	C
5	A	1526	G
5	A	1528	G
5	A	1532	U
5	A	1538	A
5	A	1539	A
5	A	1540	U
5	A	1542	C
5	A	1550	G
5	A	1551	U
5	A	1552	U
5	A	1553	A
5	A	1554	A
5	A	1555	G
5	A	1556	G
5	A	1557	C
5	A	1558	U
5	A	1560	A
5	A	1562	C
5	A	1568	U
5	A	1569	G
5	A	1571	G
5	A	1575	A
5	A	1576	A
5	A	1577	G
5	A	1578	A
5	A	1579	C
5	A	1580	A
5	A	1581	U
5	A	1582	U
5	A	1583	G
5	A	1584	U

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Mol	Chain	Res	Type
5	A	1585	G
5	A	1586	U
5	A	1587	C
5	A	1588	U
5	A	1589	U
5	A	1590	C
5	A	1592	A
5	A	1593	G
5	A	1594	U
5	A	1596	G
5	A	1598	U
5	A	1599	G
5	A	1602	U
5	A	1605	A
5	A	1606	C
5	A	1613	G
5	A	1616	A
5	A	1623	U
5	A	1624	C
5	A	1625	U
5	A	1627	G
5	A	1628	A
5	A	1629	U
5	A	1630	A
5	A	1631	G
5	A	1632	A
5	A	1633	A
5	A	1634	A
5	A	1635	A
5	A	1636	U
5	A	1637	A
5	A	1639	G
5	A	1641	G
5	A	1651	C
5	A	1652	A
5	A	1653	A
5	A	1654	A
5	A	1656	C
5	A	1657	G
5	A	1658	A
5	A	1660	A
5	A	1661	C

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Mol	Chain	Res	Type
5	A	1662	A
5	A	1666	A
5	A	1678	A
5	A	1679	A
5	A	1687	G
5	A	1690	A
5	A	1691	G
5	A	1692	C
5	A	1707	U
5	A	1717	G
5	A	1718	G
5	A	1719	C
5	A	1737	U
5	A	1740	G
5	A	1757	U
5	A	1758	A
5	A	1759	G
5	A	1760	G
5	A	1761	G
5	A	1762	U
5	A	1763	U
5	A	1764	A
5	A	1766	C
5	A	1769	C
5	A	1770	C
5	A	1771	A
5	A	1790	G
5	A	1791	G
5	A	1796	A
5	A	1797	G
5	A	1800	A
5	A	1803	G
5	A	1805	U
5	A	1806	U
5	A	1808	U
5	A	1809	C
5	A	1811	A
5	A	1813	A
5	A	1827	C
5	A	1828	U
5	A	1829	A
5	A	1835	U

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Mol	Chain	Res	Type
5	A	1843	U
5	A	1844	G
5	A	1856	A
5	A	1870	C
5	A	1871	U
5	A	1874	A
5	A	1876	G
5	A	1883	A
5	A	1886	A
5	A	1893	A
5	A	1894	G
5	A	1897	U
5	A	1898	C
5	A	1899	U
5	A	1903	A
5	A	1904	A
5	A	1905	G
5	A	1908	A
5	A	1909	C
5	A	1912	A
5	A	1919	C
5	A	1923	A
5	A	1933	G
5	A	1934	G
5	A	1938	U
5	A	1939	A
5	A	1945	A
5	A	1946	A
5	A	1948	G
5	A	1950	U
5	A	1951	C
5	A	1954	A
5	A	1956	G
5	A	1957	G
5	A	1958	U
5	A	1964	A
5	A	1965	A
5	A	1966	5MU
5	A	1967	U
5	A	1982	U
5	A	1992	C
5	A	1994	C

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Mol	Chain	Res	Type
5	A	1996	A
5	A	1997	A
5	A	1998	A
5	A	1999	G
5	A	2003	U
5	A	2008	A
5	A	2009	U
5	A	2018	U
5	A	2019	G
5	A	2020	U
5	A	2023	C
5	A	2024	A
5	A	2029	G
5	A	2048	G
5	A	2050	A
5	A	2057	A
5	A	2058	A
5	A	2059	G
5	A	2060	A
5	A	2061	U
5	A	2062	G
5	A	2070	C
5	A	2075	G
5	A	2076	A
5	A	2078	A
5	A	2082	C
5	A	2083	G
5	A	2087	A
5	A	2088	G
5	A	2089	A
5	A	2090	C
5	A	2095	U
5	A	2096	G
5	A	2107	G
5	A	2109	A
5	A	2114	G
5	A	2117	A
5	A	2119	U
5	A	2120	G
5	A	2127	G
5	A	2128	G
5	A	2129	C

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Mol	Chain	Res	Type
5	A	2130	A
5	A	2132	A
5	A	2133	G
5	A	2134	C
5	A	2135	U
5	A	2136	U
5	A	2138	U
5	A	2139	A
5	A	2140	C
5	A	2143	G
5	A	2144	A
5	A	2145	U
5	A	2146	A
5	A	2147	G
5	A	2148	G
5	A	2149	U
5	A	2153	A
5	A	2155	C
5	A	2156	C
5	A	2158	U
5	A	2159	U
5	A	2161	A
5	A	2163	A
5	A	2164	C
5	A	2169	G
5	A	2170	C
5	A	2172	C
5	A	2173	U
5	A	2175	G
5	A	2177	U
5	A	2185	A
5	A	2186	G
5	A	2188	C
5	A	2190	C
5	A	2193	G
5	A	2194	U
5	A	2195	G
5	A	2196	G
5	A	2198	A
5	A	2200	A
5	A	2204	C
5	A	2205	C

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Mol	Chain	Res	Type
5	A	2206	C
5	A	2208	A
5	A	2209	G
5	A	2210	C
5	A	2211	U
5	A	2212	G
5	A	2214	G
5	A	2215	U
5	A	2217	G
5	A	2221	U
5	A	2224	U
5	A	2225	A
5	A	2226	A
5	A	2230	G
5	A	2231	C
5	A	2232	A
5	A	2235	A
5	A	2238	U
5	A	2239	A
5	A	2240	U
5	A	2241	C
5	A	2245	G
5	A	2252	A
5	A	2265	G
5	A	2266	G
5	A	2287	C
5	A	2296	A
5	A	2306	G
5	A	2310	C
5	A	2311	U
5	A	2312	C
5	A	2313	A
5	A	2314	A
5	A	2315	A
5	A	2326	G
5	A	2328	A
5	A	2329	U
5	A	2330	G
5	A	2331	G
5	A	2332	U
5	A	2333	U
5	A	2334	G

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Mol	Chain	Res	Type
5	A	2335	G
5	A	2336	A
5	A	2337	A
5	A	2338	A
5	A	2339	U
5	A	2342	U
5	A	2345	A
5	A	2346	U
5	A	2347	A
5	A	2348	G
5	A	2349	A
5	A	2350	G
5	A	2352	G
5	A	2353	U
5	A	2354	A
5	A	2358	G
5	A	2360	A
5	A	2362	A
5	A	2364	G
5	A	2370	U
5	A	2371	U
5	A	2372	G
5	A	2374	C
5	A	2377	C
5	A	2388	A
5	A	2396	A
5	A	2397	G
5	A	2398	G
5	A	2399	G
5	A	2404	A
5	A	2408	C
5	A	2410	G
5	A	2411	A
5	A	2412	C
5	A	2416	G
5	A	2417	U
5	A	2418	G
5	A	2430	C
5	A	2433	C
5	A	2434	A
5	A	2437	G
5	A	2441	G

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Mol	Chain	Res	Type
5	A	2450	U
5	A	2451	C
5	A	2452	A
5	A	2453	A
5	A	2455	G
5	A	2456	G
5	A	2457	A
5	A	2461	A
5	A	2463	G
5	A	2468	C
5	A	2474	G
5	A	2475	A
5	A	2493	C
5	A	2497	G
5	A	2505	A
5	A	2506	U
5	A	2508	G
5	A	2521	G
5	A	2525	C
5	A	2528	C
5	A	2529	G
5	A	2531	U
5	A	2532	G
5	A	2533	U
5	A	2534	C
5	A	2543	G
5	A	2545	A
5	A	2547	C
5	A	2552	G
5	A	2554	C
5	A	2556	G
5	A	2558	A
5	A	2559	G
5	A	2562	G
5	A	2568	A
5	A	2569	A
5	A	2570	G
5	A	2574	U
5	A	2579	U
5	A	2580	G
5	A	2589	U
5	A	2592	A

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Mol	Chain	Res	Type
5	A	2593	A
5	A	2594	G
5	A	2599	A
5	A	2600	C
5	A	2601	G
5	A	2605	G
5	A	2609	G
5	A	2612	U
5	A	2613	C
5	A	2626	G
5	A	2629	A
5	A	2636	U
5	A	2640	U
5	A	2642	U
5	A	2648	G
5	A	2649	U
5	A	2650	G
5	A	2656	A
5	A	2661	A
5	A	2668	A
5	A	2672	G
5	A	2681	A
5	A	2682	G
5	A	2683	U
5	A	2684	A
5	A	2685	C
5	A	2687	A
5	A	2692	A
5	A	2693	C
5	A	2694	C
5	A	2695	G
5	A	2696	G
5	A	2700	G
5	A	2709	U
5	A	2712	G
5	A	2716	U
5	A	2728	U
5	A	2729	G
5	A	2733	A
5	A	2741	G
5	A	2745	G
5	A	2753	U

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Mol	Chain	Res	Type
5	A	2755	U
5	A	2756	G
5	A	2760	A
5	A	2761	C
5	A	2769	G
5	A	2771	G
5	A	2776	A
5	A	2777	A
5	A	2781	U
5	A	2782	C
5	A	2783	U
5	A	2784	A
5	A	2787	C
5	A	2788	A
5	A	2792	A
5	A	2794	C
5	A	2803	A
5	A	2804	G
5	A	2805	A
5	A	2806	U
5	A	2807	G
5	A	2817	A
5	A	2818	A
5	A	2819	C
5	A	2820	U
5	A	2821	U
5	A	2824	G
5	A	2826	U
5	A	2827	A
5	A	2828	U
5	A	2829	A
5	A	2830	A
5	A	2832	A
5	A	2838	C
5	A	2840	A
5	A	2844	U
5	A	2846	A
5	A	2851	G
5	A	2853	U
5	A	2855	A
5	A	2887	G
5	A	2888	A

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Mol	Chain	Res	Type
5	A	2892	G
5	A	2899	A
5	A	2900	C
5	A	2904	U
5	A	2905	C
5	A	2906	G
5	A	2913	G
5	A	2914	A
5	A	2916	U
5	A	2919	A
5	A	2920	U
6	B	3	U
6	B	6	U
6	B	10	U
6	B	14	G
6	B	16	A
6	B	17	A
6	B	20	A
6	B	22	G
6	B	23	U
6	B	24	C
6	B	25	A
6	B	26	C
6	B	27	A
6	B	30	U
6	B	31	G
6	B	33	U
6	B	36	C
6	B	37	A
6	B	39	G
6	B	40	C
6	B	41	C
6	B	42	G
6	B	43	A
6	B	45	C
6	B	49	G
6	B	50	A
6	B	51	A
6	B	52	G
6	B	53	U
6	B	54	U
6	B	55	A

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Mol	Chain	Res	Type
6	B	56	A
6	B	58	C
6	B	62	U
6	B	63	U
6	B	64	A
6	B	65	G
6	B	87	C
6	B	88	G
6	B	101	A
6	B	102	G
6	B	106	G
6	B	107	U
6	B	111	C
6	B	113	G
6	B	115	C
31	a	8	G
31	a	10	G
31	a	31	U
31	a	32	G
31	a	33	A
31	a	40	G
31	a	43	G
31	a	45	G
31	a	48	C
31	a	49	C
31	a	52	A
31	a	62	G
31	a	65	G
31	a	67	G
31	a	69	G
31	a	71	A
31	a	72	C
31	a	76	C
31	a	94	G
31	a	95	A
31	a	98	U
31	a	99	U
31	a	100	A
31	a	118	A
31	a	119	A
31	a	120	C
31	a	129	A

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Mol	Chain	Res	Type
31	a	130	A
31	a	136	C
31	a	142	G
31	a	151	A
31	a	157	G
31	a	158	G
31	a	159	G
31	a	163	C
31	a	167	A
31	a	168	G
31	a	171	A
31	a	173	U
31	a	174	A
31	a	184	A
31	a	185	U
31	a	188	U
31	a	189	G
31	a	194	G
31	a	197	U
31	a	200	U
31	a	201	U
31	a	203	A
31	a	204	A
31	a	209	G
31	a	211	A
31	a	215	C
31	a	217	G
31	a	226	U
31	a	227	C
31	a	230	U
31	a	233	U
31	a	234	A
31	a	239	G
31	a	248	U
31	a	251	A
31	a	255	G
31	a	256	C
31	a	259	G
31	a	268	G
31	a	269	U
31	a	274	G
31	a	275	C

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Mol	Chain	Res	Type
31	a	278	A
31	a	279	C
31	a	297	G
31	a	301	A
31	a	327	G
31	a	329	A
31	a	336	C
31	a	337	A
31	a	338	C
31	a	352	A
31	a	355	G
31	a	359	G
31	a	360	C
31	a	362	G
31	a	363	C
31	a	375	U
31	a	380	C
31	a	390	A
31	a	396	G
31	a	401	A
31	a	405	A
31	a	406	C
31	a	412	G
31	a	414	G
31	a	415	A
31	a	421	G
31	a	422	A
31	a	423	A
31	a	424	G
31	a	427	C
31	a	429	U
31	a	430	C
31	a	431	G
31	a	437	U
31	a	440	A
31	a	442	C
31	a	443	U
31	a	447	U
31	a	452	A
31	a	456	A
31	a	459	A
31	a	460	A

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Mol	Chain	Res	Type
31	a	461	C
31	a	466	G
31	a	468	G
31	a	473	U
31	a	484	A
31	a	485	U
31	a	486	C
31	a	487	U
31	a	488	U
31	a	489	G
31	a	492	G
31	a	499	A
31	a	501	U
31	a	503	A
31	a	504	G
31	a	508	G
31	a	514	G
31	a	517	A
31	a	519	C
31	a	526	C
31	a	529	G
31	a	532	G
31	a	535	G
31	a	538	G
31	a	539	U
31	a	540	A
31	a	541	A
31	a	542	U
31	a	543	A
31	a	544	C
31	a	548	G
31	a	553	C
31	a	555	A
31	a	567	A
31	a	572	U
31	a	578	G
31	a	580	A
31	a	581	A
31	a	584	C
31	a	585	G
31	a	587	G
31	a	590	U

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Mol	Chain	Res	Type
31	a	591	A
31	a	596	G
31	a	604	A
31	a	612	G
31	a	634	U
31	a	640	G
31	a	641	U
31	a	642	C
31	a	649	A
31	a	650	A
31	a	660	U
31	a	661	U
31	a	664	G
31	a	673	A
31	a	691	G
31	a	694	U
31	a	701	G
31	a	703	A
31	a	708	G
31	a	726	A
31	a	730	G
31	a	732	G
31	a	741	G
31	a	757	A
31	a	763	G
31	a	785	A
31	a	788	A
31	a	789	A
31	a	790	A
31	a	793	G
31	a	794	G
31	a	796	U
31	a	801	U
31	a	802	A
31	a	803	C
31	a	817	G
31	a	820	G
31	a	823	A
31	a	825	C
31	a	826	G
31	a	827	A
31	a	829	G

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Mol	Chain	Res	Type
31	a	836	A
31	a	864	G
31	a	868	C
31	a	869	A
31	a	879	U
31	a	880	U
31	a	881	A
31	a	894	G
31	a	911	G
31	a	923	A
31	a	934	G
31	a	935	G
31	a	936	G
31	a	937	G
31	a	940	C
31	a	942	G
31	a	943	C
31	a	948	G
31	a	949	C
31	a	953	G
31	a	969	U
31	a	970	U
31	a	973	A
31	a	978	A
31	a	980	G
31	a	983	A
31	a	984	A
31	a	986	A
31	a	987	A
31	a	991	U
31	a	993	C
31	a	998	U
31	a	1000	U
31	a	1001	U
31	a	1002	G
31	a	1005	A
31	a	1007	C
31	a	1008	C
31	a	1029	A
31	a	1055	A
31	a	1060	U
31	a	1064	G

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Mol	Chain	Res	Type
31	a	1067	U
31	a	1075	G
31	a	1076	U
31	a	1092	G
31	a	1097	U
31	a	1105	G
31	a	1110	G
31	a	1112	A
31	a	1113	A
31	a	1119	G
31	a	1120	C
31	a	1122	A
31	a	1124	C
31	a	1128	A
31	a	1132	U
31	a	1135	G
31	a	1137	U
31	a	1139	C
31	a	1140	C
31	a	1141	A
31	a	1143	C
31	a	1144	A
31	a	1152	G
31	a	1155	C
31	a	1156	A
31	a	1167	A
31	a	1168	C
31	a	1169	U
31	a	1172	C
31	a	1174	G
31	a	1175	U
31	a	1177	A
31	a	1178	C
31	a	1179	A
31	a	1182	C
31	a	1187	G
31	a	1189	A
31	a	1194	G
31	a	1203	G
31	a	1205	C
31	a	1206	A
31	a	1207	A

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Mol	Chain	Res	Type
31	a	1218	C
31	a	1222	U
31	a	1223	A
31	a	1225	G
31	a	1235	A
31	a	1236	C
31	a	1237	A
31	a	1239	A
31	a	1246	A
31	a	1248	A
31	a	1250	U
31	a	1254	C
31	a	1255	A
31	a	1256	A
31	a	1264	G
31	a	1266	C
31	a	1268	G
31	a	1269	C
31	a	1270	G
31	a	1271	A
31	a	1278	G
31	a	1279	A
31	a	1280	G
31	a	1283	C
31	a	1289	A
31	a	1290	A
31	a	1292	C
31	a	1296	U
31	a	1297	A
31	a	1298	A
31	a	1303	G
31	a	1307	U
31	a	1308	C
31	a	1310	G
31	a	1312	U
31	a	1313	C
31	a	1315	G
31	a	1326	G
31	a	1329	A
31	a	1330	C
31	a	1331	U
31	a	1332	C

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Mol	Chain	Res	Type
31	a	1333	G
31	a	1334	A
31	a	1335	C
31	a	1338	C
31	a	1341	G
31	a	1346	U
31	a	1347	G
31	a	1356	A
31	a	1357	G
31	a	1358	U
31	a	1363	G
31	a	1374	U
31	a	1380	G
31	a	1384	A
31	a	1385	A
31	a	1387	A
31	a	1388	C
31	a	1389	G
31	a	1390	U
31	a	1391	U
31	a	1393	C
31	a	1397	G
31	a	1401	U
31	a	1404	A
31	a	1407	C
31	a	1408	A
31	a	1409	C
31	a	1410	C
31	a	1415	G
31	a	1420	A
31	a	1429	G
31	a	1445	G
31	a	1451	G
31	a	1452	G
31	a	1456	A
31	a	1457	A
31	a	1460	U
31	a	1474	C
31	a	1475	G
31	a	1476	U
31	a	1490	A
31	a	1498	G

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Mol	Chain	Res	Type
31	a	1500	G
31	a	1504	A
31	a	1505	G
31	a	1508	G
31	a	1510	A
31	a	1514	A
31	a	1515	G
31	a	1517	U
31	a	1518	A
31	a	1528	G
31	a	1529	A
31	a	1530	A
31	a	1532	G
31	a	1540	G
31	a	1541	G
31	a	1547	C
31	a	1548	U
31	a	1549	C
31	a	1550	C

All (82) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	63	U
5	A	82	G
5	A	90	A
5	A	98	U
5	A	104	C
5	A	199	A
5	A	202	A
5	A	291	G
5	A	299	U
5	A	327	G
5	A	328	G
5	A	337	A
5	A	373	A
5	A	403	U
5	A	502	C
5	A	513	G
5	A	520	G
5	A	548	A
5	A	576	U

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Mol	Chain	Res	Type
5	A	577	A
5	A	614	U
5	A	672	A
5	A	690	U
5	A	715	A
5	A	809	A
5	A	890	G
5	A	910	C
5	A	1017	A
5	A	1028	G
5	A	1077	U
5	A	1096	C
5	A	1097	U
5	A	1130	A
5	A	1153	C
5	A	1312	A
5	A	1357	G
5	A	1361	G
5	A	1433	U
5	A	1434	U
5	A	1455	U
5	A	1458	A
5	A	1525	U
5	A	1552	U
5	A	1554	A
5	A	1555	G
5	A	1577	G
5	A	1581	U
5	A	1591	G
5	A	1593	G
5	A	1605	A
5	A	1628	A
5	A	1629	U
5	A	1634	A
5	A	1652	A
5	A	1757	U
5	A	1760	G
5	A	1789	A
5	A	1826	G
5	A	2089	A
5	A	2094	G
5	A	2137	G

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Mol	Chain	Res	Type
5	A	2224	U
5	A	2225	A
5	A	2238	U
5	A	2329	U
5	A	2347	A
5	A	2353	U
5	A	2409	G
5	A	2457	A
5	A	2495	A
5	A	2505	A
5	A	2533	U
5	A	2599	A
5	A	2628	C
5	A	2672	G
5	A	2829	A
5	A	2887	G
5	A	2912	A
6	B	22	G
6	B	37	A
6	B	50	A
6	B	105	C

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

6 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	$\# Z > 2$
5	2MA	A	2530	52,5	17,25,26	1.08	0	17,37,40	1.29	3 (17%)
5	5MU	A	792	5	19,22,23	1.48	5 (26%)	28,32,35	2.25	8 (28%)
5	5MU	A	1966	5	19,22,23	1.67	5 (26%)	28,32,35	2.32	8 (28%)
5	OMG	A	2278	5	18,26,27	1.07	1 (5%)	19,38,41	1.21	3 (15%)
5	2MG	A	2472	5	18,26,27	1.19	1 (5%)	16,38,41	1.18	2 (12%)
5	MA6	A	2085	5	18,26,27	1.06	2 (11%)	19,38,41	1.76	5 (26%)

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	2MA	A	2530	52,5	-	0/3/25/26	0/3/3/3
5	5MU	A	792	5	-	0/7/25/26	0/2/2/2
5	5MU	A	1966	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2278	5	-	1/5/27/28	0/3/3/3
5	2MG	A	2472	5	-	0/5/27/28	0/3/3/3
5	MA6	A	2085	5	-	2/7/29/30	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2472	2MG	C6-N1	-3.64	1.32	1.37
5	A	1966	5MU	C4-N3	-3.27	1.32	1.38
5	A	792	5MU	C4-N3	-3.27	1.32	1.38
5	A	1966	5MU	C6-C5	3.14	1.39	1.34
5	A	2278	OMG	C6-N1	-3.10	1.33	1.37
5	A	1966	5MU	C2-N3	-3.01	1.32	1.38
5	A	792	5MU	C6-N1	-2.74	1.33	1.38
5	A	792	5MU	C2-N3	-2.66	1.33	1.38
5	A	1966	5MU	C2-N1	2.56	1.42	1.38
5	A	1966	5MU	C4-C5	2.28	1.48	1.44
5	A	2085	MA6	C5-C4	2.17	1.46	1.40
5	A	792	5MU	C6-C5	2.16	1.38	1.34
5	A	792	5MU	C2-N1	2.14	1.41	1.38
5	A	2085	MA6	C2'-C1'	-2.10	1.50	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1966	5MU	N3-C2-N1	5.87	122.69	114.89
5	A	1966	5MU	C5-C4-N3	5.40	119.92	115.31
5	A	792	5MU	N3-C2-N1	5.33	121.97	114.89
5	A	1966	5MU	C4-N3-C2	-5.13	120.71	127.35
5	A	792	5MU	C4-N3-C2	-5.10	120.75	127.35
5	A	792	5MU	C5-C4-N3	4.03	118.75	115.31
5	A	792	5MU	O4-C4-C5	-3.98	120.29	124.90
5	A	2085	MA6	N3-C2-N1	-3.66	122.96	128.68
5	A	2085	MA6	C4-C5-N7	-3.60	105.64	109.40
5	A	2085	MA6	C10-N6-C6	-3.58	108.66	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	792	5MU	C5-C6-N1	-3.51	119.73	123.34
5	A	1966	5MU	O4-C4-C5	-3.31	121.07	124.90
5	A	1966	5MU	O2-C2-N3	-3.23	115.48	121.50
5	A	792	5MU	C3'-C2'-C1'	3.00	107.12	101.43
5	A	2278	OMG	C5-C6-N1	2.85	118.98	113.95
5	A	1966	5MU	O4'-C1'-N1	2.85	114.87	108.36
5	A	2472	2MG	C5-C6-N1	2.84	118.97	113.95
5	A	2530	2MA	O4'-C1'-C2'	-2.71	102.96	106.93
5	A	1966	5MU	C5-C6-N1	-2.61	120.65	123.34
5	A	1966	5MU	C6-N1-C2	-2.58	118.68	121.30
5	A	2085	MA6	C3'-C2'-C1'	2.58	104.86	100.98
5	A	792	5MU	C1'-N1-C2	2.58	122.24	117.57
5	A	2530	2MA	C5-C6-N1	2.57	118.45	114.02
5	A	2472	2MG	C8-N7-C5	2.56	107.86	102.99
5	A	792	5MU	O2-C2-N3	-2.50	116.84	121.50
5	A	2530	2MA	C8-N7-C5	2.41	107.59	102.99
5	A	2278	OMG	O6-C6-C5	-2.21	120.06	124.37
5	A	2085	MA6	C10-N6-C9	-2.18	109.09	116.12
5	A	2278	OMG	C8-N7-C5	2.10	106.98	102.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2085	MA6	C5-C6-N6-C10
5	A	2278	OMG	C1'-C2'-O2'-CM2
5	A	2085	MA6	N1-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 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
51	A1D6G	A	3000	52	70,73,73	2.38	24 (34%)	96,107,107	1.76	27 (28%)

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
51	A1D6G	A	3000	52	-	11/82/113/113	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	C65-N64	8.48	1.45	1.33
51	A	3000	A1D6G	C11-N13	7.15	1.50	1.34
51	A	3000	A1D6G	O10-C11	5.00	1.43	1.35
51	A	3000	A1D6G	O67-C65	4.66	1.43	1.36
51	A	3000	A1D6G	C22-C21	4.61	1.55	1.44
51	A	3000	A1D6G	O67-C68	-4.38	1.41	1.47
51	A	3000	A1D6G	O04-C03	-4.16	1.39	1.46
51	A	3000	A1D6G	C25-C26	-3.90	1.40	1.48
51	A	3000	A1D6G	C19-C20	3.49	1.56	1.47
51	A	3000	A1D6G	O04-C05	3.48	1.42	1.34
51	A	3000	A1D6G	C35-N33	-3.37	1.33	1.40
51	A	3000	A1D6G	O42-C41	3.07	1.49	1.41
51	A	3000	A1D6G	C50-C46	-3.06	1.47	1.53
51	A	3000	A1D6G	C28-C29	2.94	1.53	1.48
51	A	3000	A1D6G	C25-C35	-2.73	1.36	1.41
51	A	3000	A1D6G	C63-N64	-2.67	1.40	1.45
51	A	3000	A1D6G	O10-C09	-2.52	1.41	1.44
51	A	3000	A1D6G	C45-C46	-2.30	1.48	1.53
51	A	3000	A1D6G	O54-C52	-2.27	1.39	1.44
51	A	3000	A1D6G	O27-C26	-2.26	1.18	1.23
51	A	3000	A1D6G	O60-C59	-2.12	1.18	1.21
51	A	3000	A1D6G	C28-C26	-2.10	1.39	1.44
51	A	3000	A1D6G	C56-C52	2.07	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	C21-C20	2.02	1.22	1.19

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A	3000	A1D6G	C52-C39-C37	-4.16	107.24	113.61
51	A	3000	A1D6G	O42-C43-C45	4.12	115.45	109.14
51	A	3000	A1D6G	C02-C03-C68	-3.95	109.79	115.23
51	A	3000	A1D6G	O10-C11-N13	3.94	118.03	111.11
51	A	3000	A1D6G	C44-C43-C45	-3.83	107.38	113.40
51	A	3000	A1D6G	C41-O42-C43	3.69	118.75	112.91
51	A	3000	A1D6G	O67-C65-O66	3.36	125.53	121.66
51	A	3000	A1D6G	O04-C05-C07	3.20	118.57	111.56
51	A	3000	A1D6G	O66-C65-N64	-3.11	125.59	129.22
51	A	3000	A1D6G	O67-C68-C69	2.95	112.13	106.93
51	A	3000	A1D6G	C03-O04-C05	-2.89	113.04	118.18
51	A	3000	A1D6G	O30-C29-C28	2.82	122.84	115.83
51	A	3000	A1D6G	O10-C11-O12	-2.78	120.35	124.53
51	A	3000	A1D6G	C14-N13-C11	-2.72	117.53	121.89
51	A	3000	A1D6G	C28-C32-N33	-2.60	119.57	123.16
51	A	3000	A1D6G	C38-C37-C09	-2.55	106.83	111.40
51	A	3000	A1D6G	C56-C52-C39	-2.37	107.38	110.25
51	A	3000	A1D6G	C45-C46-N47	-2.32	109.11	115.67
51	A	3000	A1D6G	C53-C52-C39	2.18	113.07	109.75
51	A	3000	A1D6G	O12-C11-N13	-2.18	121.62	124.96
51	A	3000	A1D6G	C69-C68-C03	-2.17	108.49	112.36
51	A	3000	A1D6G	C69-C68-C63	-2.16	113.39	116.42
51	A	3000	A1D6G	O30-C29-O31	-2.13	118.74	123.61
51	A	3000	A1D6G	C57-C59-C61	2.07	122.71	119.10
51	A	3000	A1D6G	O42-C41-C50	2.03	114.65	110.35
51	A	3000	A1D6G	O67-C68-C63	2.01	105.24	103.21
51	A	3000	A1D6G	O40-C39-C52	2.01	111.20	106.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	A	3000	A1D6G	C18-C19-C20-C21
51	A	3000	A1D6G	O10-C11-N13-C14
51	A	3000	A1D6G	O12-C11-N13-C14
51	A	3000	A1D6G	C19-C20-C21-C22
51	A	3000	A1D6G	N13-C11-O10-C09

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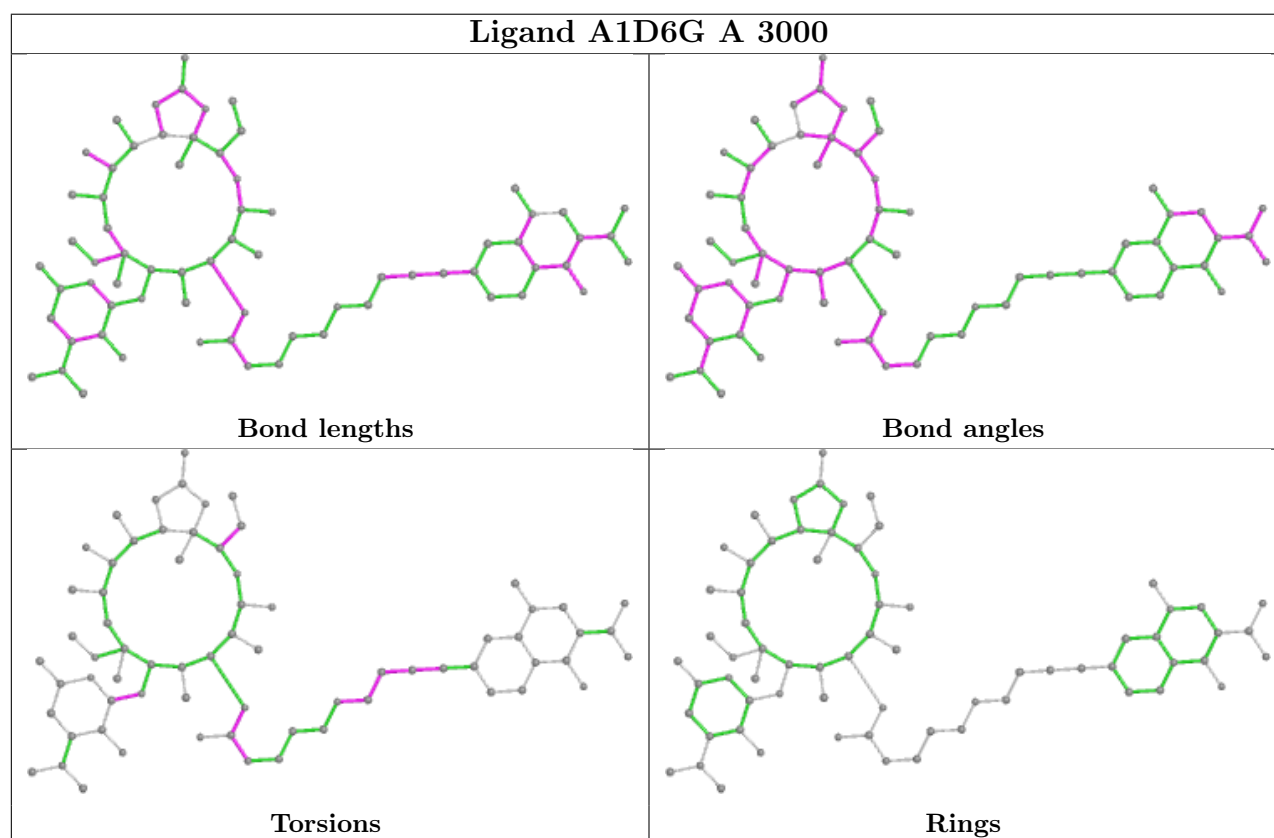
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Mol	Chain	Res	Type	Atoms
51	A	3000	A1D6G	O42-C41-O40-C39
51	A	3000	A1D6G	O12-C11-O10-C09
51	A	3000	A1D6G	C01-C02-C03-O04
51	A	3000	A1D6G	C19-C18-O17-C16
51	A	3000	A1D6G	O17-C18-C19-C20
51	A	3000	A1D6G	C50-C41-O40-C39

There are no ring outliers.

No monomer is involved in short contacts.

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



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.