



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 04:00 pm GMT

PDB ID : 8AM9
EMDB ID : EMD-15523
Title : Cryo-EM structure of the proline-rich antimicrobial peptide drosocin bound to the elongating ribosome
Authors : Koller, T.O.; Morici, M.; Wilson, D.N.
Deposited on : 2022-08-03
Resolution : 2.80 Å(reported)

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:

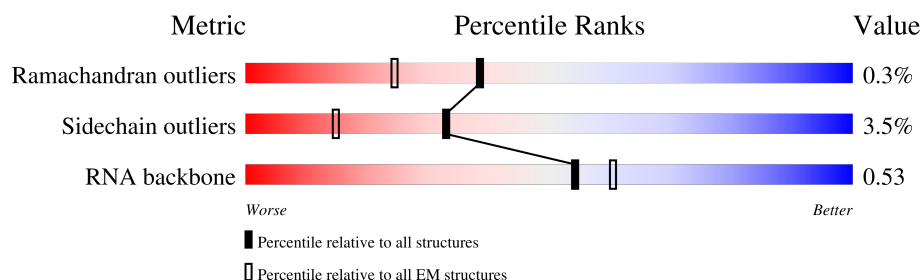
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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.






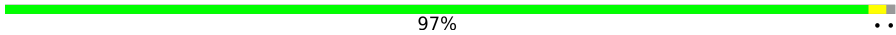
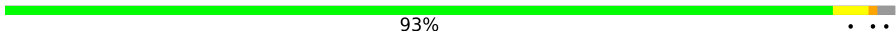




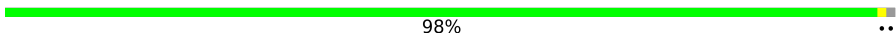
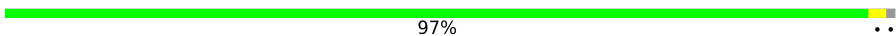
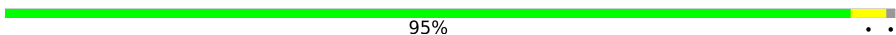







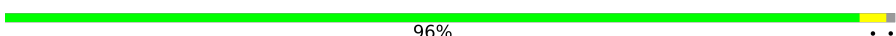
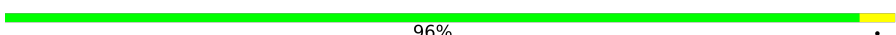
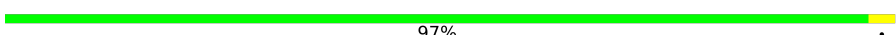
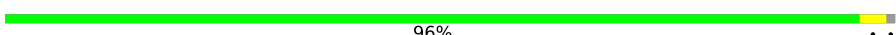


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	55	
2	1	46	
3	2	65	
4	3	38	
5	4	70	
6	B	1534	
7	C	241	
8	D	233	
9	E	206	

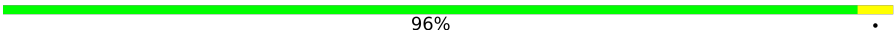
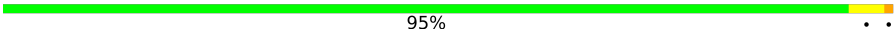
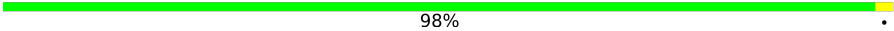
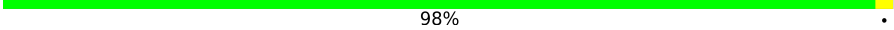

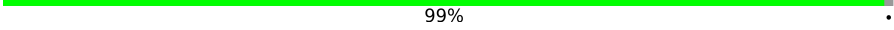
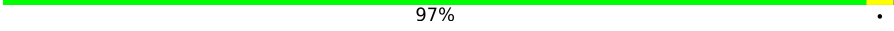
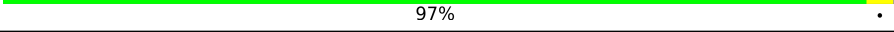
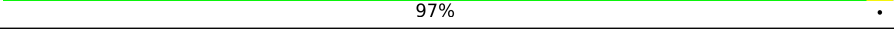
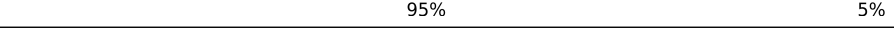

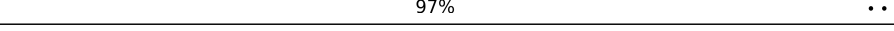
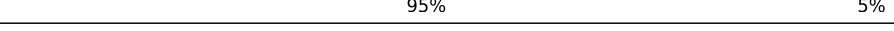

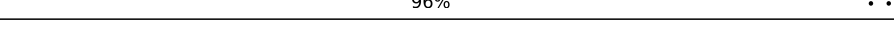
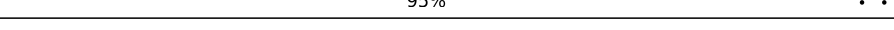
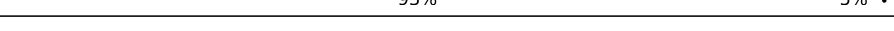
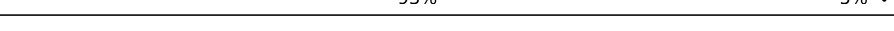

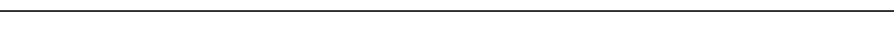

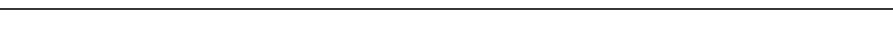
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	F	167	
11	G	135	
12	H	179	
13	I	130	
14	J	130	
15	K	103	
16	L	129	
17	M	124	
18	N	118	
19	O	101	
20	P	89	
21	Q	82	
22	R	84	
23	S	75	
24	T	92	
25	U	87	
26	V	71	
27	a	2903	
28	b	120	
29	c	273	
30	d	209	
31	e	201	
32	f	179	
33	g	177	
34	h	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
35	i	142	 96% .
36	j	123	 95% . .
37	k	144	 98% .
38	l	136	 98% .
39	m	127	 89% . 7%
40	n	117	 99% .
41	o	115	 97% . .
42	p	118	 97% . .
43	q	103	 97% .
44	r	110	 95% 5%
45	s	100	 90% . 7%
46	t	104	 97% . .
47	u	94	 95% 5%
48	v	85	 88% . 8%
49	w	78	 96% . .
50	x	63	 95% . .
51	y	59	 93% 5% .
52	z	57	 93% 5% .
53	X	12	 67% 33%
54	Y	76	 76% 22% .
55	8	85	 67% 21% 12%
56	A	19	 89% 11%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 142036 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 L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 8 is a protein called 30S ribosomal protein S3.

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

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	2753	Total	C	N	O	P	1	0
			59148	26391	10899	19104	2754		

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

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

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	12	Total	C	N	O	P	0	0
			255	114	42	87	12		

- Molecule 54 is a RNA chain called Initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Y	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 55 is a RNA chain called Leucine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	75	Total	C	N	O	P	0	0
			1602	715	291	521	75		

- Molecule 56 is a protein called Drosocin1.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	A	19	Total	C	N	O	0	0
			155	98	34	23		

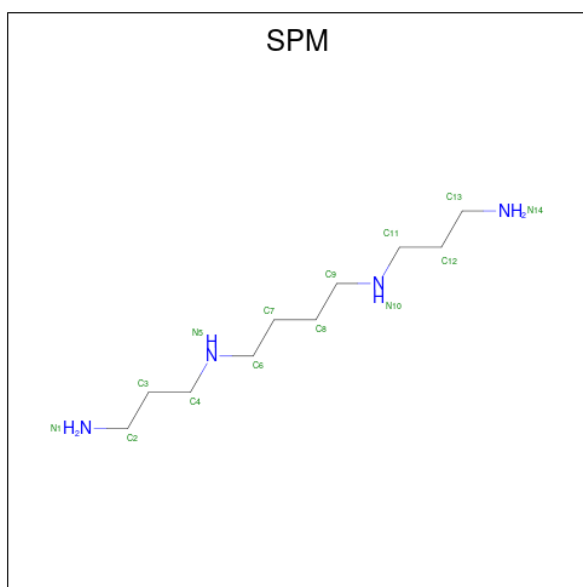
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

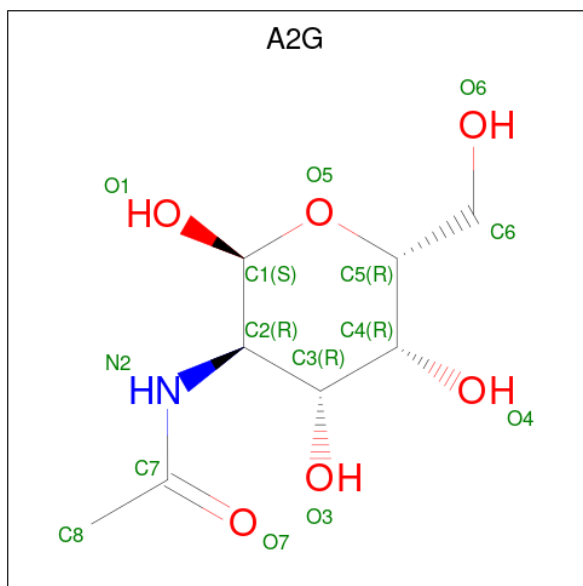
Mol	Chain	Residues	Atoms		AltConf
58	B	75	Total	Mg	0
			75	75	
58	O	1	Total	Mg	0
			1	1	
58	R	1	Total	Mg	0
			1	1	
58	a	208	Total	Mg	0
			208	208	
58	b	5	Total	Mg	0
			5	5	
58	d	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	
58	A	1	Total	Mg	0
			1	1	

- Molecule 59 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
59	a	1	Total	C	N	0
			14	10	4	

- Molecule 60 is 2-acetamido-2-deoxy- α -D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
60	A	1	Total	C	N	O	0
			14	8	1	5	


- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	a	2	Total	O	0
			2	2	

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.

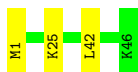
- Molecule 1: 50S ribosomal protein L33

Chain 0:  91% 7%



- Molecule 2: 50S ribosomal protein L34

Chain 1:  93% 7%



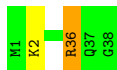
- Molecule 3: 50S ribosomal protein L35

Chain 2:  92% 6%




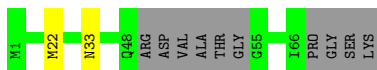
- Molecule 4: 50S ribosomal protein L36

Chain 3:  95%




- Molecule 5: 50S ribosomal protein L31

Chain 4:  83% 14%



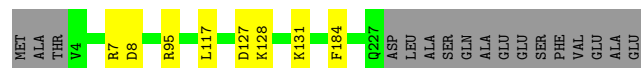
- Molecule 6: 16S ribosomal RNA

Chain B:  82% 17%



- Molecule 7: 30S ribosomal protein S2

Chain C: 90% 7%



- Molecule 8: 30S ribosomal protein S3

Chain D: 83% 6% 12%



- Molecule 9: 30S ribosomal protein S4

Chain E: 90% 8%



- Molecule 10: 30S ribosomal protein S5

Chain F: 89% 7%



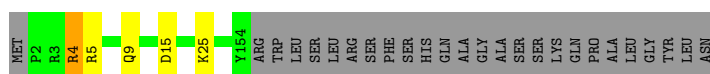
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain G: 72% 24%



- Molecule 12: 30S ribosomal protein S7

Chain H: 83% 15%



- Molecule 13: 30S ribosomal protein S8

Chain I: 97%



- Molecule 14: 30S ribosomal protein S9

Chain J: 93%



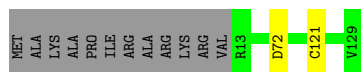
- Molecule 15: 30S ribosomal protein S10

Chain K: 85% 10% 5%



- Molecule 16: 30S ribosomal protein S11

Chain L: 89% 9%

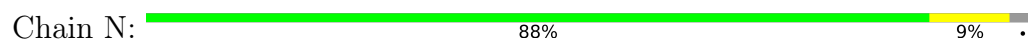


- Molecule 17: 30S ribosomal protein S12

Chain M: 91% 8%



- Molecule 18: 30S ribosomal protein S13



- Molecule 19: 30S ribosomal protein S14



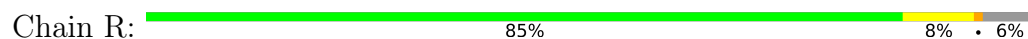
- Molecule 20: 30S ribosomal protein S15



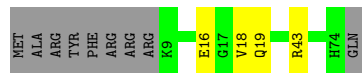
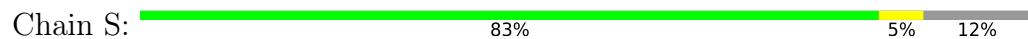
- Molecule 21: 30S ribosomal protein S16



- Molecule 22: 30S ribosomal protein S17

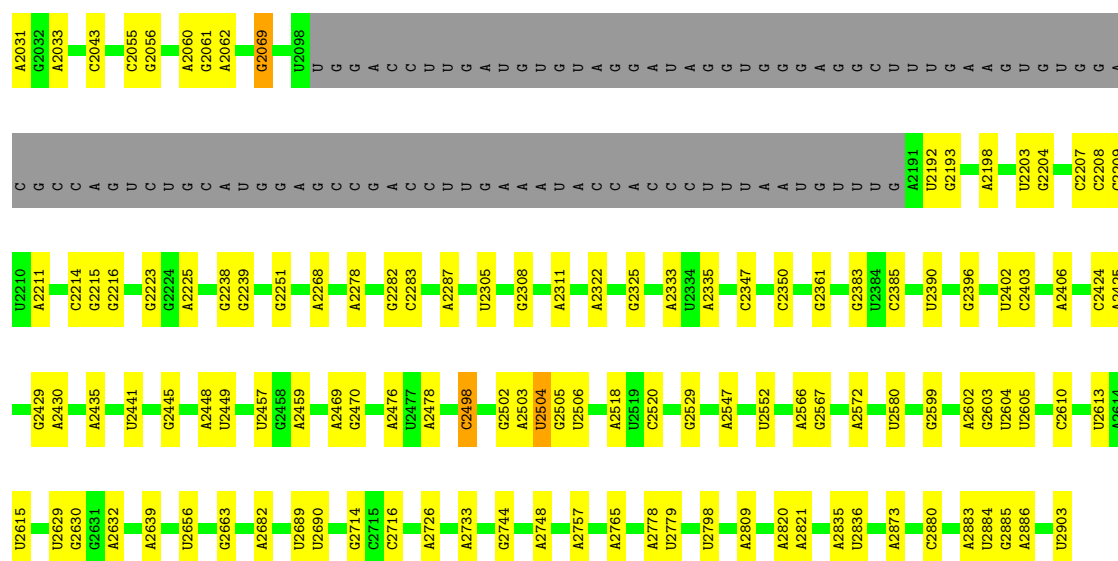


- Molecule 23: 30S ribosomal protein S18



- Molecule 24: 30S ribosomal protein S19





• Molecule 28: 5S ribosomal RNA

Chain b: 82% 17%



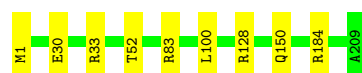
• Molecule 29: 50S ribosomal protein L2

Chain c: 96%



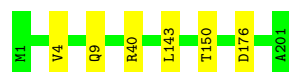
• Molecule 30: 50S ribosomal protein L3

Chain d: 96%




• Molecule 31: 50S ribosomal protein L4

Chain e: 97%



• Molecule 32: 50S ribosomal protein L5

Chain f: 96%

Chain m:  89% 7%



- Molecule 40: 50S ribosomal protein L18

Chain n:  99%



- Molecule 41: 50S ribosomal protein L19

Chain o:  97%



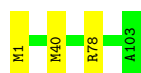
- Molecule 42: 50S ribosomal protein L20

Chain p:  97%



- Molecule 43: 50S ribosomal protein L21

Chain q:  97%




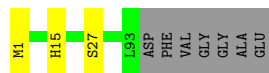
- Molecule 44: 50S ribosomal protein L22

Chain r:  95% 5%



- Molecule 45: 50S ribosomal protein L23

Chain s:  90% 7%



- Molecule 46: 50S ribosomal protein L24

Chain t:  97% ..




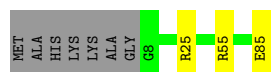
- Molecule 47: 50S ribosomal protein L25

Chain u:  95% 5%



- Molecule 48: 50S ribosomal protein L27

Chain v:  88% • 8%



- Molecule 49: 50S ribosomal protein L28

Chain w:  96% ..



- Molecule 50: 50S ribosomal protein L29

Chain x:  95% ..



- Molecule 51: 50S ribosomal protein L30

Chain y:  93% 5% •

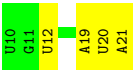


- Molecule 52: 50S ribosomal protein L32

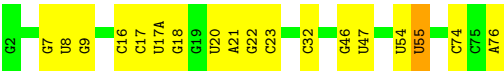
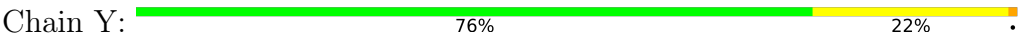
Chain z:  93% 5% •



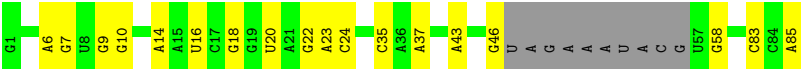
- Molecule 53: mRNA



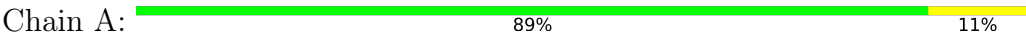
• Molecule 54: Initiator tRNA



• Molecule 55: Leucine tRNA



• Molecule 56: Drosocin1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84697	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: OMC, 5MC, 4SU, A2G, 6MZ, MEQ, 4OC, UR3, MG, 1MG, OMG, PSU, ZN, SPM, G7M, 5MU, H2U, 2MG, OMU, 2MA, MA6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.36	0/424	0.53	0/565
2	1	0.35	0/380	0.72	0/498
3	2	0.33	0/513	0.63	0/676
4	3	0.35	0/303	0.66	0/397
5	4	0.31	0/488	0.58	0/649
6	B	0.60	0/36236	0.92	1/56520 (0.0%)
7	C	0.27	0/1784	0.53	0/2403
8	D	0.30	0/1651	0.59	0/2225
9	E	0.29	0/1665	0.59	0/2227
10	F	0.32	0/1165	0.55	0/1568
11	G	0.31	0/858	0.55	0/1160
12	H	0.28	0/1219	0.58	0/1635
13	I	0.31	0/989	0.58	0/1326
14	J	0.32	0/1034	0.62	0/1375
15	K	0.31	0/796	0.60	0/1077
16	L	0.29	0/893	0.58	0/1205
17	M	0.29	0/969	0.65	0/1300
18	N	0.28	0/900	0.62	0/1204
19	O	0.32	0/817	0.61	0/1088
20	P	0.28	0/722	0.60	0/964
21	Q	0.28	0/653	0.62	0/877
22	R	0.32	0/650	0.59	0/871
23	S	0.34	0/553	0.59	0/742
24	T	0.32	0/685	0.55	0/922
25	U	0.26	0/676	0.51	0/895
26	V	0.31	0/597	0.65	0/792
27	a	0.75	0/65722	0.93	16/102528 (0.0%)
28	b	0.64	0/2850	0.91	0/4444
29	c	0.36	0/2121	0.62	0/2852
30	d	0.36	0/1576	0.56	0/2119
31	e	0.33	0/1571	0.55	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f	0.31	0/1434	0.57	0/1926
33	g	0.30	0/1343	0.57	0/1816
34	h	0.32	0/306	0.51	0/413
35	i	0.35	0/1152	0.57	0/1551
36	j	0.35	0/955	0.61	0/1279
37	k	0.33	0/1062	0.60	0/1413
38	l	0.35	0/1093	0.62	0/1460
39	m	0.34	0/958	0.65	0/1281
40	n	0.32	0/902	0.60	0/1209
41	o	0.34	0/929	0.58	0/1242
42	p	0.35	0/960	0.61	0/1278
43	q	0.34	0/829	0.59	0/1107
44	r	0.29	0/864	0.56	0/1156
45	s	0.29	0/744	0.55	0/994
46	t	0.30	0/787	0.56	0/1051
47	u	0.34	0/766	0.56	0/1025
48	v	0.36	0/593	0.58	0/785
49	w	0.31	0/635	0.65	0/848
50	x	0.27	0/502	0.58	0/667
51	y	0.30	0/453	0.62	0/605
52	z	0.34	0/450	0.62	0/599
53	X	0.64	0/284	1.01	0/440
54	Y	0.49	0/1725	0.95	1/2689 (0.0%)
55	8	0.43	0/1790	0.97	0/2786
56	A	0.42	0/162	0.68	0/221
All	All	0.61	0/153138	0.85	18/229058 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	2	0	2
4	3	0	1
7	C	0	2
8	D	0	3
9	E	0	7
10	F	0	1
12	H	0	1
14	J	0	4
15	K	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
17	M	0	5
18	N	0	5
19	O	0	1
21	Q	0	1
22	R	0	5
25	U	0	2
26	V	0	3
29	c	0	6
30	d	0	3
31	e	0	1
32	f	0	1
33	g	0	1
35	i	0	1
36	j	0	3
37	k	0	1
38	l	0	2
39	m	0	3
42	p	0	1
43	q	0	1
47	u	0	1
48	v	0	2
50	x	0	1
51	y	0	1
52	z	0	1
56	A	0	1
All	All	0	77

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	168	G	P-O3'-C3'	-10.84	106.69	119.70
27	a	160	A	P-O3'-C3'	-10.52	107.07	119.70
27	a	2216	G	P-O3'-C3'	-10.40	107.22	119.70
27	a	2208	C	P-O3'-C3'	-10.13	107.54	119.70
27	a	167	A	P-O3'-C3'	-10.12	107.56	119.70

There are no chirality outliers.

5 of 77 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	30	ARG	Sidechain
3	2	40	ARG	Sidechain
4	3	36	ARG	Sidechain
7	C	7	ARG	Sidechain
7	C	95	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
7	C	222/241 (92%)	212 (96%)	10 (4%)	0	100	100
8	D	204/233 (88%)	194 (95%)	9 (4%)	1 (0%)	25	56
9	E	203/206 (98%)	195 (96%)	7 (3%)	1 (0%)	25	56
10	F	154/167 (92%)	144 (94%)	9 (6%)	1 (1%)	22	51
11	G	101/135 (75%)	98 (97%)	2 (2%)	1 (1%)	13	39
12	H	151/179 (84%)	142 (94%)	8 (5%)	1 (1%)	19	48
13	I	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	16	44
14	J	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
15	K	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	13	39
16	L	115/129 (89%)	111 (96%)	3 (3%)	1 (1%)	14	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	M	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
18	N	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
19	O	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
20	P	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	Q	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
22	R	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
23	S	64/75 (85%)	64 (100%)	0	0	100	100
24	T	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
25	U	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	V	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
29	c	269/273 (98%)	253 (94%)	16 (6%)	0	100	100
30	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
31	e	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	25	56
32	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
33	g	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	22	51
34	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
35	i	140/142 (99%)	140 (100%)	0	0	100	100
36	j	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
37	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
38	l	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
39	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
40	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
41	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
42	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
43	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
44	r	108/110 (98%)	106 (98%)	1 (1%)	1 (1%)	14	42
45	s	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	12	37
46	t	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
47	u	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	12	37
48	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
49	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	x	60/63 (95%)	58 (97%)	1 (2%)	1 (2%)	7	26
51	y	56/59 (95%)	56 (100%)	0	0	100	100
52	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
56	A	17/19 (90%)	17 (100%)	0	0	100	100
All	All	5503/5932 (93%)	5279 (96%)	210 (4%)	14 (0%)	38	67

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	109	GLY
11	G	33	GLU
44	r	12	SER
15	K	57	VAL
47	u	67	GLY

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	0	46/49 (94%)	45 (98%)	1 (2%)	47	79
2	1	38/38 (100%)	35 (92%)	3 (8%)	10	30
3	2	51/52 (98%)	49 (96%)	2 (4%)	27	61
4	3	34/34 (100%)	32 (94%)	2 (6%)	16	44
5	4	55/62 (89%)	53 (96%)	2 (4%)	30	64
7	C	186/199 (94%)	180 (97%)	6 (3%)	34	68
8	D	170/190 (90%)	161 (95%)	9 (5%)	19	49
9	E	172/173 (99%)	159 (92%)	13 (8%)	11	32
10	F	119/126 (94%)	114 (96%)	5 (4%)	25	58
11	G	90/116 (78%)	85 (94%)	5 (6%)	17	47
12	H	126/147 (86%)	122 (97%)	4 (3%)	34	68
13	I	104/105 (99%)	102 (98%)	2 (2%)	52	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	J	105/107 (98%)	102 (97%)	3 (3%)	37	71
15	K	86/90 (96%)	80 (93%)	6 (7%)	12	36
16	L	90/99 (91%)	89 (99%)	1 (1%)	70	90
17	M	103/104 (99%)	98 (95%)	5 (5%)	21	52
18	N	93/96 (97%)	87 (94%)	6 (6%)	14	40
19	O	83/84 (99%)	83 (100%)	0	100	100
20	P	76/77 (99%)	74 (97%)	2 (3%)	41	75
21	Q	65/65 (100%)	63 (97%)	2 (3%)	35	69
22	R	73/78 (94%)	69 (94%)	4 (6%)	18	47
23	S	57/65 (88%)	53 (93%)	4 (7%)	12	36
24	T	72/79 (91%)	71 (99%)	1 (1%)	62	87
25	U	65/66 (98%)	62 (95%)	3 (5%)	23	55
26	V	60/61 (98%)	55 (92%)	5 (8%)	9	28
29	c	216/218 (99%)	214 (99%)	2 (1%)	75	92
30	d	163/163 (100%)	158 (97%)	5 (3%)	35	69
31	e	165/165 (100%)	161 (98%)	4 (2%)	44	77
32	f	148/150 (99%)	143 (97%)	5 (3%)	32	66
33	g	137/138 (99%)	129 (94%)	8 (6%)	17	45
34	h	32/114 (28%)	30 (94%)	2 (6%)	15	42
35	i	116/116 (100%)	112 (97%)	4 (3%)	32	66
36	j	104/104 (100%)	100 (96%)	4 (4%)	28	62
37	k	103/103 (100%)	101 (98%)	2 (2%)	52	82
38	l	109/109 (100%)	108 (99%)	1 (1%)	75	92
39	m	98/103 (95%)	96 (98%)	2 (2%)	50	81
40	n	86/87 (99%)	86 (100%)	0	100	100
41	o	99/100 (99%)	96 (97%)	3 (3%)	36	70
42	p	89/90 (99%)	87 (98%)	2 (2%)	47	79
43	q	84/84 (100%)	82 (98%)	2 (2%)	44	77
44	r	93/93 (100%)	89 (96%)	4 (4%)	25	57
45	s	80/84 (95%)	78 (98%)	2 (2%)	42	75
46	t	83/85 (98%)	82 (99%)	1 (1%)	67	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	u	78/78 (100%)	75 (96%)	3 (4%)	28	62
48	v	58/63 (92%)	57 (98%)	1 (2%)	56	84
49	w	67/68 (98%)	65 (97%)	2 (3%)	36	70
50	x	54/55 (98%)	54 (100%)	0	100	100
51	y	48/49 (98%)	46 (96%)	2 (4%)	25	58
52	z	47/48 (98%)	45 (96%)	2 (4%)	25	57
56	A	18/18 (100%)	17 (94%)	1 (6%)	17	47
All	All	4594/4847 (95%)	4434 (96%)	160 (4%)	33	65

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	g	52	PHE
44	r	66	ILE
33	g	155	GLU
37	k	112	LEU
47	u	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	39	HIS
16	L	119	ASN
32	f	5	HIS
44	r	61	ASN
49	w	34	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	a	2746/2903 (94%)	373 (13%)	0
28	b	118/120 (98%)	20 (16%)	0
53	X	11/12 (91%)	4 (36%)	0
54	Y	75/76 (98%)	12 (16%)	4 (5%)
55	8	73/85 (85%)	18 (24%)	2 (2%)
6	B	1513/1534 (98%)	244 (16%)	38 (2%)
All	All	4536/4730 (95%)	671 (14%)	44 (0%)

5 of 671 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	4	U
6	B	5	U
6	B	6	G
6	B	8	A
6	B	9	G

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	B	1145	A
6	B	1397	C
6	B	1181	G
6	B	1239	A
6	B	1505	G

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

38 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	$\# Z > 2$
27	PSU	a	1917	27	18,21,22	1.16	2 (11%)	22,30,33	1.84	4 (18%)
54	PSU	Y	55	54	18,21,22	1.17	2 (11%)	22,30,33	1.63	3 (13%)
27	5MU	a	747	27	19,22,23	7.49	7 (36%)	28,32,35	3.17	10 (35%)
27	PSU	a	2504	27	18,21,22	1.14	2 (11%)	22,30,33	1.79	3 (13%)
54	4SU	Y	8	54	18,21,22	3.54	8 (44%)	26,30,33	2.06	4 (15%)
6	2MG	B	1516	6	18,26,27	2.41	7 (38%)	16,38,41	1.51	4 (25%)
27	OMU	a	2552	27	19,22,23	2.92	8 (42%)	26,31,34	1.80	5 (19%)
6	2MG	B	966	6	18,26,27	2.45	7 (38%)	16,38,41	1.40	3 (18%)
6	G7M	B	527	6	20,26,27	2.41	7 (35%)	17,39,42	1.12	2 (11%)
6	UR3	B	1498	6	19,22,23	2.88	8 (42%)	26,32,35	1.46	2 (7%)
6	4OC	B	1402	6	20,23,24	2.96	8 (40%)	26,32,35	1.02	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	MEQ	d	150	30	8,9,10	0.93	0	5,10,12	1.28	1 (20%)
27	PSU	a	955	27	18,21,22	1.05	1 (5%)	22,30,33	1.86	3 (13%)
27	OMC	a	2498	27,58	19,22,23	2.79	8 (42%)	26,31,34	0.76	0
27	PSU	a	2580	27	18,21,22	1.23	2 (11%)	22,30,33	2.00	6 (27%)
27	H2U	a	2449	27	18,21,22	3.25	6 (33%)	21,30,33	2.23	5 (23%)
27	2MA	a	2503	27,58	19,25,26	3.49	7 (36%)	21,37,40	1.82	4 (19%)
6	MA6	B	1518	6	18,26,27	1.20	1 (5%)	19,38,41	2.81	2 (10%)
6	5MC	B	967	6	18,22,23	3.60	7 (38%)	26,32,35	0.95	1 (3%)
6	5MC	B	1407	6	18,22,23	3.56	7 (38%)	26,32,35	1.03	3 (11%)
27	PSU	a	2604	27	18,21,22	1.11	2 (11%)	22,30,33	1.96	4 (18%)
27	6MZ	a	1618	27	18,25,26	2.53	2 (11%)	16,36,39	1.98	4 (25%)
6	2MG	B	1207	6	18,26,27	2.49	7 (38%)	16,38,41	1.37	3 (18%)
27	5MC	a	1962	27	18,22,23	3.59	7 (38%)	26,32,35	1.12	3 (11%)
27	5MU	a	1939	27	19,22,23	7.52	7 (36%)	28,32,35	3.12	9 (32%)
6	PSU	B	516	6	18,21,22	1.09	2 (11%)	22,30,33	1.77	4 (18%)
27	1MG	a	745	27	18,26,27	2.72	6 (33%)	19,39,42	1.63	5 (26%)
6	MA6	B	1519	6	18,26,27	1.22	1 (5%)	19,38,41	2.86	2 (10%)
27	PSU	a	746	27,58	18,21,22	1.14	2 (11%)	22,30,33	1.71	3 (13%)
27	PSU	a	2457	27	18,21,22	1.17	1 (5%)	22,30,33	1.81	4 (18%)
54	5MC	Y	32	54	18,22,23	3.59	7 (38%)	26,32,35	0.97	1 (3%)
27	G7M	a	2069	27	20,26,27	2.31	7 (35%)	17,39,42	1.12	2 (11%)
27	OMG	a	2251	27,54,58	18,26,27	2.62	7 (38%)	19,38,41	1.47	4 (21%)
27	PSU	a	2605	27	18,21,22	1.07	2 (11%)	22,30,33	1.83	4 (18%)
27	2MG	a	2445	27	18,26,27	2.38	7 (38%)	16,38,41	1.48	4 (25%)
27	PSU	a	1911	27	18,21,22	1.09	2 (11%)	22,30,33	1.75	3 (13%)
54	5MU	Y	54	54	19,22,23	7.47	7 (36%)	28,32,35	3.05	9 (32%)
27	2MG	a	1835	27	18,26,27	2.39	7 (38%)	16,38,41	1.36	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PSU	a	1917	27	-	0/7/25/26	0/2/2/2
54	PSU	Y	55	54	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	5MU	a	747	27	-	0/7/25/26	0/2/2/2
27	PSU	a	2504	27	-	0/7/25/26	0/2/2/2
54	4SU	Y	8	54	-	0/7/25/26	0/2/2/2
6	2MG	B	1516	6	-	0/5/27/28	0/3/3/3
27	OMU	a	2552	27	-	0/9/27/28	0/2/2/2
6	2MG	B	966	6	-	2/5/27/28	0/3/3/3
6	G7M	B	527	6	-	1/3/25/26	0/3/3/3
6	UR3	B	1498	6	-	0/7/25/26	0/2/2/2
6	4OC	B	1402	6	-	0/9/29/30	0/2/2/2
30	MEQ	d	150	30	-	2/8/9/11	-
27	PSU	a	955	27	-	0/7/25/26	0/2/2/2
27	OMC	a	2498	27,58	-	0/9/27/28	0/2/2/2
27	PSU	a	2580	27	-	0/7/25/26	0/2/2/2
27	H2U	a	2449	27	-	0/7/38/39	0/2/2/2
27	2MA	a	2503	27,58	-	2/3/25/26	0/3/3/3
6	MA6	B	1518	6	-	0/7/29/30	0/3/3/3
6	5MC	B	967	6	-	0/7/25/26	0/2/2/2
6	5MC	B	1407	6	-	0/7/25/26	0/2/2/2
27	PSU	a	2604	27	-	0/7/25/26	0/2/2/2
27	6MZ	a	1618	27	-	1/5/27/28	0/3/3/3
6	2MG	B	1207	6	-	0/5/27/28	0/3/3/3
27	5MC	a	1962	27	-	4/7/25/26	0/2/2/2
27	5MU	a	1939	27	-	0/7/25/26	0/2/2/2
6	PSU	B	516	6	-	0/7/25/26	0/2/2/2
27	1MG	a	745	27	-	0/3/25/26	0/3/3/3
6	MA6	B	1519	6	-	0/7/29/30	0/3/3/3
27	PSU	a	746	27,58	-	3/7/25/26	0/2/2/2
27	PSU	a	2457	27	-	0/7/25/26	0/2/2/2
54	5MC	Y	32	54	-	0/7/25/26	0/2/2/2
27	G7M	a	2069	27	-	1/3/25/26	0/3/3/3
27	OMG	a	2251	27,54,58	-	1/5/27/28	0/3/3/3
27	PSU	a	2605	27	-	0/7/25/26	0/2/2/2
27	2MG	a	2445	27	-	0/5/27/28	0/3/3/3
27	PSU	a	1911	27	-	0/7/25/26	0/2/2/2
54	5MU	Y	54	54	-	2/7/25/26	0/2/2/2
27	2MG	a	1835	27	-	0/5/27/28	0/3/3/3

The worst 5 of 188 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	747	5MU	C4-C5	21.48	1.80	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	1939	5MU	C4-C5	21.40	1.80	1.44
54	Y	54	5MU	C4-C5	21.18	1.79	1.44
54	Y	54	5MU	C6-N1	16.00	1.65	1.38
27	a	1939	5MU	C6-N1	15.68	1.64	1.38

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1519	MA6	N1-C6-N6	-10.99	105.49	117.06
6	B	1518	MA6	N1-C6-N6	-10.40	106.11	117.06
54	Y	54	5MU	C5-C4-N3	9.89	123.75	115.31
27	a	1939	5MU	C5-C4-N3	9.82	123.69	115.31
27	a	747	5MU	C5-C4-N3	9.48	123.40	115.31

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	a	746	PSU	C2'-C1'-C5-C4
27	a	746	PSU	O4'-C1'-C5-C6
27	a	1618	6MZ	C4'-C5'-O5'-P
30	d	150	MEQ	NE2-CD-CG-CB
30	d	150	MEQ	OE1-CD-CG-CB

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 297 ligands modelled in this entry, 295 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	A2G	A	101	56	14,14,15	0.47	0	17,19,21	0.58	0
59	SPM	a	3209	-	13,13,13	0.31	0	12,12,12	0.86	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
60	A2G	A	101	56	-	0/6/23/26	0/1/1/1
59	SPM	a	3209	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

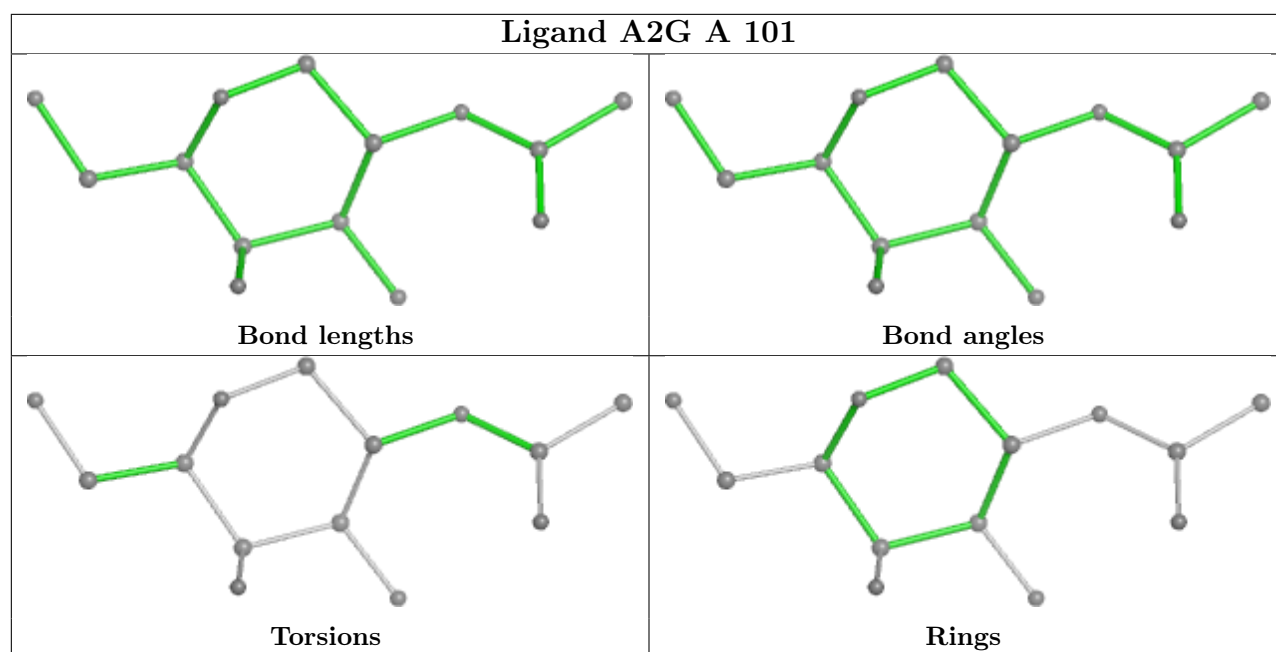
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	a	3209	SPM	C12-C11-N10-C9
59	a	3209	SPM	C3-C4-N5-C6

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.