



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 03:45 pm GMT

PDB ID : 8R8M
EMDB ID : EMD-19004
Title : 70S Escherichia coli ribosome with Paenilamicin B2 bound with hybrid A/P- and hybrid P/E-tRNA.
Authors : Koller, T.O.; Wilson, D.N.
Deposited on : 2023-11-29
Resolution : 2.40 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 : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

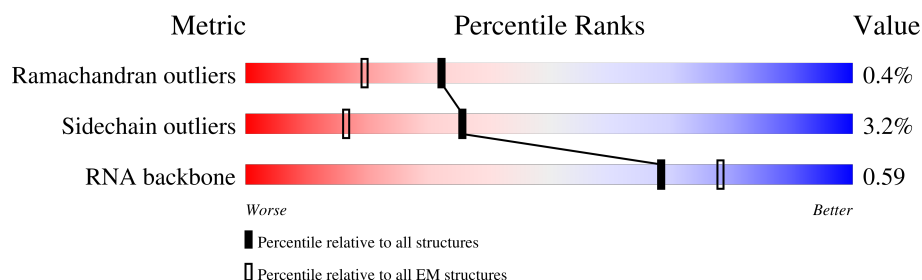
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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.



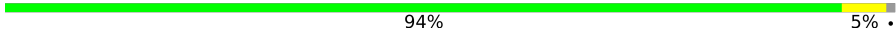

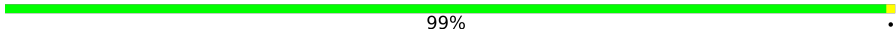
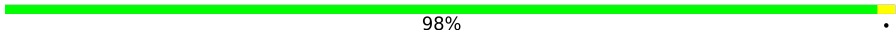
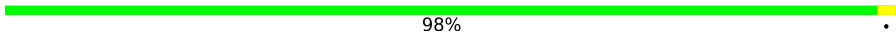
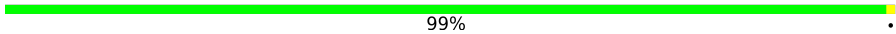

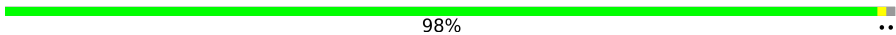
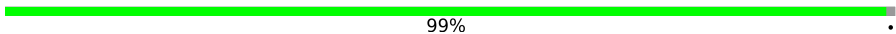
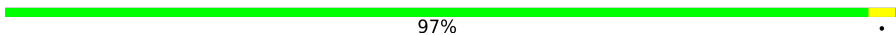
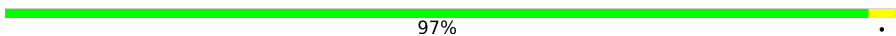
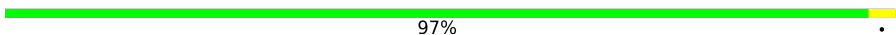

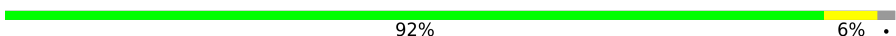
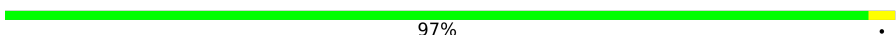

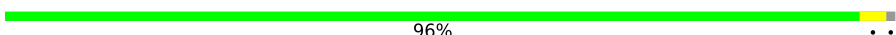

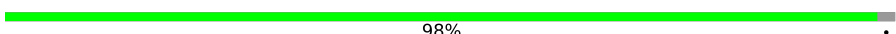
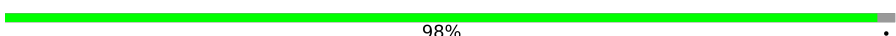





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	b	120	
6	c	273	
7	d	209	
8	e	201	
9	f	179	

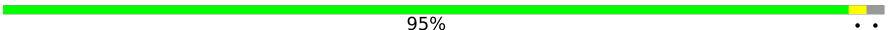

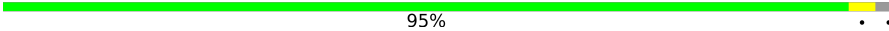
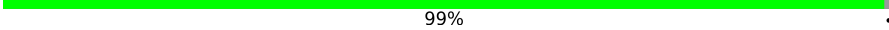



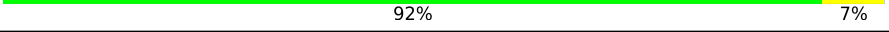
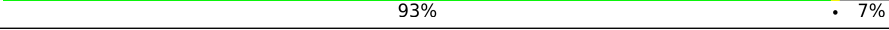

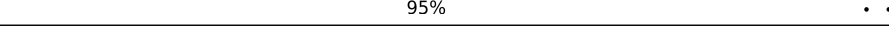
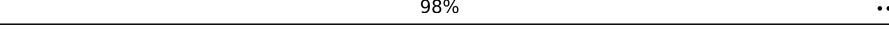
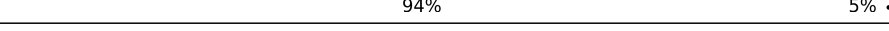


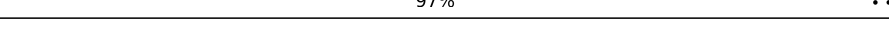
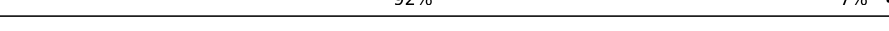

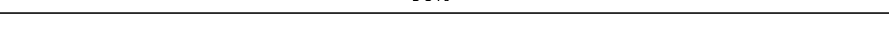
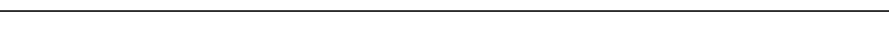

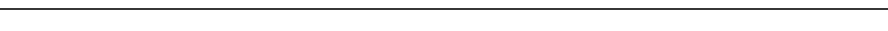
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Mol	Chain	Length	Quality of chain
10	g	177	
11	h	149	
12	i	142	
13	j	123	
14	k	144	
15	l	136	
16	m	127	
17	n	117	
18	o	115	
19	p	118	
20	q	103	
21	r	110	
22	s	100	
23	t	104	
24	u	94	
25	v	85	
26	w	78	
27	x	63	
28	y	59	
29	z	57	
30	X	10	
31	4	70	
32	a	2903	
33	A	1534	
34	C	233	

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Mol	Chain	Length	Quality of chain
35	I	130	 95% ..
36	J	103	 87% 8% 5%
37	M	118	 95% ..
38	N	101	 99% .
39	S	92	 88% . 9%
40	G	179	 80% 5% 15%
41	B	241	 90% . 7%
42	D	206	 92% 7%
43	E	167	 93% . 7%
44	F	135	 74% . 24%
45	H	130	 95% ..
46	O	89	 98% ..
47	P	82	 94% 5% .
48	Q	84	 90% . 6%
49	R	75	 87% . 12%
50	T	87	 97% ..
51	U	71	 92% 7% .
52	K	129	 88% . 9%
53	L	124	 96% ..
54	Z	85	 64% 21% 15%
55	Y	76	 76% 20% .
56	5	8	 88% 12%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 141380 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 bL33.

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 Large ribosomal subunit protein bL34.

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 Large ribosomal subunit protein bL35.

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 Large ribosomal subunit protein bL36A.

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 RNA chain called 5S ribosomal RNA.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL9.

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

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

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

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

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	variant	UNP P0ADY7

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

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

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

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

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

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

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	10	Total	C	N	O	P	0	0
			212	95	35	72	10		

- Molecule 31 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	48	Total	C	N	O	S	0	0
			373	232	66	69	6		

- Molecule 32 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	2738	Total	C	N	O	P	0	0
			58815	26243	10844	18990	2738		

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A	1519	Total	C	N	O	P	0	0
			32608	14548	5986	10555	1519		

- Molecule 34 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 35 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 37 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 38 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 39 is a protein called Small ribosomal subunit protein uS19.

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

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

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

- Molecule 41 is a protein called 30S ribosomal protein S2.

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

- Molecule 42 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 43 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 44 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

- Molecule 45 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 46 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 49 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 52 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 53 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 54 is a RNA chain called Leucine-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Z	72	Total	C	N	O	P	S	0	0
			1547	693	281	500	72	1		

- Molecule 55 is a RNA chain called Isoleucine-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Y	73	Total	C	N	O	P		0	0
			1564	700	283	509	72			

- Molecule 56 is a protein called Paenilamicin B2.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	5	8	Total	C	N	O	0	0
			71	42	16	13		

- 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	5	Total	Mg	0
			5	5	
58	c	1	Total	Mg	0
			1	1	
58	d	1	Total	Mg	0
			1	1	
58	p	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	
58	a	207	Total	Mg	0
			207	207	
58	A	91	Total	Mg	0
			91	91	

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	d	1	Total 1	K 1	0
59	5	1	Total 1	K 1	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	X	3	Total 3	O 3	0
60	a	1	Total 1	O 1	0
60	A	19	Total 19	O 19	0
60	C	1	Total 1	O 1	0
60	Z	2	Total 2	O 2	0
60	5	10	Total 10	O 10	0

3 Residue-property plots [i](#)

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

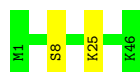
- Molecule 1: Large ribosomal subunit protein bL33

Chain 0:  89% 7%



- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  96%



- Molecule 3: Large ribosomal subunit protein bL35

Chain 2:  89% 9%



- Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:  97%



- Molecule 5: 5S ribosomal RNA

Chain b:  92% 8%



- Molecule 6: Large ribosomal subunit protein uL2

Chain c:  98%



- Molecule 7: Large ribosomal subunit protein uL3

Chain d: 98% .



- Molecule 8: Large ribosomal subunit protein uL4

Chain e: 98% .



- Molecule 9: Large ribosomal subunit protein uL5

Chain f: 96% . .



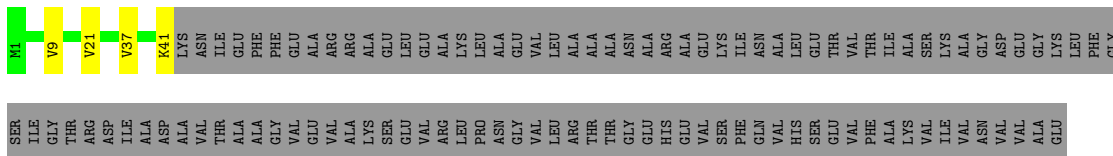
- Molecule 10: Large ribosomal subunit protein uL6

Chain g: 94% 5% .



- Molecule 11: Large ribosomal subunit protein bL9

Chain h: 25% . 72%



- Molecule 12: Large ribosomal subunit protein uL13

Chain i: 99% .



- Molecule 13: Large ribosomal subunit protein uL14

Chain j:  98% .



- Molecule 14: 50S ribosomal protein L15

Chain k:  98% .



- Molecule 15: Large ribosomal subunit protein uL16

Chain l:  99% .



- Molecule 16: Large ribosomal subunit protein bL17

Chain m:  91% . 7%



- Molecule 17: Large ribosomal subunit protein uL18

Chain n:  98% ..



- Molecule 18: Large ribosomal subunit protein bL19

Chain o:  99% .



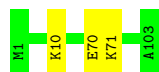
- Molecule 19: Large ribosomal subunit protein bL20

Chain p:  97% ..



- Molecule 20: Large ribosomal subunit protein bL21

Chain q:  97%



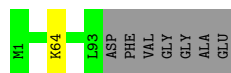
- Molecule 21: Large ribosomal subunit protein uL22

Chain r:  97%



- Molecule 22: Large ribosomal subunit protein uL23

Chain s:  92% 7%



- Molecule 23: Large ribosomal subunit protein uL24

Chain t:  92% 6%



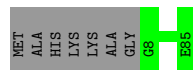
- Molecule 24: 50S ribosomal protein L25

Chain u:  97%



- Molecule 25: Large ribosomal subunit protein bL27

Chain v:  92% 8%



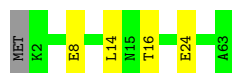
- Molecule 26: Large ribosomal subunit protein bL28

Chain w:  96%



- Molecule 27: Large ribosomal subunit protein uL29

Chain x:  92% 6%



- Molecule 28: Large ribosomal subunit protein uL30

Chain y:  98%




- Molecule 29: Large ribosomal subunit protein bL32

Chain z:  98%



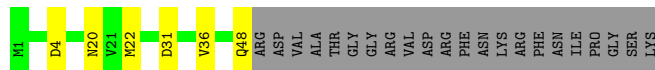
- Molecule 30: mRNA

Chain X:  90% 10%




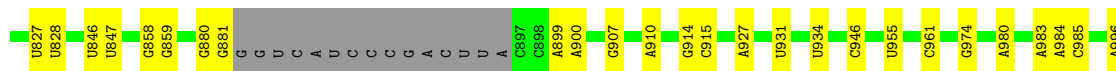
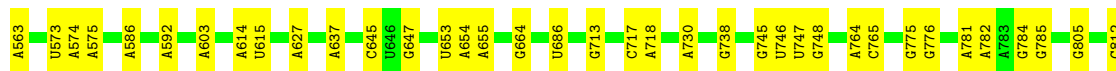
- Molecule 31: Large ribosomal subunit protein bL31A

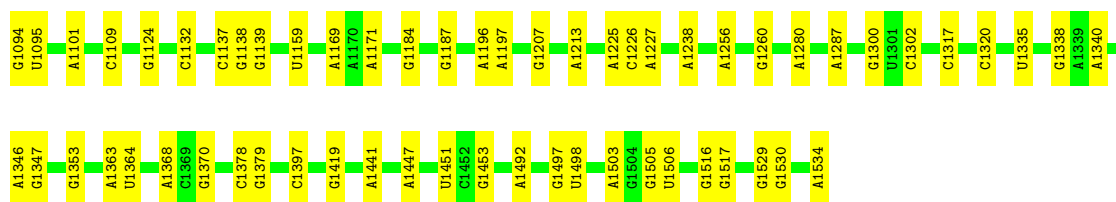
Chain 4:  60% 9% 31%



- Molecule 32: 23S ribosomal RNA

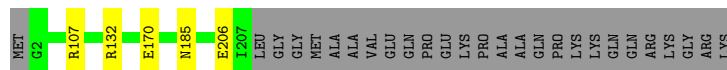
Chain a:  82% 12% 6%





- Molecule 34: Small ribosomal subunit protein uS3

Chain C: 86% 12%



- Molecule 35: Small ribosomal subunit protein uS9

Chain I: 95% 5%



- Molecule 36: Small ribosomal subunit protein uS10

Chain J: 87% 8% 5%



- Molecule 37: Small ribosomal subunit protein uS13

Chain M: 95% 5%



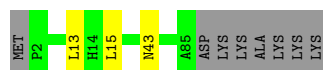
- Molecule 38: Small ribosomal subunit protein uS14

Chain N: 99% 1%




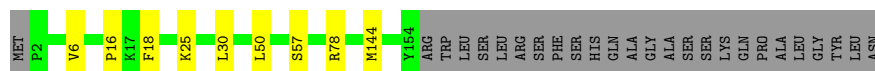
- Molecule 39: Small ribosomal subunit protein uS19

Chain S: 88% 9% 3%



- Molecule 40: 30S ribosomal protein S7

Chain G:  80% 5% 15%



- Molecule 41: 30S ribosomal protein S2

Chain B:  90% 7%



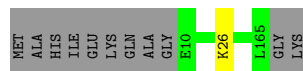
- Molecule 42: Small ribosomal subunit protein uS4

Chain D:  92% 7%



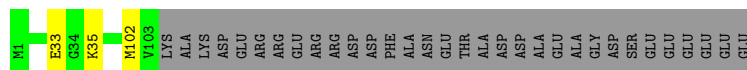
- Molecule 43: Small ribosomal subunit protein uS5

Chain E:  93% 7%



- Molecule 44: 30S ribosomal protein S6, fully modified isoform

Chain F:  74% 24%



- Molecule 45: Small ribosomal subunit protein uS8

Chain H:  95%



- Molecule 46: Small ribosomal subunit protein uS15

Chain O:  98%




- Molecule 47: 30S ribosomal protein S16

Chain P:  94% 5%



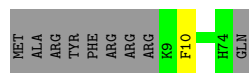
- Molecule 48: Small ribosomal subunit protein uS17

Chain Q:  90% 6%



- Molecule 49: Small ribosomal subunit protein bS18

Chain R:  87% 12%



- Molecule 50: 30S ribosomal protein S20

Chain T:  97%




- Molecule 51: Small ribosomal subunit protein bS21

Chain U:  92% 7%



- Molecule 52: Small ribosomal subunit protein uS11

Chain K:  88% 9%



- Molecule 53: Small ribosomal subunit protein uS12

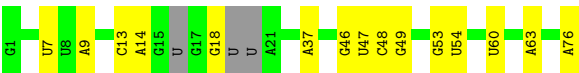
Chain L:  96%



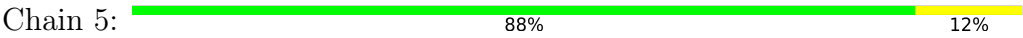
- Molecule 54: Leucine-tRNA



● Molecule 55: Isoleucine-tRNA



● Molecule 56: Paenilamicin B2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13681	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 ($e^-/\text{\AA}^2$)	60	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: 4OC, OMC, DAL, MIA, 1MG, OMG, YF5, YFZ, D2T, SPD, MG, H2U, PSU, K, YFQ, MKX, 5MC, 2MA, ORD, MEQ, 6MZ, IAS, ZN, OMU, 5MU, 4D4, G7M, 2MG, MS6, UR3, 3TD

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	0.39	0/424	0.63	0/565
2	1	0.48	0/380	0.71	0/498
3	2	0.49	0/513	0.66	0/676
4	3	0.43	0/303	0.68	0/397
5	b	0.52	0/2850	0.96	0/4444
6	c	0.43	0/2121	0.67	0/2852
7	d	0.42	0/1576	0.62	0/2119
8	e	0.40	0/1571	0.59	0/2113
9	f	0.36	0/1434	0.58	0/1926
10	g	0.34	0/1343	0.62	0/1816
11	h	0.36	0/306	0.74	0/413
12	i	0.37	0/1152	0.57	0/1551
13	j	0.38	0/955	0.65	0/1279
14	k	0.45	0/1062	0.60	0/1413
15	l	0.37	0/1073	0.61	0/1433
16	m	0.43	0/958	0.64	1/1281 (0.1%)
17	n	0.35	0/902	0.56	0/1209
18	o	0.41	0/929	0.63	0/1242
19	p	0.44	0/960	0.66	0/1278
20	q	0.42	0/829	0.65	0/1107
21	r	0.42	0/864	0.60	0/1156
22	s	0.38	0/744	0.57	0/994
23	t	0.38	0/787	0.64	0/1051
24	u	0.36	0/766	0.60	0/1025
25	v	0.45	0/599	0.58	0/792
26	w	0.44	0/635	0.64	0/848
27	x	0.33	0/502	0.57	0/667
28	y	0.37	0/453	0.59	0/605
29	z	0.46	0/450	0.65	0/599
30	X	0.55	0/236	0.85	0/365
31	4	0.36	0/380	0.60	0/508

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	a	0.60	0/65299	1.00	37/101863 (0.0%)
33	A	0.51	0/36287	0.96	5/56602 (0.0%)
34	C	0.33	0/1651	0.55	0/2225
35	I	0.38	0/1034	0.60	0/1375
36	J	0.34	0/796	0.61	0/1077
37	M	0.35	0/900	0.56	0/1204
38	N	0.35	0/817	0.54	0/1088
39	S	0.35	0/685	0.55	0/922
40	G	0.35	0/1219	0.56	0/1635
41	B	0.35	0/1784	0.56	0/2403
42	D	0.36	0/1665	0.60	0/2227
43	E	0.35	0/1165	0.57	0/1568
44	F	0.34	0/858	0.56	0/1160
45	H	0.35	0/989	0.57	0/1326
46	O	0.36	0/722	0.50	0/964
47	P	0.35	0/653	0.62	0/877
48	Q	0.33	0/650	0.59	0/871
49	R	0.35	0/553	0.56	0/742
50	T	0.34	0/676	0.53	0/895
51	U	0.36	0/597	0.59	0/792
52	K	0.37	0/884	0.57	1/1191 (0.1%)
53	L	0.34	0/960	0.65	0/1286
54	Z	0.58	0/1693	1.01	0/2628
55	Y	0.60	0/1711	0.98	0/2659
56	5	0.52	0/3	1.08	0/2
All	All	0.52	0/152308	0.90	44/227804 (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
32	a	0	5
52	K	0	1
56	5	0	1
All	All	0	7

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	512	G	O4'-C1'-N9	7.95	114.56	108.20
32	a	2724	U	O5'-P-OP2	-6.90	99.49	105.70
32	a	2848	G	O4'-C1'-N9	6.59	113.47	108.20
32	a	1936	A	O4'-C1'-N9	6.39	113.31	108.20
32	a	204	A	O3'-P-O5'	-6.29	92.06	104.00
32	a	1565	C	O3'-P-O5'	-6.22	92.18	104.00
32	a	542	C	O3'-P-O5'	-6.09	92.44	104.00
32	a	1790	C	O5'-P-OP2	-6.03	100.27	105.70
33	A	686	U	C3'-C2'-C1'	-5.96	96.73	101.50
32	a	543	G	O3'-P-O5'	-5.95	92.69	104.00
32	a	748	G	C1'-O4'-C4'	-5.94	105.15	109.90
32	a	1246	A	O3'-P-O5'	-5.93	92.73	104.00
32	a	1025	G	O3'-P-O5'	5.82	115.05	104.00
32	a	2873	A	C1'-O4'-C4'	-5.75	105.30	109.90
32	a	242	G	C3'-C2'-C1'	-5.72	96.93	101.50
32	a	1648	U	O3'-P-O5'	-5.69	93.19	104.00
32	a	781	A	O3'-P-O5'	-5.67	93.23	104.00
32	a	2447	G	C3'-C2'-C1'	-5.65	96.98	101.50
32	a	2050	C	O3'-P-O5'	-5.63	93.31	104.00
52	K	89	PRO	N-CA-CB	-5.62	96.42	102.60
32	a	310	A	O3'-P-O5'	-5.58	93.40	104.00
32	a	2715	C	O5'-P-OP2	-5.56	100.70	105.70
32	a	1128	G	C1'-O4'-C4'	-5.49	105.51	109.90
32	a	1293	C	O3'-P-O5'	-5.48	93.58	104.00
32	a	528	A	O3'-P-O5'	-5.46	93.63	104.00
32	a	1936	A	C1'-O4'-C4'	-5.42	105.57	109.90
33	A	561	U	O3'-P-O5'	-5.41	93.72	104.00
32	a	1969	A	O3'-P-O5'	-5.41	93.72	104.00
32	a	2222	C	O3'-P-O5'	-5.40	93.74	104.00
32	a	574	A	O5'-P-OP1	-5.38	100.85	105.70
32	a	1929	G	O4'-C1'-N9	5.32	112.46	108.20
33	A	746	A	O3'-P-O5'	-5.31	93.91	104.00
32	a	1643	G	O3'-P-O5'	-5.30	93.92	104.00
32	a	2645	G	O4'-C1'-N9	5.26	112.41	108.20
33	A	1347	G	C3'-C2'-C1'	-5.25	97.30	101.50
32	a	512	G	C1'-O4'-C4'	-5.16	105.78	109.90
32	a	2382	G	O3'-P-O5'	-5.14	94.24	104.00
32	a	2761	A	O3'-P-O5'	-5.12	94.26	104.00
16	m	1	MET	CG-SD-CE	-5.11	92.02	100.20
32	a	1025	G	O4'-C1'-N9	-5.08	104.14	108.20
32	a	2446	G	OP2-P-O3'	5.07	116.35	105.20
33	A	1053	G	C3'-C2'-C1'	-5.05	97.46	101.50
32	a	1918	A	O4'-C1'-N9	5.01	112.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	199	A	C1'-O4'-C4'	-5.01	105.89	109.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	5	4	ORD	Peptide
52	K	82	LEU	Peptide
32	a	249	C	Sidechain
32	a	2595	G	Sidechain
32	a	463	G	Sidechain
32	a	512	G	Sidechain
32	a	980	A	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%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	8	11
4	3	36/38 (95%)	36 (100%)	0	0	100	100
6	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
7	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
8	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
9	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	g	174/177 (98%)	167 (96%)	6 (3%)	1 (1%)	22	33
11	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
12	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
13	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
14	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	19	29
15	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
16	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
17	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
18	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
19	p	115/118 (98%)	115 (100%)	0	0	100	100
20	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
21	r	108/110 (98%)	107 (99%)	0	1 (1%)	14	22
22	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
23	t	100/104 (96%)	92 (92%)	7 (7%)	1 (1%)	13	20
24	u	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	12	18
25	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
26	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
27	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
28	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
29	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
31	4	46/70 (66%)	43 (94%)	2 (4%)	1 (2%)	5	6
34	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
35	I	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
36	J	96/103 (93%)	88 (92%)	5 (5%)	3 (3%)	3	3
37	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
38	N	98/101 (97%)	98 (100%)	0	0	100	100
39	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
40	G	151/179 (84%)	142 (94%)	6 (4%)	3 (2%)	6	8
41	B	222/241 (92%)	212 (96%)	10 (4%)	0	100	100
42	D	203/206 (98%)	197 (97%)	4 (2%)	2 (1%)	13	20
43	E	154/167 (92%)	148 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	F	101/135 (75%)	97 (96%)	3 (3%)	1 (1%)	13	20
45	H	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	16	26
46	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	P	79/82 (96%)	69 (87%)	8 (10%)	2 (2%)	4	5
48	Q	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
49	R	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
50	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
51	U	68/71 (96%)	67 (98%)	0	1 (2%)	8	12
52	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
53	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
All	All	5471/5913 (92%)	5269 (96%)	182 (3%)	20 (0%)	32	44

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	G	6	VAL
40	G	57	SER
42	D	10	LYS
42	D	98	LEU
24	u	58	SER
36	J	57	VAL
47	P	51	ARG
51	U	3	VAL
36	J	27	GLU
44	F	33	GLU
47	P	80	LYS
14	k	29	LYS
21	r	12	SER
31	4	4	ASP
10	g	176	LYS
3	2	28	ASN
23	t	39	ILE
36	J	36	VAL
40	G	16	PRO
45	H	75	ILE

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%)	44 (96%)	2 (4%)	25	42
2	1	38/38 (100%)	36 (95%)	2 (5%)	19	33
3	2	51/52 (98%)	46 (90%)	5 (10%)	6	10
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	58
6	c	216/218 (99%)	213 (99%)	3 (1%)	62	79
7	d	163/163 (100%)	159 (98%)	4 (2%)	42	63
8	e	165/165 (100%)	161 (98%)	4 (2%)	44	64
9	f	148/150 (99%)	143 (97%)	5 (3%)	32	52
10	g	137/138 (99%)	129 (94%)	8 (6%)	17	29
11	h	32/114 (28%)	28 (88%)	4 (12%)	3	5
12	i	116/116 (100%)	114 (98%)	2 (2%)	56	75
13	j	104/104 (100%)	102 (98%)	2 (2%)	52	72
14	k	103/103 (100%)	101 (98%)	2 (2%)	52	72
15	l	107/107 (100%)	106 (99%)	1 (1%)	75	88
16	m	98/103 (95%)	96 (98%)	2 (2%)	50	70
17	n	86/87 (99%)	85 (99%)	1 (1%)	67	82
18	o	99/100 (99%)	99 (100%)	0	100	100
19	p	89/90 (99%)	86 (97%)	3 (3%)	32	52
20	q	84/84 (100%)	81 (96%)	3 (4%)	30	49
21	r	93/93 (100%)	91 (98%)	2 (2%)	47	67
22	s	80/84 (95%)	79 (99%)	1 (1%)	65	81
23	t	83/85 (98%)	78 (94%)	5 (6%)	16	27
24	u	78/78 (100%)	76 (97%)	2 (3%)	41	62
25	v	59/63 (94%)	59 (100%)	0	100	100
26	w	67/68 (98%)	65 (97%)	2 (3%)	36	57
27	x	54/55 (98%)	50 (93%)	4 (7%)	11	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	y	48/49 (98%)	48 (100%)	0	100	100
29	z	47/48 (98%)	47 (100%)	0	100	100
31	4	44/62 (71%)	39 (89%)	5 (11%)	4	6
34	C	170/190 (90%)	165 (97%)	5 (3%)	37	58
35	I	105/107 (98%)	102 (97%)	3 (3%)	37	58
36	J	86/90 (96%)	81 (94%)	5 (6%)	17	29
37	M	93/96 (97%)	90 (97%)	3 (3%)	34	54
38	N	83/84 (99%)	83 (100%)	0	100	100
39	S	72/79 (91%)	69 (96%)	3 (4%)	25	43
40	G	126/147 (86%)	120 (95%)	6 (5%)	21	37
41	B	186/199 (94%)	180 (97%)	6 (3%)	34	54
42	D	172/173 (99%)	159 (92%)	13 (8%)	11	18
43	E	119/126 (94%)	118 (99%)	1 (1%)	79	90
44	F	90/116 (78%)	88 (98%)	2 (2%)	47	67
45	H	104/105 (99%)	100 (96%)	4 (4%)	28	47
46	O	76/77 (99%)	75 (99%)	1 (1%)	65	81
47	P	65/65 (100%)	63 (97%)	2 (3%)	35	56
48	Q	73/78 (94%)	70 (96%)	3 (4%)	26	44
49	R	57/65 (88%)	56 (98%)	1 (2%)	54	73
50	T	65/66 (98%)	63 (97%)	2 (3%)	35	56
51	U	60/61 (98%)	56 (93%)	4 (7%)	13	23
52	K	89/98 (91%)	86 (97%)	3 (3%)	32	52
53	L	102/103 (99%)	99 (97%)	3 (3%)	37	58
All	All	4562/4825 (94%)	4417 (97%)	145 (3%)	36	54

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
1	0	54	ILE
2	1	8	SER
2	1	25	LYS
3	2	15	LYS
3	2	31	HIS

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Mol	Chain	Res	Type
3	2	47	LYS
3	2	54	ASP
3	2	57	LEU
4	3	36	ARG
6	c	4	VAL
6	c	37	ASN
6	c	203	ARG
7	d	1	MET
7	d	12	THR
7	d	32	ASN
7	d	157	LYS
8	e	6	LYS
8	e	55	SER
8	e	80	SER
8	e	88	ARG
9	f	42	GLU
9	f	50	LEU
9	f	117	LEU
9	f	140	GLU
9	f	150	ARG
10	g	3	ARG
10	g	18	LYS
10	g	20	ASN
10	g	30	ASN
10	g	43	VAL
10	g	90	VAL
10	g	103	ILE
10	g	155	GLU
11	h	9	VAL
11	h	21	VAL
11	h	37	VAL
11	h	41	LYS
12	i	4	PHE
12	i	5	THR
13	j	49	ARG
13	j	93	GLN
14	k	112	LEU
14	k	129	LYS
15	l	135	VAL
16	m	6	SER
16	m	51	LEU
17	n	2	ASP

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Mol	Chain	Res	Type
19	p	11	ARG
19	p	51	ARG
19	p	112	LYS
20	q	10	LYS
20	q	70	GLU
20	q	71	LYS
21	r	7	HIS
21	r	92	ARG
22	s	64	LYS
23	t	15	THR
23	t	53	ASN
23	t	54	GLN
23	t	74	ASN
23	t	81	ASP
24	u	34	LYS
24	u	61	LEU
26	w	16	ASN
26	w	54	LYS
27	x	8	GLU
27	x	14	LEU
27	x	16	THR
27	x	24	GLU
31	4	20	ASN
31	4	22	MET
31	4	31	ASP
31	4	36	VAL
31	4	48	GLN
34	C	107	ARG
34	C	132	ARG
34	C	170	GLU
34	C	185	ASN
34	C	206	GLU
35	I	85	ARG
35	I	89	GLU
35	I	123	ARG
36	J	5	ARG
36	J	30	LYS
36	J	81	GLU
36	J	83	THR
36	J	88	MET
37	M	16	VAL
37	M	27	LYS

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Mol	Chain	Res	Type
37	M	113	ARG
39	S	13	LEU
39	S	15	LEU
39	S	43	ASN
40	G	18	PHE
40	G	25	LYS
40	G	30	LEU
40	G	50	LEU
40	G	78	ARG
40	G	144	MET
41	B	23	TRP
41	B	63	ARG
41	B	89	GLN
41	B	93	ASN
41	B	105	LYS
41	B	161	LEU
42	D	8	LYS
42	D	14	ARG
42	D	21	LEU
42	D	29	ASP
42	D	45	LYS
42	D	48	LEU
42	D	58	LYS
42	D	116	GLN
42	D	128	ARG
42	D	131	ASN
42	D	138	SER
42	D	183	LYS
42	D	202	GLU
43	E	26	LYS
44	F	35	LYS
44	F	102	MET
45	H	54	ASP
45	H	56	LYS
45	H	60	GLU
45	H	89	LYS
46	O	17	ARG
47	P	1	MET
47	P	56	ARG
48	Q	20	SER
48	Q	65	ARG
48	Q	74	THR

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Mol	Chain	Res	Type
49	R	10	PHE
50	T	40	GLU
50	T	84	ASN
51	U	8	GLU
51	U	21	ARG
51	U	58	LYS
51	U	64	ASN
52	K	72	ASP
52	K	89	PRO
52	K	94	GLU
53	L	18	LYS
53	L	51	LYS
53	L	55	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	31	HIS
6	c	37	ASN
6	c	197	ASN
6	c	243	HIS
9	f	63	GLN
10	g	30	ASN
12	i	128	ASN
13	j	89	ASN
16	m	18	GLN
18	o	12	GLN
19	p	52	GLN
21	r	40	ASN
22	s	48	GLN
23	t	53	ASN
24	u	49	ASN
34	C	139	GLN
34	C	140	ASN
36	J	56	HIS
38	N	35	ASN
40	G	68	ASN
41	B	89	GLN
41	B	103	ASN
42	D	100	ASN
42	D	152	GLN
43	E	82	GLN

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Mol	Chain	Res	Type
46	O	35	GLN
50	T	48	GLN
50	T	52	ASN
50	T	84	ASN
51	U	64	ASN
52	K	81	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	X	9/10 (90%)	1 (11%)	0
32	a	2729/2903 (94%)	297 (10%)	0
33	A	1515/1534 (98%)	198 (13%)	31 (2%)
5	b	118/120 (98%)	9 (7%)	0
54	Z	68/85 (80%)	16 (23%)	4 (5%)
55	Y	69/76 (90%)	11 (15%)	4 (5%)
All	All	4508/4728 (95%)	532 (11%)	39 (0%)

All (532) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	b	25	U
5	b	36	C
5	b	44	G
5	b	56	G
5	b	67	G
5	b	89	U
5	b	90	C
5	b	99	A
5	b	109	A
30	X	14	U
32	a	10	A
32	a	12	U
32	a	34	U
32	a	58	G
32	a	71	A
32	a	74	A
32	a	75	G
32	a	101	A
32	a	102	U
32	a	118	A

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Mol	Chain	Res	Type
32	a	119	A
32	a	120	U
32	a	131	A
32	a	139	U
32	a	142	A
32	a	165	A
32	a	181	A
32	a	196	A
32	a	199	A
32	a	200	U
32	a	215	G
32	a	216	A
32	a	221	A
32	a	222	A
32	a	233	A
32	a	248	G
32	a	272	A
32	a	276	U
32	a	277	G
32	a	278	A
32	a	289	G
32	a	311	A
32	a	329	G
32	a	330	A
32	a	345	A
32	a	353	C
32	a	356	G
32	a	361	G
32	a	386	G
32	a	404	A
32	a	405	U
32	a	411	G
32	a	412	A
32	a	425	G
32	a	451	U
32	a	456	C
32	a	481	G
32	a	491	G
32	a	503	A
32	a	504	A
32	a	505	A
32	a	509	C

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Mol	Chain	Res	Type
32	a	530	G
32	a	532	A
32	a	533	G
32	a	538	A
32	a	545	U
32	a	546	U
32	a	547	A
32	a	548	G
32	a	549	G
32	a	563	A
32	a	573	U
32	a	575	A
32	a	586	A
32	a	592	A
32	a	603	A
32	a	614	A
32	a	615	U
32	a	627	A
32	a	637	A
32	a	645	C
32	a	647	G
32	a	653	U
32	a	654	A
32	a	655	A
32	a	664	G
32	a	686	U
32	a	713	G
32	a	717	C
32	a	718	A
32	a	730	A
32	a	738	G
32	a	747	5MU
32	a	764	A
32	a	765	C
32	a	775	G
32	a	776	G
32	a	782	A
32	a	784	G
32	a	785	G
32	a	805	G
32	a	812	C
32	a	827	U

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Mol	Chain	Res	Type
32	a	828	U
32	a	846	U
32	a	847	U
32	a	858	G
32	a	859	G
32	a	880	G
32	a	881	G
32	a	899	A
32	a	900	A
32	a	907	G
32	a	910	A
32	a	914	G
32	a	915	C
32	a	927	A
32	a	931	U
32	a	934	U
32	a	946	C
32	a	961	C
32	a	974	G
32	a	983	A
32	a	984	A
32	a	985	C
32	a	996	A
32	a	1012	U
32	a	1013	C
32	a	1022	G
32	a	1026	G
32	a	1033	U
32	a	1040	A
32	a	1045	C
32	a	1046	A
32	a	1047	G
32	a	1109	C
32	a	1110	G
32	a	1111	A
32	a	1112	G
32	a	1116	G
32	a	1122	G
32	a	1128	G
32	a	1129	A
32	a	1132	U
32	a	1133	A

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Mol	Chain	Res	Type
32	a	1134	A
32	a	1135	C
32	a	1142	A
32	a	1171	G
32	a	1172	C
32	a	1187	G
32	a	1253	A
32	a	1256	G
32	a	1271	G
32	a	1272	A
32	a	1294	U
32	a	1300	G
32	a	1301	A
32	a	1352	U
32	a	1365	A
32	a	1379	U
32	a	1383	A
32	a	1386	C
32	a	1409	U
32	a	1416	G
32	a	1417	C
32	a	1427	A
32	a	1428	C
32	a	1434	A
32	a	1435	G
32	a	1452	G
32	a	1453	A
32	a	1459	G
32	a	1482	G
32	a	1493	C
32	a	1508	A
32	a	1509	A
32	a	1510	G
32	a	1515	A
32	a	1529	G
32	a	1535	A
32	a	1536	C
32	a	1537	G
32	a	1569	A
32	a	1578	U
32	a	1583	A
32	a	1584	U

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Mol	Chain	Res	Type
32	a	1585	C
32	a	1586	A
32	a	1608	A
32	a	1609	A
32	a	1647	U
32	a	1648	U
32	a	1649	G
32	a	1674	G
32	a	1715	G
32	a	1729	U
32	a	1730	C
32	a	1732	C
32	a	1738	G
32	a	1764	C
32	a	1773	A
32	a	1782	U
32	a	1800	C
32	a	1801	A
32	a	1808	A
32	a	1816	C
32	a	1829	A
32	a	1839	G
32	a	1848	A
32	a	1858	A
32	a	1870	C
32	a	1871	A
32	a	1907	G
32	a	1910	G
32	a	1925	C
32	a	1926	U
32	a	1930	G
32	a	1937	A
32	a	1938	A
32	a	1955	U
32	a	1967	C
32	a	1970	A
32	a	1971	U
32	a	1972	G
32	a	1987	A
32	a	1991	U
32	a	1993	U
32	a	2023	C

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Mol	Chain	Res	Type
32	a	2027	G
32	a	2031	A
32	a	2033	A
32	a	2043	C
32	a	2055	C
32	a	2056	G
32	a	2060	A
32	a	2061	G
32	a	2062	A
32	a	2069	G7M
32	a	2198	A
32	a	2203	U
32	a	2204	G
32	a	2211	A
32	a	2225	A
32	a	2238	G
32	a	2239	G
32	a	2268	A
32	a	2283	C
32	a	2287	A
32	a	2303	G
32	a	2305	U
32	a	2308	G
32	a	2310	C
32	a	2312	U
32	a	2322	A
32	a	2325	G
32	a	2333	A
32	a	2335	A
32	a	2347	C
32	a	2361	G
32	a	2372	U
32	a	2383	G
32	a	2385	C
32	a	2396	G
32	a	2402	U
32	a	2406	A
32	a	2425	A
32	a	2429	G
32	a	2430	A
32	a	2435	A
32	a	2441	U

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Mol	Chain	Res	Type
32	a	2448	A
32	a	2464	G
32	a	2476	A
32	a	2478	A
32	a	2502	G
32	a	2505	G
32	a	2518	A
32	a	2525	G
32	a	2529	G
32	a	2547	A
32	a	2566	A
32	a	2567	G
32	a	2573	C
32	a	2602	A
32	a	2609	U
32	a	2613	U
32	a	2629	U
32	a	2663	G
32	a	2682	A
32	a	2689	U
32	a	2690	U
32	a	2714	G
32	a	2724	U
32	a	2726	A
32	a	2744	G
32	a	2748	A
32	a	2757	A
32	a	2765	A
32	a	2778	A
32	a	2791	G
32	a	2798	U
32	a	2800	A
32	a	2820	A
32	a	2821	A
32	a	2884	U
33	A	4	U
33	A	5	U
33	A	7	A
33	A	9	G
33	A	22	G
33	A	32	A
33	A	39	G

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Mol	Chain	Res	Type
33	A	44	A
33	A	47	C
33	A	48	C
33	A	51	A
33	A	71	A
33	A	72	A
33	A	75	G
33	A	83	C
33	A	84	U
33	A	85	U
33	A	87	C
33	A	88	U
33	A	94	G
33	A	95	C
33	A	119	A
33	A	120	A
33	A	122	G
33	A	131	A
33	A	142	G
33	A	144	G
33	A	159	G
33	A	163	C
33	A	164	G
33	A	182	A
33	A	197	A
33	A	226	G
33	A	240	G
33	A	245	U
33	A	247	G
33	A	251	G
33	A	266	G
33	A	267	C
33	A	289	G
33	A	321	A
33	A	328	C
33	A	329	A
33	A	345	C
33	A	347	G
33	A	348	G
33	A	352	C
33	A	354	G
33	A	367	U

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Mol	Chain	Res	Type
33	A	372	C
33	A	376	G
33	A	391	G
33	A	392	C
33	A	406	G
33	A	412	A
33	A	413	G
33	A	414	A
33	A	417	G
33	A	421	U
33	A	422	C
33	A	423	G
33	A	424	G
33	A	429	U
33	A	430	A
33	A	439	U
33	A	446	G
33	A	451	A
33	A	453	G
33	A	456	A
33	A	457	G
33	A	458	U
33	A	467	U
33	A	468	A
33	A	481	G
33	A	484	G
33	A	486	U
33	A	511	C
33	A	513	C
33	A	518	C
33	A	530	G
33	A	531	U
33	A	532	A
33	A	533	A
33	A	542	G
33	A	547	A
33	A	559	A
33	A	572	A
33	A	573	A
33	A	576	C
33	A	577	G
33	A	579	A

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Mol	Chain	Res	Type
33	A	588	G
33	A	596	A
33	A	633	G
33	A	642	A
33	A	650	G
33	A	653	U
33	A	654	G
33	A	656	G
33	A	661	G
33	A	665	A
33	A	723	U
33	A	724	G
33	A	734	G
33	A	748	G
33	A	755	G
33	A	777	A
33	A	793	U
33	A	794	A
33	A	815	A
33	A	817	C
33	A	851	G
33	A	857	C
33	A	874	G
33	A	887	G
33	A	890	G
33	A	914	A
33	A	926	G
33	A	934	C
33	A	935	A
33	A	936	C
33	A	958	A
33	A	960	U
33	A	966	2MG
33	A	969	A
33	A	975	A
33	A	976	G
33	A	977	A
33	A	978	A
33	A	984	C
33	A	993	G
33	A	994	A
33	A	996	A

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Mol	Chain	Res	Type
33	A	1003	G
33	A	1004	A
33	A	1005	A
33	A	1008	U
33	A	1009	U
33	A	1027	C
33	A	1028	C
33	A	1031	C
33	A	1033	G
33	A	1034	G
33	A	1036	A
33	A	1044	A
33	A	1065	U
33	A	1085	U
33	A	1094	G
33	A	1095	U
33	A	1101	A
33	A	1132	C
33	A	1137	C
33	A	1138	G
33	A	1139	G
33	A	1159	U
33	A	1169	A
33	A	1171	A
33	A	1184	G
33	A	1187	G
33	A	1196	A
33	A	1197	A
33	A	1213	A
33	A	1225	A
33	A	1226	C
33	A	1227	A
33	A	1238	A
33	A	1256	A
33	A	1260	G
33	A	1280	A
33	A	1287	A
33	A	1300	G
33	A	1302	C
33	A	1317	C
33	A	1320	C
33	A	1338	G

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Mol	Chain	Res	Type
33	A	1340	A
33	A	1346	A
33	A	1353	G
33	A	1363	A
33	A	1364	U
33	A	1368	A
33	A	1370	G
33	A	1378	C
33	A	1379	G
33	A	1397	C
33	A	1419	G
33	A	1441	A
33	A	1451	U
33	A	1453	G
33	A	1492	A
33	A	1497	G
33	A	1503	A
33	A	1505	G
33	A	1506	U
33	A	1517	G
33	A	1529	G
33	A	1530	G
33	A	1534	A
54	Z	4	G
54	Z	5	A
54	Z	6	A
54	Z	7	G
54	Z	8	U
54	Z	19	G
54	Z	23	A
54	Z	24	C
54	Z	43	A
54	Z	44	C
54	Z	45	C
54	Z	46	G
54	Z	47	U
54	Z	58	G
54	Z	70	C
54	Z	85	A
55	Y	9	A
55	Y	14	A
55	Y	18	G

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Mol	Chain	Res	Type
55	Y	46	G
55	Y	47	U
55	Y	48	C
55	Y	49	G
55	Y	53	G
55	Y	54	U
55	Y	63	A
55	Y	76	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	A	7	A
33	A	70	U
33	A	83	C
33	A	86	G
33	A	94	G
33	A	119	A
33	A	199	A
33	A	367	U
33	A	412	A
33	A	429	U
33	A	438	U
33	A	485	U
33	A	530	G
33	A	532	A
33	A	587	G
33	A	641	U
33	A	653	U
33	A	733	G
33	A	776	G
33	A	793	U
33	A	858	G
33	A	992	U
33	A	1008	U
33	A	1035	A
33	A	1045	C
33	A	1046	A
33	A	1109	C
33	A	1124	G
33	A	1225	A
33	A	1335	U

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Mol	Chain	Res	Type
33	A	1447	A
54	Z	6	A
54	Z	7	G
54	Z	22	G
54	Z	44	C
55	Y	7	U
55	Y	13	C
55	Y	46	G
55	Y	60	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	ORD	5	4	56	6,7,8	0.51	0	2,7,9	0.29	0
32	PSU	a	2605	32	18,21,22	0.96	1 (5%)	22,30,33	0.91	1 (4%)
33	4OC	A	1402	33	20,23,24	0.39	0	26,32,35	0.64	0
33	2MG	A	966	33	18,26,27	1.11	2 (11%)	16,38,41	0.63	0
32	1MG	a	745	32	18,26,27	1.15	3 (16%)	19,39,42	0.43	0
32	H2U	a	2449	32	18,21,22	0.73	1 (5%)	21,30,33	0.87	2 (9%)
32	PSU	a	955	32	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
32	5MC	a	1962	32	18,22,23	0.43	0	26,32,35	0.73	0
33	5MC	A	1407	33	18,22,23	0.32	0	26,32,35	0.74	0
54	MIA	Z	38	54	24,31,32	0.79	1 (4%)	26,44,47	3.28	2 (7%)
32	6MZ	a	1618	32	18,25,26	0.62	0	16,36,39	0.80	1 (6%)
32	6MZ	a	2030	32	18,25,26	0.75	0	16,36,39	0.81	1 (6%)
33	UR3	A	1498	33	19,22,23	0.34	0	26,32,35	0.71	1 (3%)
33	2MG	A	1207	33	18,26,27	1.02	2 (11%)	16,38,41	0.75	0
33	5MC	A	967	33	18,22,23	0.36	0	26,32,35	0.61	0
55	MKX	Y	37	55	27,33,35	0.85	1 (3%)	29,49,54	1.32	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	2MG	a	1835	32	18,26,27	1.04	2 (11%)	16,38,41	0.73	0
33	G7M	A	527	33	20,26,27	1.11	2 (10%)	17,39,42	0.67	0
32	5MU	a	747	32	19,22,23	0.35	0	28,32,35	0.40	0
32	PSU	a	1911	32	18,21,22	0.92	1 (5%)	22,30,33	0.65	0
33	PSU	A	516	58,33	18,21,22	1.02	1 (5%)	22,30,33	0.77	1 (4%)
32	PSU	a	2504	32	18,21,22	0.96	1 (5%)	22,30,33	0.75	0
32	PSU	a	2604	32	18,21,22	1.02	1 (5%)	22,30,33	0.83	0
32	G7M	a	2069	32	20,26,27	1.17	3 (15%)	17,39,42	0.60	0
32	2MA	a	2503	58,32	19,25,26	1.23	3 (15%)	21,37,40	1.68	4 (19%)
56	YFZ	5	5	56	11,11,12	0.42	0	9,13,15	0.69	0
32	2MG	a	2445	32	18,26,27	1.21	3 (16%)	16,38,41	0.75	0
32	OMU	a	2552	32	19,22,23	0.34	0	26,31,34	0.46	0
15	4D4	l	81	15	9,11,12	0.59	0	8,13,15	0.56	0
32	PSU	a	2580	58,32	18,21,22	1.04	1 (5%)	22,30,33	0.73	0
32	PSU	a	2457	32	18,21,22	1.03	1 (5%)	22,30,33	0.69	0
32	5MU	a	1939	32	19,22,23	0.49	0	28,32,35	0.36	0
53	D2T	L	89	53	7,9,10	0.94	0	6,11,13	1.74	3 (50%)
56	YF5	5	1	56	15,17,18	0.48	0	16,21,23	0.88	0
56	YFQ	5	3	56	3,6,7	0.69	0	0,6,8	-	-
52	IAS	K	119	52	6,7,8	0.87	0	6,8,10	0.95	0
56	DAL	5	2	56	3,4,5	0.57	0	2,4,6	1.06	0
33	2MG	A	1516	33	18,26,27	1.11	2 (11%)	16,38,41	0.81	0
32	OMC	a	2498	58,32	19,22,23	0.47	0	26,31,34	0.58	0
32	3TD	a	1915	32	18,22,23	0.96	1 (5%)	22,32,35	0.78	0
32	PSU	a	1917	32	18,21,22	0.93	1 (5%)	22,30,33	0.63	0
32	OMG	a	2251	55,32	18,26,27	1.11	3 (16%)	19,38,41	0.67	0
7	MEQ	d	150	7	8,9,10	0.54	0	5,10,12	0.85	0
56	YFQ	5	6	56	3,6,7	0.74	0	0,6,8	-	-
32	PSU	a	746	58,32	18,21,22	0.98	1 (5%)	22,30,33	0.60	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
56	ORD	5	4	56	-	2/5/6/8	-
32	PSU	a	2605	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	4OC	A	1402	33	-	0/9/29/30	0/2/2/2
33	2MG	A	966	33	-	0/5/27/28	0/3/3/3
32	1MG	a	745	32	-	0/3/25/26	0/3/3/3
32	H2U	a	2449	32	-	0/7/38/39	0/2/2/2
32	PSU	a	955	32	-	0/7/25/26	0/2/2/2
32	5MC	a	1962	32	-	2/7/25/26	0/2/2/2
33	5MC	A	1407	33	-	0/7/25/26	0/2/2/2
54	MIA	Z	38	54	-	2/11/33/34	0/3/3/3
32	6MZ	a	1618	32	-	0/5/27/28	0/3/3/3
32	6MZ	a	2030	32	-	1/5/27/28	0/3/3/3
33	UR3	A	1498	33	-	0/7/25/26	0/2/2/2
33	2MG	A	1207	33	-	0/5/27/28	0/3/3/3
33	5MC	A	967	33	-	0/7/25/26	0/2/2/2
55	MKX	Y	37	55	-	4/10/48/50	0/4/4/4
32	2MG	a	1835	32	-	0/5/27/28	0/3/3/3
33	G7M	A	527	33	-	1/3/25/26	0/3/3/3
32	5MU	a	747	32	-	0/7/25/26	0/2/2/2
32	PSU	a	1911	32	-	0/7/25/26	0/2/2/2
33	PSU	A	516	58,33	-	0/7/25/26	0/2/2/2
32	PSU	a	2504	32	-	0/7/25/26	0/2/2/2
32	PSU	a	2604	32	-	0/7/25/26	0/2/2/2
32	G7M	a	2069	32	-	2/3/25/26	0/3/3/3
32	2MA	a	2503	58,32	-	1/3/25/26	0/3/3/3
56	YFZ	5	5	56	-	3/13/13/14	-
32	2MG	a	2445	32	-	0/5/27/28	0/3/3/3
32	OMU	a	2552	32	-	0/9/27/28	0/2/2/2
15	4D4	l	81	15	-	3/11/12/14	-
32	PSU	a	2580	58,32	-	0/7/25/26	0/2/2/2
32	PSU	a	2457	32	-	0/7/25/26	0/2/2/2
32	5MU	a	1939	32	-	0/7/25/26	0/2/2/2
53	D2T	L	89	53	-	3/7/12/14	-
56	YF5	5	1	56	-	4/19/21/23	-
56	YFQ	5	3	56	-	0/2/5/7	-
52	IAS	K	119	52	-	0/7/7/8	-
56	DAL	5	2	56	-	0/0/2/4	-
33	2MG	A	1516	33	-	0/5/27/28	0/3/3/3
32	OMC	a	2498	58,32	-	0/9/27/28	0/2/2/2
32	3TD	a	1915	32	-	2/7/25/26	0/2/2/2
32	PSU	a	1917	32	-	0/7/25/26	0/2/2/2
32	OMG	a	2251	55,32	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEQ	d	150	7	-	2/8/9/11	-
56	YFQ	5	6	56	-	0/2/5/7	-
32	PSU	a	746	58,32	-	1/7/25/26	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	516	PSU	C6-C5	3.96	1.39	1.35
32	a	1915	3TD	C6-C5	3.64	1.39	1.35
32	a	2604	PSU	C6-C5	3.62	1.39	1.35
32	a	1917	PSU	C6-C5	3.59	1.39	1.35
32	a	1911	PSU	C6-C5	3.58	1.39	1.35
32	a	2580	PSU	C6-C5	3.58	1.39	1.35
32	a	2457	PSU	C6-C5	3.51	1.39	1.35
33	A	527	G7M	C8-N9	3.43	1.39	1.33
32	a	746	PSU	C6-C5	3.42	1.39	1.35
32	a	2069	G7M	C8-N9	3.20	1.39	1.33
32	a	2605	PSU	C6-C5	3.12	1.39	1.35
32	a	2445	2MG	C5-C6	-3.11	1.41	1.47
32	a	2504	PSU	C6-C5	3.11	1.38	1.35
32	a	2251	OMG	C5-C6	-3.01	1.41	1.47
32	a	2069	G7M	C5-C6	-2.87	1.38	1.45
32	a	955	PSU	C6-C5	2.87	1.38	1.35
33	A	1516	2MG	C5-C6	-2.67	1.42	1.47
33	A	527	G7M	C8-N7	2.61	1.37	1.33
32	a	2503	2MA	C6-N1	2.61	1.38	1.33
32	a	745	1MG	C5-C4	-2.59	1.36	1.43
33	A	966	2MG	C5-C6	-2.57	1.42	1.47
32	a	1835	2MG	C5-C6	-2.46	1.42	1.47
32	a	2251	OMG	C8-N7	-2.41	1.30	1.35
33	A	1207	2MG	C5-C6	-2.36	1.42	1.47
32	a	745	1MG	C5-C6	-2.35	1.40	1.47
32	a	2503	2MA	C2-N1	2.25	1.38	1.34
54	Z	38	MIA	C6-N1	2.21	1.35	1.32
32	a	2251	OMG	C5-C4	-2.21	1.37	1.43
32	a	2069	G7M	C8-N7	2.21	1.37	1.33
55	Y	37	MKX	C8-N7	-2.20	1.30	1.34
33	A	966	2MG	C8-N7	-2.20	1.31	1.35
32	a	2503	2MA	C2-N3	2.16	1.37	1.34
33	A	1207	2MG	C8-N7	-2.13	1.31	1.35
32	a	745	1MG	C6-N1	2.09	1.43	1.39
32	a	2449	H2U	C2-N3	-2.08	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	2445	2MG	C5-C4	-2.08	1.37	1.43
33	A	1516	2MG	C8-N7	-2.05	1.31	1.35
32	a	1835	2MG	C8-N7	-2.03	1.31	1.35
32	a	2445	2MG	C8-N7	-2.02	1.31	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Z	38	MIA	C11-S10-C2	16.06	114.26	102.27
32	a	2503	2MA	C5-C6-N1	-4.84	117.83	121.01
55	Y	37	MKX	C14-C12-N11	-3.48	109.76	113.75
32	a	2503	2MA	C5-C6-N6	3.45	125.60	120.35
54	Z	38	MIA	C5-C6-N1	-3.10	118.23	120.81
32	a	2503	2MA	CM2-C2-N1	3.05	121.92	117.15
55	Y	37	MKX	C13-N6-C10	-2.95	108.47	111.28
55	Y	37	MKX	C6-N6-C10	2.86	126.69	123.20
32	a	2503	2MA	N3-C2-N1	-2.64	120.90	125.73
53	L	89	D2T	OD1-CG-CB	-2.51	117.18	122.44
33	A	516	PSU	C3'-C2'-C1'	2.47	104.51	101.64
55	Y	37	MKX	C14-C12-C13	2.38	115.44	109.52
32	a	2449	H2U	N3-C2-N1	2.33	119.12	116.65
53	L	89	D2T	OD2-CG-CB	2.18	117.86	113.15
53	L	89	D2T	O-C-CA	-2.15	119.14	124.78
32	a	2605	PSU	C2'-C3'-C4'	-2.12	98.52	102.64
32	a	2449	H2U	O2-C2-N1	-2.08	120.50	123.11
32	a	2030	6MZ	C2-N1-C6	2.05	118.35	116.59
32	a	1618	6MZ	C2-N1-C6	2.04	118.34	116.59
33	A	1498	UR3	C6-N1-C2	-2.04	119.96	121.79

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	L	89	D2T	O-C-CA-CB
55	Y	37	MKX	C5-C6-N6-C10
55	Y	37	MKX	C5-C6-N6-C13
55	Y	37	MKX	N1-C6-N6-C10
55	Y	37	MKX	N1-C6-N6-C13
32	a	1915	3TD	O4'-C1'-C5-C4
32	a	1915	3TD	O4'-C1'-C5-C6
56	5	4	ORD	O-C-CA-CB
56	5	5	YFZ	CD-CE-CZ-OH

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Mol	Chain	Res	Type	Atoms
56	5	5	YFZ	N-CE-CZ-OH
54	Z	38	MIA	O4'-C4'-C5'-O5'
54	Z	38	MIA	C3'-C4'-C5'-O5'
56	5	1	YF5	CZ-CZ1-CZ2-NZ3
7	d	150	MEQ	NE2-CD-CG-CB
7	d	150	MEQ	OE1-CD-CG-CB
56	5	1	YF5	CE-CZ-CZ1-CZ2
56	5	4	ORD	C-CA-CB-CG
15	l	81	4D4	NH1-CZ-NE-CD
56	5	1	YF5	NZ6-CZ4-NZ3-CZ2
56	5	1	YF5	NZ5-CZ4-NZ3-CZ2
56	5	5	YFZ	O-C-CA-CB
32	a	2069	G7M	C4'-C5'-O5'-P
15	l	81	4D4	CG-CD-NE-CZ
53	L	89	D2T	SB-CB-CG-OD2
32	a	2030	6MZ	O4'-C4'-C5'-O5'
32	a	1962	5MC	O4'-C1'-N1-C6
53	L	89	D2T	CG-CB-SB-CB1
32	a	746	PSU	O4'-C1'-C5-C6
32	a	2069	G7M	O4'-C4'-C5'-O5'
32	a	2503	2MA	O4'-C4'-C5'-O5'
32	a	1962	5MC	C2'-C1'-N1-C6
15	l	81	4D4	O-C-CA-CB
33	A	527	G7M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 311 ligands modelled in this entry, 311 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.