



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 02:51 pm GMT

PDB ID : 8R6C  
EMDB ID : EMD-18950  
Title : 70S Escherichia coli ribosome with Paenilamicin B2 bound with A- and P-site tRNA.  
Authors : Koller, T.O.; Wilson, D.N.  
Deposited on : 2023-11-22  
Resolution : 2.20 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](mailto: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>.

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

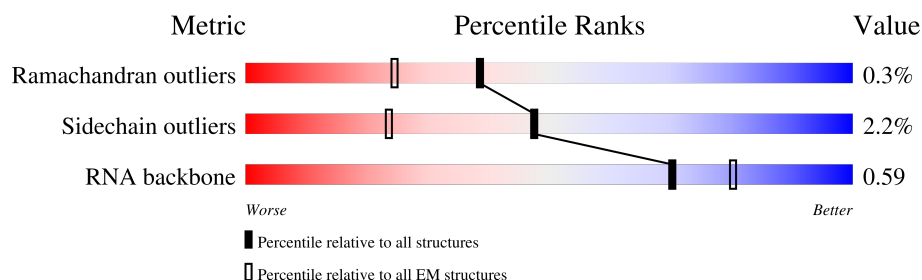
EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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 2.20 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.



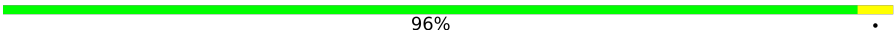
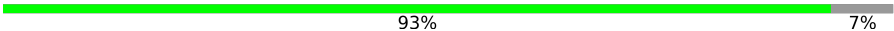


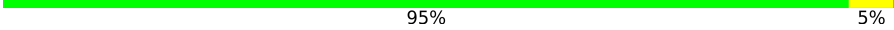
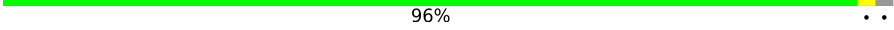


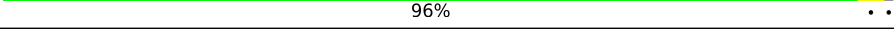
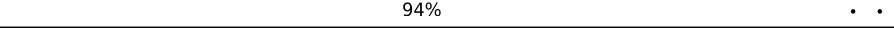
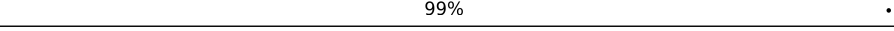
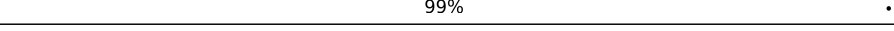
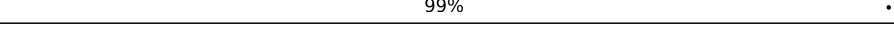
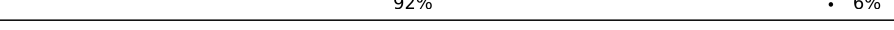


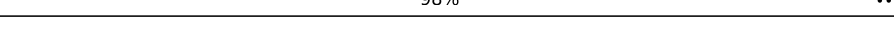
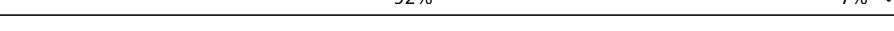
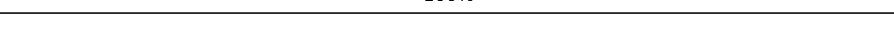
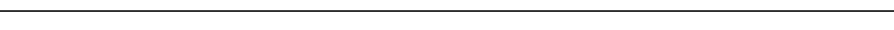

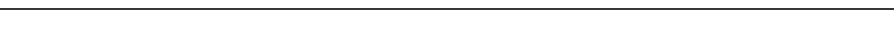
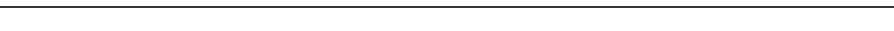


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	89% 7%
2	1	46	98% .
3	2	65	92% 6% .
4	3	38	97% .
5	4	70	84% 14%
6	5	77	97%
7	A	1534	84% 15% .
8	B	241	90% 7%
9	C	233	88% 12%


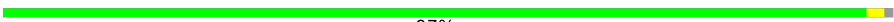









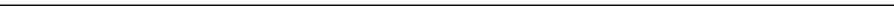


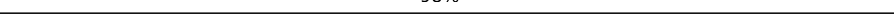


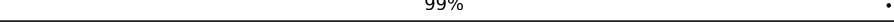
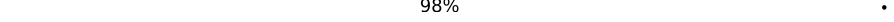
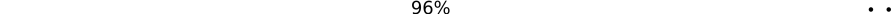
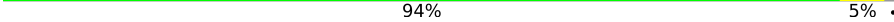
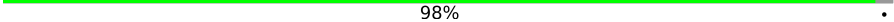
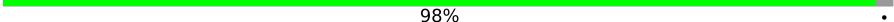
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Mol	Chain	Length	Quality of chain
10	D	206	
11	E	167	
12	F	135	
13	G	179	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	U	71	
28	X	10	
29	Y	76	
30	Z	85	
31	a	2903	
32	b	120	
33	c	273	
34	d	209	

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Mol	Chain	Length	Quality of chain
35	e	201	 100%
36	f	179	 97% ..
37	g	177	 96% ..
38	h	149	 27% . 72%
39	i	142	 100%
40	j	123	 94% . .
41	k	144	 98% .
42	l	136	 99% .
43	m	127	 92% . 7%
44	n	117	 98% ..
45	o	115	 99% .
46	p	118	 97% ..
47	q	103	 95% 5%
48	r	110	 98% .
49	s	100	 90% .. 7%
50	t	104	 91% 7% .
51	u	94	 99% .
52	v	85	 98% .
53	w	78	 96% ..
54	x	63	 94% 5% .
55	y	59	 98% .
56	z	57	 98% .
57	6	8	 88% 12%

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 145010 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 protein called Large ribosomal subunit protein bL31A.

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 N-Formylmethionine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

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

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

- Molecule 8 is a protein called 30S ribosomal protein S2.

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

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

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

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

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

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

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

- Molecule 12 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

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

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

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

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

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

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS10.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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 18 is a protein called Small ribosomal subunit protein uS12.

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

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

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

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

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called 30S ribosomal protein S20.

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

- Molecule 27 is a protein called Small ribosomal subunit protein bS21.



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

- Molecule 28 is a RNA chain called mRNA.

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

- Molecule 29 is a RNA chain called Isoeucine-tRNA.

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

- Molecule 30 is a RNA chain called Leucine-tRNA.

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	118	Total	C	N	O	S	0	0
			901	567	170	158	6		

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

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	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 43 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	83	Total	C	N	O	S	0	0
			629	388	128	112	1		

- Molecule 53 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 55 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 56 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 57 is a protein called Paenilamicin B2.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	6	8	Total	C	N	O	0	0
			71	42	16	13		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	3	1	Total	Zn	0
			1	1	
58	4	1	Total	Zn	0
			1	1	

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	A	90	Total	Mg	0
			90	90	
59	N	1	Total	Mg	0
			1	1	
59	X	1	Total	Mg	0
			1	1	
59	a	206	Total	Mg	0
			206	206	
59	b	5	Total	Mg	0
			5	5	

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Mol	Chain	Residues	Atoms		AltConf
59	c	1	Total 1	Mg 1	0
59	d	2	Total 2	Mg 2	0
59	p	1	Total 1	Mg 1	0
59	z	1	Total 1	Mg 1	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
60	A	1	Total 1	K 1	0
60	a	1	Total 1	K 1	0
60	d	1	Total 1	K 1	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	0	6	Total 6	O 6	0
61	1	7	Total 7	O 7	0
61	2	15	Total 15	O 15	0
61	3	1	Total 1	O 1	0
61	A	317	Total 317	O 317	0
61	B	2	Total 2	O 2	0
61	C	1	Total 1	O 1	0
61	D	1	Total 1	O 1	0
61	E	2	Total 2	O 2	0
61	F	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
61	G	1	Total 1	O 1	0
61	H	1	Total 1	O 1	0
61	I	1	Total 1	O 1	0
61	J	1	Total 1	O 1	0
61	K	2	Total 2	O 2	0
61	L	4	Total 4	O 4	0
61	M	2	Total 2	O 2	0
61	N	1	Total 1	O 1	0
61	O	1	Total 1	O 1	0
61	U	1	Total 1	O 1	0
61	X	9	Total 9	O 9	0
61	Y	3	Total 3	O 3	0
61	Z	6	Total 6	O 6	0
61	a	2502	Total 2502	O 2502	0
61	b	25	Total 25	O 25	0
61	c	49	Total 49	O 49	0
61	d	34	Total 34	O 34	0
61	e	28	Total 28	O 28	0
61	g	2	Total 2	O 2	0
61	h	1	Total 1	O 1	0
61	i	12	Total 12	O 12	0

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Mol	Chain	Residues	Atoms		AltConf
61	j	8	Total 8	O 8	0
61	k	21	Total 21	O 21	0
61	l	14	Total 14	O 14	0
61	m	11	Total 11	O 11	0
61	n	2	Total 2	O 2	0
61	o	7	Total 7	O 7	0
61	p	27	Total 27	O 27	0
61	q	9	Total 9	O 9	0
61	r	18	Total 18	O 18	0
61	s	2	Total 2	O 2	0
61	t	4	Total 4	O 4	0
61	u	5	Total 5	O 5	0
61	v	8	Total 8	O 8	0
61	w	6	Total 6	O 6	0
61	x	1	Total 1	O 1	0
61	y	3	Total 3	O 3	0
61	z	17	Total 17	O 17	0
61	6	6	Total 6	O 6	0

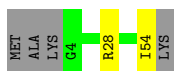


### 3 Residue-property plots [i](#)

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:  98%



- Molecule 3: Large ribosomal subunit protein bL35

Chain 2:  92% 6%




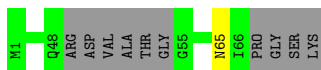
- Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:  97%



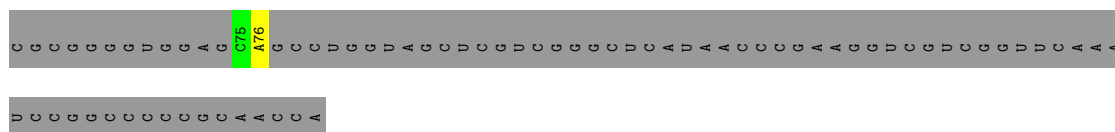
- Molecule 5: Large ribosomal subunit protein bL31A

Chain 4:  84% 14%



- Molecule 6: N-Formylmethionine tRNA

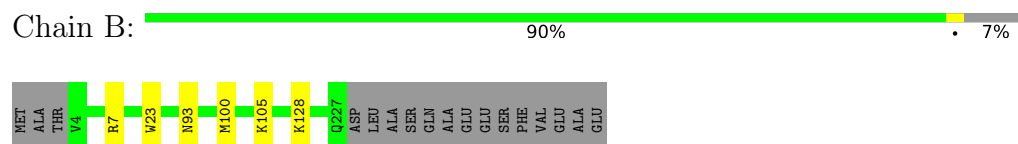
Chain 5:  97%



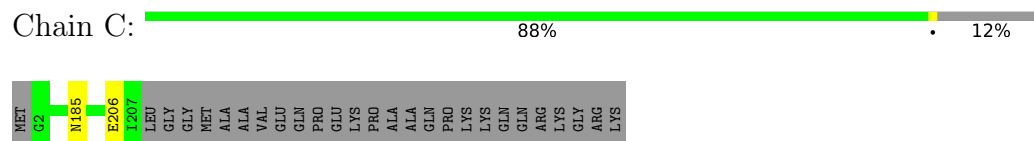
• Molecule 7: 16S ribosomal RNA



• Molecule 8: 30S ribosomal protein S2



• Molecule 9: Small ribosomal subunit protein uS3



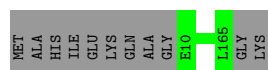
• Molecule 10: Small ribosomal subunit protein uS4





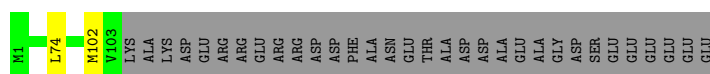
- Molecule 11: Small ribosomal subunit protein uS5

Chain E: 93% 7%



- Molecule 12: 30S ribosomal protein S6, fully modified isoform

Chain F: 75% 24%



- Molecule 13: 30S ribosomal protein S7

Chain G: 81% 15%



- Molecule 14: Small ribosomal subunit protein uS8

Chain H: 95% 5%



- Molecule 15: Small ribosomal subunit protein uS9

Chain I: 96% 2%



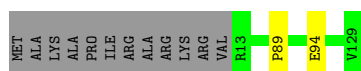
- Molecule 16: Small ribosomal subunit protein uS10

Chain J: 90% 5% 5%



- Molecule 17: Small ribosomal subunit protein uS11

Chain K: 89% 9%



- Molecule 18: Small ribosomal subunit protein uS12

Chain L: 96%



- Molecule 19: Small ribosomal subunit protein uS13

Chain M: 94%



- Molecule 20: Small ribosomal subunit protein uS14

Chain N: 99%



- Molecule 21: Small ribosomal subunit protein uS15

Chain O: 99%



- Molecule 22: 30S ribosomal protein S16

Chain P: 99%



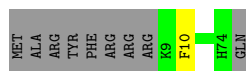
- Molecule 23: Small ribosomal subunit protein uS17

Chain Q: 92% 6%



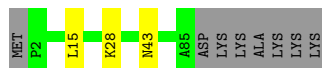
- Molecule 24: Small ribosomal subunit protein bS18

Chain R: 87% 12%



- Molecule 25: Small ribosomal subunit protein uS19

Chain S: 88% 9%



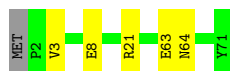
- Molecule 26: 30S ribosomal protein S20

Chain T: 98%



- Molecule 27: Small ribosomal subunit protein bS21

Chain U: 92% 7%



- Molecule 28: mRNA

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 29: Isoeucine-tRNA

Chain Y: 84% 12%



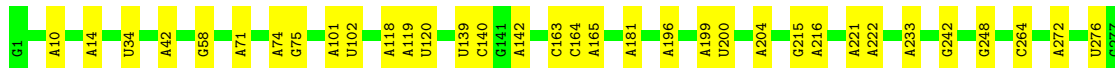
- Molecule 30: Leucine-tRNA

Chain Z: 68% 16% 15%



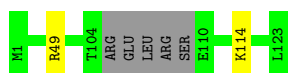
- Molecule 31: 23S ribosomal RNA

Chain a: 82% 12% 5%









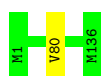
- Molecule 41: 50S ribosomal protein L15

Chain k: 98% .



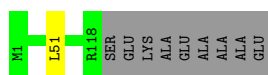
- Molecule 42: Large ribosomal subunit protein uL16

Chain l: 99% .



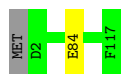
- Molecule 43: Large ribosomal subunit protein bL17

Chain m: 92% • 7%



- Molecule 44: Large ribosomal subunit protein uL18

Chain n: 98% ..



- Molecule 45: Large ribosomal subunit protein bL19

Chain o: 99% .



- Molecule 46: Large ribosomal subunit protein bL20

Chain p: 97% ..



- Molecule 47: Large ribosomal subunit protein bL21

Chain q: 95% 5%





- Molecule 48: Large ribosomal subunit protein uL22

Chain r: 98% .



- Molecule 49: Large ribosomal subunit protein uL23

Chain s: 90% .. 7%



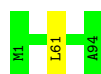
- Molecule 50: Large ribosomal subunit protein uL24

Chain t: 91% 7% .



- Molecule 51: 50S ribosomal protein L25

Chain u: 99% .



- Molecule 52: Large ribosomal subunit protein bL27

Chain v: 98% .



- Molecule 53: Large ribosomal subunit protein bL28

Chain w: 96% ..



- Molecule 54: Large ribosomal subunit protein uL29

Chain x: 94% 5% .



- Molecule 55: Large ribosomal subunit protein uL30

Chain y:  98% .




- Molecule 56: Large ribosomal subunit protein bL32

Chain z:  98% .



- Molecule 57: Paenilamicin B2

Chain 6:  88% 12%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176827	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: D2T, 4D4, 2MA, H2U, MS6, 1MG, ORD, PSU, G7M, 6MZ, YF5, ZN, MEQ, IAS, 4OC, MKX, OMG, MIA, OMC, 5MU, UR3, YFZ, SPD, MG, 5MC, K, OMU, YFQ, DAL, 3TD, 2MG

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	0.62	0/565
2	1	0.44	0/380	0.76	0/498
3	2	0.45	0/513	0.68	0/676
4	3	0.44	0/303	0.71	0/397
5	4	0.39	0/488	0.58	0/649
6	5	0.77	0/46	0.93	0/69
7	A	0.52	0/36287	0.97	6/56602 (0.0%)
8	B	0.36	0/1784	0.59	0/2403
9	C	0.35	0/1651	0.59	0/2225
10	D	0.35	0/1665	0.60	0/2227
11	E	0.37	0/1165	0.61	0/1568
12	F	0.34	0/858	0.60	0/1160
13	G	0.36	0/1219	0.61	0/1635
14	H	0.36	0/989	0.62	0/1326
15	I	0.38	0/1034	0.62	0/1375
16	J	0.35	0/796	0.66	0/1077
17	K	0.38	0/884	0.60	0/1191
18	L	0.36	0/960	0.69	0/1286
19	M	0.36	0/900	0.63	0/1204
20	N	0.36	0/817	0.58	0/1088
21	O	0.35	0/722	0.54	0/964
22	P	0.34	0/653	0.64	0/877
23	Q	0.34	0/650	0.63	0/871
24	R	0.36	0/553	0.63	0/742
25	S	0.37	0/685	0.61	0/922
26	T	0.34	0/676	0.54	0/895
27	U	0.38	0/597	0.68	0/792
28	X	0.67	0/236	0.93	0/365
29	Y	0.57	0/1711	0.96	0/2659
30	Z	0.61	0/1693	1.00	0/2628
31	a	0.58	0/65651	1.02	53/102413 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	b	0.51	0/2850	0.98	0/4444
33	c	0.40	0/2121	0.70	0/2852
34	d	0.40	0/1576	0.63	0/2119
35	e	0.38	0/1571	0.61	0/2113
36	f	0.35	0/1434	0.58	0/1926
37	g	0.35	0/1343	0.63	0/1816
38	h	0.36	0/306	0.68	0/413
39	i	0.38	0/1152	0.59	0/1551
40	j	0.39	0/909	0.65	0/1217
41	k	0.43	0/1062	0.60	0/1413
42	l	0.37	0/1073	0.65	0/1433
43	m	0.40	0/958	0.70	0/1281
44	n	0.36	0/902	0.60	0/1209
45	o	0.41	0/929	0.65	0/1242
46	p	0.42	0/960	0.66	0/1278
47	q	0.42	0/829	0.66	0/1107
48	r	0.43	0/864	0.65	0/1156
49	s	0.37	0/744	0.60	0/994
50	t	0.36	0/787	0.63	0/1051
51	u	0.36	0/766	0.62	0/1025
52	v	0.42	0/637	0.63	0/841
53	w	0.40	0/635	0.70	0/848
54	x	0.33	0/502	0.59	0/667
55	y	0.37	0/453	0.63	0/605
56	z	0.42	0/450	0.69	0/599
57	6	0.47	0/3	0.99	0/2
All	All	0.51	0/152806	0.92	59/228551 (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
7	A	0	1
31	a	0	6
38	h	0	1
49	s	0	1
53	w	0	1
57	6	0	1
All	All	0	11

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1965	C	O5'-P-OP2	-11.15	95.66	105.70
31	a	1790	C	O5'-P-OP2	-10.21	96.51	105.70
31	a	512	G	O4'-C1'-N9	8.15	114.72	108.20
31	a	730	A	O5'-P-OP1	-7.51	98.94	105.70
31	a	1779	U	O5'-P-OP2	-7.50	98.95	105.70
31	a	204	A	O3'-P-O5'	-7.25	90.23	104.00
31	a	2513	A	O5'-P-OP2	-7.02	99.38	105.70
31	a	574	A	O5'-P-OP1	-6.63	99.73	105.70
7	A	22	G	O5'-P-OP2	-6.59	99.77	105.70
31	a	2724	U	O5'-P-OP2	-6.45	99.89	105.70
31	a	1378	A	O3'-P-O5'	-6.40	91.83	104.00
31	a	2546	U	O3'-P-O5'	-6.38	91.89	104.00
31	a	2222	C	O3'-P-O5'	-6.32	92.00	104.00
31	a	733	G	O5'-P-OP2	-6.29	100.03	105.70
31	a	1025	G	O3'-P-O5'	6.14	115.66	104.00
31	a	242	G	C3'-C2'-C1'	-6.12	96.60	101.50
31	a	1565	C	O3'-P-O5'	-6.11	92.40	104.00
31	a	329	G	O3'-P-O5'	-6.10	92.41	104.00
31	a	1936	A	O4'-C1'-N9	6.01	113.01	108.20
31	a	310	A	O3'-P-O5'	-5.99	92.62	104.00
31	a	1936	A	C1'-O4'-C4'	-5.99	105.11	109.90
31	a	1293	C	O3'-P-O5'	-5.91	92.78	104.00
31	a	395	U	O4'-C1'-N1	5.83	112.87	108.20
31	a	2698	U	O5'-P-OP2	-5.63	100.64	105.70
31	a	1638	C	O5'-P-OP2	-5.62	100.64	105.70
31	a	777	G	O5'-P-OP1	-5.62	100.64	105.70
7	A	561	U	O3'-P-O5'	-5.56	93.43	104.00
31	a	781	A	O3'-P-O5'	-5.56	93.43	104.00
31	a	2050	C	O3'-P-O5'	-5.56	93.44	104.00
31	a	818	G	O3'-P-O5'	-5.54	93.48	104.00
31	a	517	C	O5'-P-OP2	-5.48	100.77	105.70
31	a	2458	G	O3'-P-O5'	-5.44	93.66	104.00
31	a	2383	G	O3'-P-O5'	-5.43	93.69	104.00
31	a	1131	G	O3'-P-O5'	-5.40	93.73	104.00
7	A	809	G	O5'-P-OP2	-5.31	100.92	105.70
31	a	677	A	OP2-P-O3'	5.26	116.78	105.20
31	a	763	G	O3'-P-O5'	-5.24	94.04	104.00
31	a	2431	U	O5'-P-OP2	-5.22	101.00	105.70
31	a	1778	U	OP2-P-O3'	5.21	116.65	105.20
31	a	2620	C	O3'-P-O5'	-5.19	94.14	104.00
31	a	2357	G	OP2-P-O3'	5.19	116.62	105.20
31	a	1128	G	C1'-O4'-C4'	-5.17	105.77	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	14	A	O3'-P-O5'	-5.16	94.19	104.00
31	a	2504	PSU	OP2-P-O3'	5.16	116.55	105.20
31	a	1959	G	O3'-P-O5'	-5.15	94.22	104.00
31	a	528	A	OP2-P-O3'	5.09	116.41	105.20
31	a	1643	G	O3'-P-O5'	-5.09	94.32	104.00
31	a	1789	A	OP2-P-O3'	5.08	116.38	105.20
31	a	838	C	O5'-P-OP2	-5.08	101.13	105.70
31	a	2848	G	O4'-C1'-N9	5.07	112.26	108.20
31	a	1929	G	O3'-P-O5'	-5.06	94.39	104.00
31	a	1905	C	O3'-P-O5'	-5.05	94.40	104.00
7	A	921	U	O3'-P-O5'	-5.04	94.42	104.00
31	a	748	G	C1'-O4'-C4'	-5.03	105.88	109.90
7	A	686	U	C3'-C2'-C1'	-5.02	97.48	101.50
31	a	2477	U	O3'-P-O5'	-5.02	94.47	104.00
31	a	972	A	O3'-P-O5'	-5.01	94.47	104.00
31	a	1775	U	O3'-P-O5'	-5.01	94.49	104.00
7	A	792	A	C3'-C2'-C1'	-5.00	97.50	101.50

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
57	6	4	ORD	Peptide
7	A	898	G	Sidechain
31	a	1253	A	Sidechain
31	a	2037	A	Sidechain
31	a	2595	G	Sidechain
31	a	395	U	Sidechain
31	a	463	G	Sidechain
31	a	512	G	Sidechain
38	h	9	VAL	Peptide
49	s	88	LYS	Peptide
53	w	16	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	6
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	53 (95%)	2 (4%)	1 (2%)	7	5
8	B	222/241 (92%)	215 (97%)	7 (3%)	0	100	100
9	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
10	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
11	E	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
12	F	101/135 (75%)	95 (94%)	6 (6%)	0	100	100
13	G	151/179 (84%)	144 (95%)	6 (4%)	1 (1%)	19	19
14	H	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	16	16
15	I	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
16	J	96/103 (93%)	89 (93%)	4 (4%)	3 (3%)	3	1
17	K	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
18	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
19	M	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
22	P	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
23	Q	77/84 (92%)	74 (96%)	2 (3%)	1 (1%)	10	8
24	R	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
25	S	82/92 (89%)	77 (94%)	5 (6%)	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	68/71 (96%)	66 (97%)	1 (2%)	1 (2%)	8	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
34	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
35	e	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	25	28
36	f	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
37	g	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
38	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
39	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
40	j	114/123 (93%)	111 (97%)	3 (3%)	0	100	100
41	k	142/144 (99%)	137 (96%)	4 (3%)	1 (1%)	19	19
42	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
43	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
44	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
45	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
46	p	115/118 (98%)	115 (100%)	0	0	100	100
47	q	101/103 (98%)	97 (96%)	2 (2%)	2 (2%)	6	4
48	r	108/110 (98%)	107 (99%)	0	1 (1%)	14	14
49	s	91/100 (91%)	87 (96%)	3 (3%)	1 (1%)	12	10
50	t	100/104 (96%)	93 (93%)	5 (5%)	2 (2%)	6	4
51	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
52	v	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
53	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
54	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
56	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5479/5913 (93%)	5294 (97%)	168 (3%)	17 (0%)	38	42

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
47	q	45	GLU
5	4	65	ASN
16	J	57	VAL
16	J	83	THR
16	J	84	VAL

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Mol	Chain	Res	Type
27	U	3	VAL
3	2	28	ASN
48	r	12	SER
13	G	57	SER
49	s	89	GLU
41	k	29	LYS
47	q	44	GLY
50	t	75	ALA
23	Q	50	ASN
35	e	71	GLY
14	H	75	ILE
50	t	39	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	32
2	1	38/38 (100%)	37 (97%)	1 (3%)	41	54
3	2	51/52 (98%)	48 (94%)	3 (6%)	16	20
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	50
5	4	55/62 (89%)	55 (100%)	0	100	100
8	B	186/199 (94%)	180 (97%)	6 (3%)	34	45
9	C	170/190 (90%)	168 (99%)	2 (1%)	67	80
10	D	172/173 (99%)	164 (95%)	8 (5%)	22	29
11	E	119/126 (94%)	119 (100%)	0	100	100
12	F	90/116 (78%)	88 (98%)	2 (2%)	47	61
13	G	126/147 (86%)	119 (94%)	7 (6%)	17	21
14	H	104/105 (99%)	99 (95%)	5 (5%)	21	28
15	I	105/107 (98%)	103 (98%)	2 (2%)	52	67
16	J	86/90 (96%)	84 (98%)	2 (2%)	45	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	K	89/98 (91%)	87 (98%)	2 (2%)	47	61
18	L	102/103 (99%)	99 (97%)	3 (3%)	37	50
19	M	93/96 (97%)	89 (96%)	4 (4%)	25	32
20	N	83/84 (99%)	83 (100%)	0	100	100
21	O	76/77 (99%)	76 (100%)	0	100	100
22	P	65/65 (100%)	65 (100%)	0	100	100
23	Q	73/78 (94%)	72 (99%)	1 (1%)	62	77
24	R	57/65 (88%)	56 (98%)	1 (2%)	54	69
25	S	72/79 (91%)	69 (96%)	3 (4%)	25	33
26	T	65/66 (98%)	64 (98%)	1 (2%)	60	75
27	U	60/61 (98%)	56 (93%)	4 (7%)	13	15
33	c	216/218 (99%)	212 (98%)	4 (2%)	52	67
34	d	163/163 (100%)	161 (99%)	2 (1%)	67	80
35	e	165/165 (100%)	165 (100%)	0	100	100
36	f	148/150 (99%)	144 (97%)	4 (3%)	40	53
37	g	137/138 (99%)	131 (96%)	6 (4%)	24	31
38	h	32/114 (28%)	31 (97%)	1 (3%)	35	47
39	i	116/116 (100%)	116 (100%)	0	100	100
40	j	99/104 (95%)	97 (98%)	2 (2%)	50	65
41	k	103/103 (100%)	101 (98%)	2 (2%)	52	67
42	l	107/107 (100%)	106 (99%)	1 (1%)	75	86
43	m	98/103 (95%)	97 (99%)	1 (1%)	73	84
44	n	86/87 (99%)	85 (99%)	1 (1%)	67	80
45	o	99/100 (99%)	99 (100%)	0	100	100
46	p	89/90 (99%)	87 (98%)	2 (2%)	47	61
47	q	84/84 (100%)	81 (96%)	3 (4%)	30	40
48	r	93/93 (100%)	92 (99%)	1 (1%)	70	82
49	s	80/84 (95%)	78 (98%)	2 (2%)	42	56
50	t	83/85 (98%)	78 (94%)	5 (6%)	16	19
51	u	78/78 (100%)	77 (99%)	1 (1%)	65	78
52	v	62/63 (98%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	w	67/68 (98%)	66 (98%)	1 (2%)	60	75
54	x	54/55 (98%)	51 (94%)	3 (6%)	17	21
55	y	48/49 (98%)	48 (100%)	0	100	100
56	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4571/4825 (95%)	4469 (98%)	102 (2%)	47	61

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
1	0	54	ILE
2	1	25	LYS
3	2	31	HIS
3	2	47	LYS
3	2	57	LEU
4	3	36	ARG
8	B	7	ARG
8	B	23	TRP
8	B	93	ASN
8	B	100	MET
8	B	105	LYS
8	B	128	LYS
9	C	185	ASN
9	C	206	GLU
10	D	14	ARG
10	D	34	ILE
10	D	45	LYS
10	D	128	ARG
10	D	131	ASN
10	D	138	SER
10	D	184	ARG
10	D	202	GLU
12	F	74	LEU
12	F	102	MET
13	G	5	ARG
13	G	25	LYS
13	G	78	ARG
13	G	92	ARG
13	G	133	THR
13	G	137	LYS
13	G	144	MET

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Mol	Chain	Res	Type
14	H	27	MET
14	H	54	ASP
14	H	56	LYS
14	H	89	LYS
14	H	117	ARG
15	I	100	LYS
15	I	123	ARG
16	J	17	LEU
16	J	88	MET
17	K	89	PRO
17	K	94	GLU
18	L	45	PRO
18	L	54	ARG
18	L	111	LYS
19	M	14	HIS
19	M	16	VAL
19	M	27	LYS
19	M	113	ARG
23	Q	65	ARG
24	R	10	PHE
25	S	15	LEU
25	S	28	LYS
25	S	43	ASN
26	T	40	GLU
27	U	8	GLU
27	U	21	ARG
27	U	63	GLU
27	U	64	ASN
33	c	34	LEU
33	c	37	ASN
33	c	182	ARG
33	c	203	ARG
34	d	12	THR
34	d	32	ASN
36	f	30	ARG
36	f	47	LYS
36	f	120	LYS
36	f	165	GLU
37	g	3	ARG
37	g	25	THR
37	g	30	ASN
37	g	90	VAL

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Mol	Chain	Res	Type
37	g	103	ILE
37	g	155	GLU
38	h	9	VAL
40	j	49	ARG
40	j	114	LYS
41	k	112	LEU
41	k	129	LYS
42	l	80	VAL
43	m	51	LEU
44	n	84	GLU
46	p	51	ARG
46	p	112	LYS
47	q	20	VAL
47	q	70	GLU
47	q	71	LYS
48	r	7	HIS
49	s	64	LYS
49	s	89	GLU
50	t	15	THR
50	t	53	ASN
50	t	54	GLN
50	t	74	ASN
50	t	81	ASP
51	u	61	LEU
53	w	54	LYS
54	x	8	GLU
54	x	14	LEU
54	x	24	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
8	B	89	GLN
8	B	103	ASN
9	C	100	GLN
9	C	140	ASN
10	D	100	ASN
11	E	82	GLN
17	K	118	HIS
20	N	35	ASN
20	N	66	GLN
26	T	48	GLN

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Mol	Chain	Res	Type
26	T	52	ASN
26	T	84	ASN
27	U	64	ASN
33	c	37	ASN
33	c	90	ASN
33	c	197	ASN
39	i	47	HIS
39	i	128	ASN
40	j	89	ASN
45	o	12	GLN
46	p	52	GLN
47	q	66	HIS
48	r	40	ASN
50	t	53	ASN
50	t	74	ASN
51	u	49	ASN
53	w	6	GLN
54	x	15	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	X	9/10 (90%)	0	0
29	Y	69/76 (90%)	8 (11%)	2 (2%)
30	Z	68/85 (80%)	10 (14%)	5 (7%)
31	a	2745/2903 (94%)	297 (10%)	0
32	b	118/120 (98%)	12 (10%)	0
6	5	1/77 (1%)	1 (100%)	0
7	A	1515/1534 (98%)	202 (13%)	29 (1%)
All	All	4525/4805 (94%)	530 (11%)	36 (0%)

All (530) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
7	A	4	U
7	A	5	U
7	A	6	G
7	A	22	G
7	A	32	A
7	A	39	G

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Mol	Chain	Res	Type
7	A	44	A
7	A	47	C
7	A	48	C
7	A	51	A
7	A	71	A
7	A	83	C
7	A	84	U
7	A	85	U
7	A	86	G
7	A	87	C
7	A	88	U
7	A	94	G
7	A	95	C
7	A	119	A
7	A	120	A
7	A	122	G
7	A	131	A
7	A	141	G
7	A	143	A
7	A	144	G
7	A	159	G
7	A	163	C
7	A	164	G
7	A	182	A
7	A	183	C
7	A	197	A
7	A	202	G
7	A	226	G
7	A	240	G
7	A	245	U
7	A	247	G
7	A	251	G
7	A	266	G
7	A	267	C
7	A	289	G
7	A	321	A
7	A	328	C
7	A	329	A
7	A	347	G
7	A	348	G
7	A	352	C
7	A	354	G

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Mol	Chain	Res	Type
7	A	367	U
7	A	372	C
7	A	373	A
7	A	376	G
7	A	384	G
7	A	406	G
7	A	411	A
7	A	412	A
7	A	413	G
7	A	414	A
7	A	415	A
7	A	421	U
7	A	422	C
7	A	423	G
7	A	424	G
7	A	429	U
7	A	446	G
7	A	453	G
7	A	457	G
7	A	458	U
7	A	467	U
7	A	468	A
7	A	479	U
7	A	481	G
7	A	484	G
7	A	486	U
7	A	511	C
7	A	518	C
7	A	531	U
7	A	547	A
7	A	559	A
7	A	562	U
7	A	572	A
7	A	573	A
7	A	576	C
7	A	577	G
7	A	579	A
7	A	588	G
7	A	596	A
7	A	628	G
7	A	633	G
7	A	650	G

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Mol	Chain	Res	Type
7	A	653	U
7	A	661	G
7	A	665	A
7	A	703	G
7	A	721	G
7	A	723	U
7	A	724	G
7	A	734	G
7	A	748	G
7	A	755	G
7	A	777	A
7	A	793	U
7	A	794	A
7	A	815	A
7	A	817	C
7	A	840	C
7	A	849	G
7	A	857	C
7	A	887	G
7	A	890	G
7	A	914	A
7	A	926	G
7	A	934	C
7	A	935	A
7	A	936	C
7	A	960	U
7	A	966	2MG
7	A	969	A
7	A	971	G
7	A	975	A
7	A	976	G
7	A	977	A
7	A	984	C
7	A	993	G
7	A	994	A
7	A	996	A
7	A	1003	G
7	A	1004	A
7	A	1005	A
7	A	1009	U
7	A	1027	C
7	A	1028	C

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Mol	Chain	Res	Type
7	A	1030	U
7	A	1031	C
7	A	1032	G
7	A	1033	G
7	A	1034	G
7	A	1036	A
7	A	1039	G
7	A	1053	G
7	A	1065	U
7	A	1085	U
7	A	1094	G
7	A	1095	U
7	A	1101	A
7	A	1124	G
7	A	1132	C
7	A	1135	U
7	A	1137	C
7	A	1138	G
7	A	1139	G
7	A	1140	C
7	A	1159	U
7	A	1171	A
7	A	1184	G
7	A	1196	A
7	A	1197	A
7	A	1213	A
7	A	1226	C
7	A	1227	A
7	A	1238	A
7	A	1256	A
7	A	1257	A
7	A	1260	G
7	A	1275	A
7	A	1280	A
7	A	1286	U
7	A	1287	A
7	A	1300	G
7	A	1302	C
7	A	1317	C
7	A	1319	A
7	A	1320	C
7	A	1338	G

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Mol	Chain	Res	Type
7	A	1340	A
7	A	1346	A
7	A	1350	A
7	A	1353	G
7	A	1363	A
7	A	1368	A
7	A	1370	G
7	A	1378	C
7	A	1379	G
7	A	1381	U
7	A	1382	C
7	A	1397	C
7	A	1419	G
7	A	1429	A
7	A	1441	A
7	A	1451	U
7	A	1453	G
7	A	1487	G
7	A	1492	A
7	A	1494	G
7	A	1497	G
7	A	1503	A
7	A	1505	G
7	A	1506	U
7	A	1517	G
7	A	1529	G
7	A	1530	G
7	A	1533	C
29	Y	14	A
29	Y	18	G
29	Y	46	G
29	Y	47	U
29	Y	48	C
29	Y	70	G
29	Y	73	A
29	Y	74	C
30	Z	6	A
30	Z	7	G
30	Z	14	A
30	Z	23	A
30	Z	24	C
30	Z	46	G

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Mol	Chain	Res	Type
30	Z	47	U
30	Z	58	G
30	Z	81	C
30	Z	85	A
31	a	10	A
31	a	34	U
31	a	42	A
31	a	58	G
31	a	71	A
31	a	74	A
31	a	75	G
31	a	101	A
31	a	102	U
31	a	118	A
31	a	119	A
31	a	120	U
31	a	139	U
31	a	140	C
31	a	142	A
31	a	163	C
31	a	164	C
31	a	165	A
31	a	181	A
31	a	196	A
31	a	199	A
31	a	200	U
31	a	215	G
31	a	216	A
31	a	221	A
31	a	222	A
31	a	233	A
31	a	248	G
31	a	264	C
31	a	272	A
31	a	276	U
31	a	278	A
31	a	289	G
31	a	291	G
31	a	311	A
31	a	329	G
31	a	330	A
31	a	345	A

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Mol	Chain	Res	Type
31	a	361	G
31	a	362	A
31	a	386	G
31	a	404	A
31	a	405	U
31	a	411	G
31	a	412	A
31	a	451	U
31	a	481	G
31	a	491	G
31	a	504	A
31	a	505	A
31	a	509	C
31	a	530	G
31	a	531	C
31	a	532	A
31	a	533	G
31	a	544	C
31	a	545	U
31	a	546	U
31	a	547	A
31	a	549	G
31	a	563	A
31	a	573	U
31	a	575	A
31	a	586	A
31	a	592	A
31	a	603	A
31	a	614	A
31	a	615	U
31	a	618	G
31	a	627	A
31	a	637	A
31	a	645	C
31	a	647	G
31	a	653	U
31	a	654	A
31	a	655	A
31	a	686	U
31	a	717	C
31	a	730	A
31	a	738	G

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Mol	Chain	Res	Type
31	a	747	5MU
31	a	764	A
31	a	765	C
31	a	775	G
31	a	776	G
31	a	782	A
31	a	784	G
31	a	785	G
31	a	792	A
31	a	805	G
31	a	812	C
31	a	827	U
31	a	828	U
31	a	846	U
31	a	847	U
31	a	858	G
31	a	859	G
31	a	881	G
31	a	884	U
31	a	890	C
31	a	891	G
31	a	895	U
31	a	896	A
31	a	897	C
31	a	910	A
31	a	914	G
31	a	915	C
31	a	927	A
31	a	931	U
31	a	934	U
31	a	946	C
31	a	961	C
31	a	974	G
31	a	983	A
31	a	984	A
31	a	985	C
31	a	996	A
31	a	1012	U
31	a	1013	C
31	a	1022	G
31	a	1026	G
31	a	1033	U

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Mol	Chain	Res	Type
31	a	1040	A
31	a	1045	C
31	a	1046	A
31	a	1047	G
31	a	1109	C
31	a	1110	G
31	a	1111	A
31	a	1112	G
31	a	1116	G
31	a	1122	G
31	a	1128	G
31	a	1129	A
31	a	1132	U
31	a	1133	A
31	a	1135	C
31	a	1142	A
31	a	1169	A
31	a	1172	C
31	a	1187	G
31	a	1253	A
31	a	1256	G
31	a	1271	G
31	a	1272	A
31	a	1300	G
31	a	1301	A
31	a	1352	U
31	a	1365	A
31	a	1379	U
31	a	1383	A
31	a	1386	C
31	a	1416	G
31	a	1427	A
31	a	1428	C
31	a	1452	G
31	a	1453	A
31	a	1482	G
31	a	1483	G
31	a	1493	C
31	a	1504	A
31	a	1508	A
31	a	1509	A
31	a	1510	G

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Mol	Chain	Res	Type
31	a	1515	A
31	a	1535	A
31	a	1536	C
31	a	1537	G
31	a	1569	A
31	a	1578	U
31	a	1583	A
31	a	1584	U
31	a	1585	C
31	a	1608	A
31	a	1609	A
31	a	1647	U
31	a	1648	U
31	a	1649	G
31	a	1674	G
31	a	1715	G
31	a	1729	U
31	a	1730	C
31	a	1732	C
31	a	1738	G
31	a	1750	G
31	a	1764	C
31	a	1773	A
31	a	1782	U
31	a	1800	C
31	a	1801	A
31	a	1807	G
31	a	1808	A
31	a	1816	C
31	a	1829	A
31	a	1842	G
31	a	1847	A
31	a	1848	A
31	a	1858	A
31	a	1870	C
31	a	1871	A
31	a	1873	G
31	a	1906	G
31	a	1907	G
31	a	1929	G
31	a	1930	G
31	a	1937	A

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Mol	Chain	Res	Type
31	a	1938	A
31	a	1955	U
31	a	1965	C
31	a	1967	C
31	a	1970	A
31	a	1971	U
31	a	1972	G
31	a	1991	U
31	a	1993	U
31	a	2023	C
31	a	2027	G
31	a	2033	A
31	a	2043	C
31	a	2055	C
31	a	2056	G
31	a	2060	A
31	a	2061	G
31	a	2062	A
31	a	2069	G7M
31	a	2198	A
31	a	2203	U
31	a	2204	G
31	a	2211	A
31	a	2225	A
31	a	2238	G
31	a	2239	G
31	a	2268	A
31	a	2283	C
31	a	2287	A
31	a	2305	U
31	a	2308	G
31	a	2312	U
31	a	2322	A
31	a	2325	G
31	a	2333	A
31	a	2335	A
31	a	2347	C
31	a	2361	G
31	a	2372	U
31	a	2383	G
31	a	2385	C
31	a	2396	G

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Mol	Chain	Res	Type
31	a	2402	U
31	a	2403	C
31	a	2406	A
31	a	2424	C
31	a	2425	A
31	a	2429	G
31	a	2430	A
31	a	2435	A
31	a	2441	U
31	a	2448	A
31	a	2474	U
31	a	2476	A
31	a	2480	C
31	a	2491	U
31	a	2494	G
31	a	2502	G
31	a	2505	G
31	a	2518	A
31	a	2529	G
31	a	2547	A
31	a	2554	U
31	a	2556	C
31	a	2566	A
31	a	2567	G
31	a	2573	C
31	a	2602	A
31	a	2609	U
31	a	2613	U
31	a	2629	U
31	a	2630	G
31	a	2663	G
31	a	2689	U
31	a	2690	U
31	a	2714	G
31	a	2726	A
31	a	2744	G
31	a	2748	A
31	a	2757	A
31	a	2778	A
31	a	2791	G
31	a	2798	U
31	a	2800	A

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Mol	Chain	Res	Type
31	a	2820	A
31	a	2821	A
31	a	2880	C
31	a	2883	A
31	a	2884	U
31	a	2885	G
31	a	2894	G
32	b	25	U
32	b	35	C
32	b	36	C
32	b	44	G
32	b	45	A
32	b	56	G
32	b	67	G
32	b	88	C
32	b	89	U
32	b	90	C
32	b	99	A
32	b	109	A

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	4	U
7	A	5	U
7	A	70	U
7	A	84	U
7	A	86	G
7	A	94	G
7	A	119	A
7	A	181	A
7	A	199	A
7	A	361	G
7	A	468	A
7	A	481	G
7	A	587	G
7	A	653	U
7	A	776	G
7	A	793	U
7	A	858	G
7	A	992	U
7	A	993	G

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Mol	Chain	Res	Type
7	A	1035	A
7	A	1045	C
7	A	1046	A
7	A	1109	C
7	A	1124	G
7	A	1139	G
7	A	1225	A
7	A	1319	A
7	A	1320	C
7	A	1505	G
29	Y	46	G
29	Y	47	U
30	Z	6	A
30	Z	9	G
30	Z	22	G
30	Z	46	G
30	Z	80	G

## 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	$\# Z  > 2$
31	PSU	a	955	31	18,21,22	1.02	1 (5%)	22,30,33	0.77	0
31	2MG	a	2445	31	18,26,27	1.16	3 (16%)	16,38,41	0.70	0
18	D2T	L	89	18	7,9,10	0.97	0	6,11,13	1.71	3 (50%)
7	2MG	A	1207	7	18,26,27	1.09	3 (16%)	16,38,41	0.79	0
7	G7M	A	527	7	20,26,27	1.24	3 (15%)	17,39,42	0.56	0
34	MEQ	d	150	34	8,9,10	0.51	0	5,10,12	0.81	0
31	6MZ	a	1618	31	18,25,26	0.67	0	16,36,39	0.70	0
31	H2U	a	2449	31	18,21,22	0.52	0	21,30,33	0.87	2 (9%)
31	3TD	a	1915	31	18,22,23	0.97	1 (5%)	22,32,35	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	YFQ	6	3	57	3,6,7	0.75	0	0,6,8	-	-
7	2MG	A	1516	7	18,26,27	0.99	2 (11%)	16,38,41	0.84	0
31	OMU	a	2552	31	19,22,23	0.32	0	26,31,34	0.53	0
30	MIA	Z	38	30	24,31,32	0.83	1 (4%)	26,44,47	4.66	2 (7%)
31	PSU	a	2605	31	18,21,22	0.95	1 (5%)	22,30,33	0.91	1 (4%)
31	2MA	a	2503	59,31	19,25,26	1.16	2 (10%)	21,37,40	1.68	4 (19%)
31	5MC	a	1962	31	18,22,23	0.35	0	26,32,35	0.56	0
31	6MZ	a	2030	31	18,25,26	0.83	0	16,36,39	0.76	1 (6%)
31	5MU	a	747	31	19,22,23	0.31	0	28,32,35	0.35	0
31	PSU	a	746	59,31	18,21,22	1.02	1 (5%)	22,30,33	0.54	0
57	DAL	6	2	57	3,4,5	0.68	0	2,4,6	0.95	0
57	ORD	6	4	57	6,7,8	0.52	0	2,7,9	0.33	0
31	1MG	a	745	31	18,26,27	0.93	1 (5%)	19,39,42	0.54	0
42	4D4	l	81	42	9,11,12	0.75	0	8,13,15	0.51	0
7	4OC	A	1402	7	20,23,24	0.43	0	26,32,35	0.57	0
31	PSU	a	2457	31	18,21,22	1.15	1 (5%)	22,30,33	0.63	0
57	YFQ	6	6	57	3,6,7	0.86	0	0,6,8	-	-
31	OMG	a	2251	30,31	18,26,27	1.04	3 (16%)	19,38,41	0.80	0
7	2MG	A	966	7	18,26,27	1.10	2 (11%)	16,38,41	0.61	0
31	PSU	a	2580	31	18,21,22	1.12	1 (5%)	22,30,33	0.70	1 (4%)
57	YF5	6	1	57	15,17,18	0.47	0	16,21,23	0.89	0
31	G7M	a	2069	31	20,26,27	1.20	3 (15%)	17,39,42	0.59	0
31	PSU	a	1917	31	18,21,22	0.91	1 (5%)	22,30,33	0.68	0
31	PSU	a	2604	31	18,21,22	1.03	1 (5%)	22,30,33	0.83	1 (4%)
31	PSU	a	2504	60,31	18,21,22	1.07	1 (5%)	22,30,33	0.75	1 (4%)
17	IAS	K	119	17	6,7,8	0.92	0	6,8,10	0.90	0
7	PSU	A	516	59,7	18,21,22	0.94	1 (5%)	22,30,33	0.60	0
7	5MC	A	1407	7	18,22,23	0.45	0	26,32,35	0.81	0
7	5MC	A	967	7	18,22,23	0.35	0	26,32,35	0.65	0
31	5MU	a	1939	31	19,22,23	0.35	0	28,32,35	0.41	0
31	2MG	a	1835	31	18,26,27	1.14	2 (11%)	16,38,41	0.60	0
31	PSU	a	1911	31	18,21,22	0.91	1 (5%)	22,30,33	0.66	0
31	OMC	a	2498	59,31	19,22,23	0.41	0	26,31,34	0.44	0
57	YFZ	6	5	57	11,11,12	0.44	0	9,13,15	0.66	0
7	UR3	A	1498	7	19,22,23	0.36	0	26,32,35	0.71	0
29	MKX	Y	37	29	27,33,35	0.92	1 (3%)	29,49,54	1.22	1 (3%)

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
31	PSU	a	955	31	-	0/7/25/26	0/2/2/2
31	2MG	a	2445	31	-	0/5/27/28	0/3/3/3
18	D2T	L	89	18	-	4/7/12/14	-
7	2MG	A	1207	7	-	0/5/27/28	0/3/3/3
7	G7M	A	527	7	-	1/3/25/26	0/3/3/3
34	MEQ	d	150	34	-	3/8/9/11	-
31	6MZ	a	1618	31	-	0/5/27/28	0/3/3/3
31	H2U	a	2449	31	-	0/7/38/39	0/2/2/2
31	3TD	a	1915	31	-	0/7/25/26	0/2/2/2
57	YFQ	6	3	57	-	0/2/5/7	-
7	2MG	A	1516	7	-	0/5/27/28	0/3/3/3
31	OMU	a	2552	31	-	0/9/27/28	0/2/2/2
30	MIA	Z	38	30	-	3/11/33/34	0/3/3/3
31	PSU	a	2605	31	-	0/7/25/26	0/2/2/2
31	2MA	a	2503	59,31	-	1/3/25/26	0/3/3/3
31	5MC	a	1962	31	-	0/7/25/26	0/2/2/2
31	6MZ	a	2030	31	-	2/5/27/28	0/3/3/3
31	5MU	a	747	31	-	1/7/25/26	0/2/2/2
31	PSU	a	746	59,31	-	3/7/25/26	0/2/2/2
57	DAL	6	2	57	-	0/0/2/4	-
57	ORD	6	4	57	-	1/5/6/8	-
31	1MG	a	745	31	-	0/3/25/26	0/3/3/3
42	4D4	l	81	42	-	1/11/12/14	-
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
31	PSU	a	2457	31	-	0/7/25/26	0/2/2/2
57	YFQ	6	6	57	-	1/2/5/7	-
31	OMG	a	2251	30,31	-	0/5/27/28	0/3/3/3
7	2MG	A	966	7	-	0/5/27/28	0/3/3/3
31	PSU	a	2580	31	-	0/7/25/26	0/2/2/2
57	YF5	6	1	57	-	4/19/21/23	-
31	G7M	a	2069	31	-	2/3/25/26	0/3/3/3
31	PSU	a	1917	31	-	0/7/25/26	0/2/2/2
31	PSU	a	2604	31	-	0/7/25/26	0/2/2/2
31	PSU	a	2504	60,31	-	0/7/25/26	0/2/2/2
17	IAS	K	119	17	-	0/7/7/8	-
7	PSU	A	516	59,7	-	0/7/25/26	0/2/2/2
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	5MU	a	1939	31	-	0/7/25/26	0/2/2/2
31	2MG	a	1835	31	-	0/5/27/28	0/3/3/3
31	PSU	a	1911	31	-	0/7/25/26	0/2/2/2
31	OMC	a	2498	59,31	-	0/9/27/28	0/2/2/2
57	YFZ	6	5	57	-	1/13/13/14	-
7	UR3	A	1498	7	-	0/7/25/26	0/2/2/2
29	MKX	Y	37	29	-	7/10/48/50	0/4/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	2580	PSU	C6-C5	4.23	1.40	1.35
31	a	2457	PSU	C6-C5	4.22	1.40	1.35
31	a	1915	3TD	C6-C5	3.81	1.39	1.35
31	a	2504	PSU	C6-C5	3.78	1.39	1.35
31	a	746	PSU	C6-C5	3.69	1.39	1.35
31	a	2604	PSU	C6-C5	3.56	1.39	1.35
7	A	516	PSU	C6-C5	3.56	1.39	1.35
31	a	955	PSU	C6-C5	3.54	1.39	1.35
7	A	527	G7M	C8-N9	3.50	1.39	1.33
31	a	1911	PSU	C6-C5	3.48	1.39	1.35
31	a	1917	PSU	C6-C5	3.43	1.39	1.35
31	a	2605	PSU	C6-C5	3.37	1.39	1.35
31	a	2069	G7M	C8-N9	3.29	1.39	1.33
7	A	527	G7M	C8-N7	2.94	1.38	1.33
31	a	1835	2MG	C5-C6	-2.87	1.41	1.47
31	a	2251	OMG	C5-C6	-2.84	1.41	1.47
29	Y	37	MKX	C6-N6	-2.74	1.38	1.42
7	A	966	2MG	C5-C6	-2.69	1.41	1.47
7	A	1207	2MG	C5-C6	-2.41	1.42	1.47
31	a	2069	G7M	C5-C6	-2.39	1.39	1.45
31	a	1835	2MG	C8-N7	-2.37	1.31	1.35
31	a	2069	G7M	C8-N7	2.36	1.37	1.33
31	a	2445	2MG	C5-C6	-2.35	1.42	1.47
7	A	527	G7M	C5-C6	-2.31	1.39	1.45
31	a	2503	2MA	C6-N1	2.30	1.38	1.33
31	a	745	1MG	C5-C4	-2.26	1.37	1.43
31	a	2445	2MG	C8-N7	-2.26	1.31	1.35
7	A	1207	2MG	C8-N7	-2.21	1.31	1.35
31	a	2445	2MG	C5-C4	-2.18	1.37	1.43
7	A	1516	2MG	C5-C6	-2.12	1.43	1.47
7	A	966	2MG	C8-N7	-2.11	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	2251	OMG	C5-C4	-2.08	1.37	1.43
31	a	2251	OMG	C8-N7	-2.08	1.31	1.35
31	a	2503	2MA	C2-N1	2.06	1.37	1.34
30	Z	38	MIA	C6-N1	2.03	1.35	1.32
7	A	1516	2MG	C5-C4	-2.01	1.38	1.43
7	A	1207	2MG	C6-N1	2.00	1.40	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Z	38	MIA	C11-S10-C2	23.27	119.64	102.27
31	a	2503	2MA	C5-C6-N1	-4.99	117.73	121.01
31	a	2503	2MA	C5-C6-N6	3.68	125.94	120.35
29	Y	37	MKX	C6-N6-C10	3.38	127.33	123.20
30	Z	38	MIA	C5-C6-N1	-3.31	118.06	120.81
31	a	2503	2MA	CM2-C2-N1	2.76	121.45	117.15
18	L	89	D2T	OD1-CG-CB	-2.48	117.25	122.44
31	a	2503	2MA	N3-C2-N1	-2.38	121.38	125.73
31	a	2604	PSU	C2'-C3'-C4'	-2.24	98.30	102.64
31	a	2449	H2U	O2-C2-N1	-2.22	120.32	123.11
18	L	89	D2T	O-C-CA	-2.16	119.11	124.78
18	L	89	D2T	OD2-CG-CB	2.13	117.75	113.15
31	a	2030	6MZ	C2-N1-C6	2.12	118.41	116.59
31	a	2504	PSU	C2'-C3'-C4'	-2.09	98.58	102.64
31	a	2449	H2U	C4-N3-C2	-2.06	124.08	125.79
31	a	2605	PSU	C5-C6-N1	-2.02	119.07	122.11
31	a	2580	PSU	C3'-C2'-C1'	2.02	103.99	101.64

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	Y	37	MKX	C13-C12-C14-C15
29	Y	37	MKX	C13-C12-C14-O14
29	Y	37	MKX	C5-C6-N6-C10
29	Y	37	MKX	C5-C6-N6-C13
29	Y	37	MKX	N1-C6-N6-C10
29	Y	37	MKX	N1-C6-N6-C13
31	a	746	PSU	C2'-C1'-C5-C4
31	a	746	PSU	C2'-C1'-C5-C6
31	a	746	PSU	O4'-C1'-C5-C6
57	6	4	ORD	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
57	6	1	YF5	CZ-CZ1-CZ2-NZ3
34	d	150	MEQ	OE1-CD-CG-CB
34	d	150	MEQ	NE2-CD-CG-CB
31	a	2030	6MZ	O4'-C4'-C5'-O5'
31	a	2069	G7M	C4'-C5'-O5'-P
29	Y	37	MKX	N11-C12-C14-C15
30	Z	38	MIA	O4'-C4'-C5'-O5'
57	6	1	YF5	N-CE-CZ-CZ1
18	L	89	D2T	CA-CB-CG-OD1
18	L	89	D2T	CA-CB-CG-OD2
7	A	527	G7M	C4'-C5'-O5'-P
57	6	5	YFZ	O-C-CA-CB
30	Z	38	MIA	N6-C12-C13-C14
18	L	89	D2T	SB-CB-CG-OD2
31	a	747	5MU	C3'-C4'-C5'-O5'
57	6	6	YFQ	C-CA-CB-NG
57	6	1	YF5	CZ1-CZ2-NZ3-CZ4
18	L	89	D2T	CG-CB-SB-CB1
31	a	2030	6MZ	C3'-C4'-C5'-O5'
30	Z	38	MIA	C3'-C4'-C5'-O5'
31	a	2069	G7M	O4'-C4'-C5'-O5'
31	a	2503	2MA	O4'-C4'-C5'-O5'
42	l	81	4D4	O-C-CA-CB
34	d	150	MEQ	CA-CB-CG-CD
57	6	1	YF5	CE-CZ-CZ1-CZ2

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 313 ligands modelled in this entry, 313 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.