



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 05:20 pm GMT

PDB ID : 8B7Y  
EMDB ID : EMD-15905  
Title : Cryo-EM structure of the E.coli 70S ribosome in complex with the antibiotic Myxovalargin B.  
Authors : Koller, T.O.; Graf, M.; Wilson, D.N.  
Deposited on : 2022-10-03  
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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

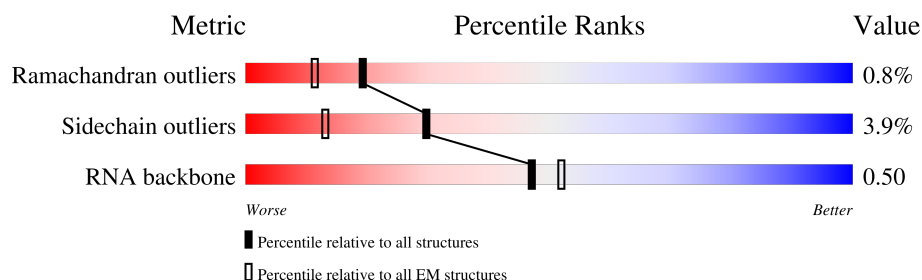
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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.



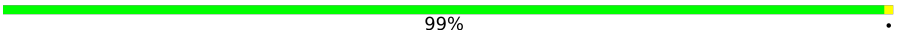



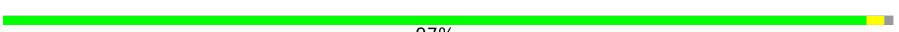







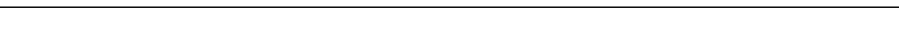

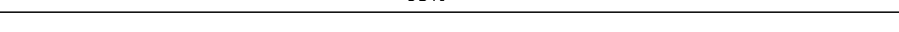

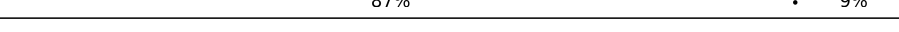
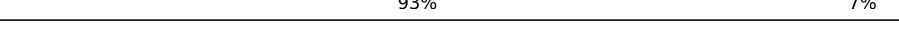

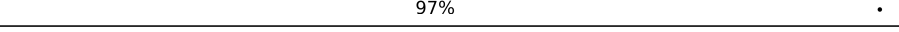





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	I	2904	80% 19%
2	J	118	75% 25%
3	K	273	98% ..
4	L	209	97% .
5	M	201	98% .
6	O	177	96% ..
7	R	142	96% .
8	S	123	96% ..
9	T	144	97% .



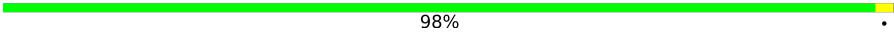
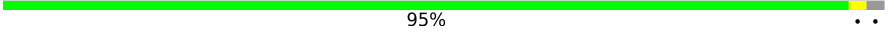


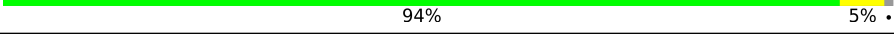
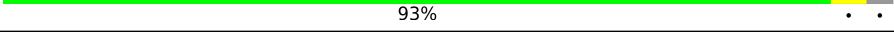
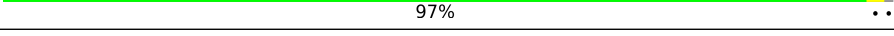
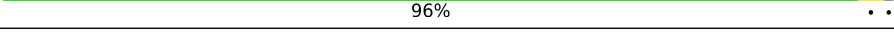
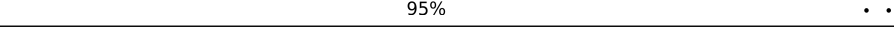


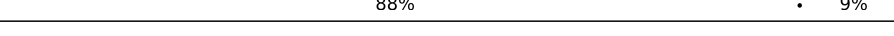
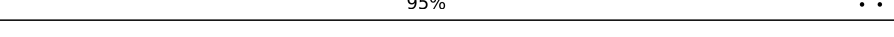
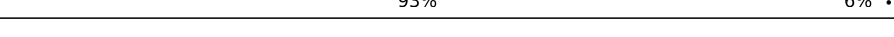
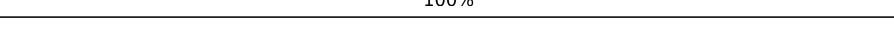

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Mol	Chain	Length	Quality of chain
10	U	136	 99% .
11	V	127	 92% . 6%
12	W	117	 93% 6% .
13	X	115	 94% 5% .
14	Y	118	 97% ..
15	Z	103	 92% 8%
16	a	110	 97% .
17	b	100	 90% . 7%
18	c	104	 95% . .
19	d	94	 98% .
20	e	85	 86% . 12%
21	f	78	 99% .
22	g	63	 92% 6% .
23	h	59	 95% . .
24	i	57	 91% 7% .
25	j	55	 87% . 9%
26	k	46	 93% 7%
27	l	65	 92% 6% .
28	m	38	 97% .
29	n	76	 . 67% 30%
30	C	1533	 79% 20% .
31	D	241	 89% . 7%
32	E	233	 86% . 12%
33	F	206	 83% 15% .
34	G	167	 92% . 7%

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Mol	Chain	Length	Quality of chain
35	H	135	
36	N	179	
37	P	130	
38	Q	130	
39	o	103	
40	p	129	
41	q	124	
42	r	118	
43	s	101	
44	t	89	
45	u	82	
46	v	84	
47	w	75	
48	x	92	
49	y	87	
50	5	71	
51	6	3	
52	z	16	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 141008 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	2898	Total	C	N	O	P	0	0
			62225	27764	11448	20115	2898		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L6.

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

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 12 is a protein called 50S ribosomal protein L18.

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

- Molecule 13 is a protein called 50S ribosomal protein L19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

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

- Molecule 18 is a protein called 50S ribosomal protein L24.

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

- Molecule 19 is a protein called 50S ribosomal protein L25.

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

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

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

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	j	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 26 is a protein called 50S ribosomal protein L34.

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

- Molecule 27 is a protein called 50S ribosomal protein L35.

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

- Molecule 28 is a protein called 50S ribosomal protein L36.



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

- Molecule 29 is a RNA chain called P-tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	n	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 30 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	1519	Total	C	N	O	P	0	0
			32599	14539	5986	10555	1519		

- Molecule 31 is a protein called 30S ribosomal protein S2.

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

- Molecule 32 is a protein called 30S ribosomal protein S3.

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

- Molecule 33 is a protein called 30S ribosomal protein S4.

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

- Molecule 34 is a protein called 30S ribosomal protein S5.

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

- Molecule 35 is a protein called 30S ribosomal protein S6.

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

- Molecule 36 is a protein called 30S ribosomal protein S7.

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

- Molecule 37 is a protein called 30S ribosomal protein S8.

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

- Molecule 38 is a protein called 30S ribosomal protein S9.

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

- Molecule 39 is a protein called 30S ribosomal protein S10.

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

- Molecule 40 is a protein called 30S ribosomal protein S11.

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

- Molecule 41 is a protein called 30S ribosomal protein S12.

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

- Molecule 42 is a protein called 30S ribosomal protein S13.

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

- Molecule 43 is a protein called 30S ribosomal protein S14.

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

- Molecule 44 is a protein called 30S ribosomal protein S15.

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

- Molecule 45 is a protein called 30S ribosomal protein S16.

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

- Molecule 46 is a protein called 30S ribosomal protein S17.

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

- Molecule 47 is a protein called 30S ribosomal protein S18.

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

- Molecule 48 is a protein called 30S ribosomal protein S19.

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

- Molecule 49 is a protein called 30S ribosomal protein S20.

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

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	5	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 51 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	6	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 52 is a protein (with D amino acids) called Myxovalargin B.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	z	16	Total	C	N	O	0	0
			118	80	21	17		

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	I	136	Total	Mg	0
			136	136	
53	J	2	Total	Mg	0
			2	2	
53	K	1	Total	Mg	0
			1	1	
53	T	1	Total	Mg	0
			1	1	
53	V	1	Total	Mg	0
			1	1	
53	a	2	Total	Mg	0
			2	2	
53	d	1	Total	Mg	0
			1	1	
53	h	1	Total	Mg	0
			1	1	
53	C	87	Total	Mg	0
			87	87	

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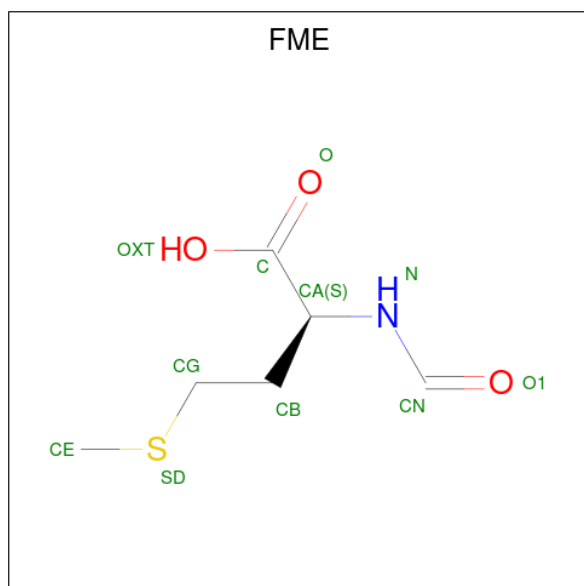
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Mol	Chain	Residues	Atoms		AltConf
53	G	1	Total	Mg	0
			1	1	
53	q	1	Total	Mg	0
			1	1	
53	s	1	Total	Mg	0
			1	1	
53	5	1	Total	Mg	0
			1	1	
53	6	1	Total	Mg	0
			1	1	

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

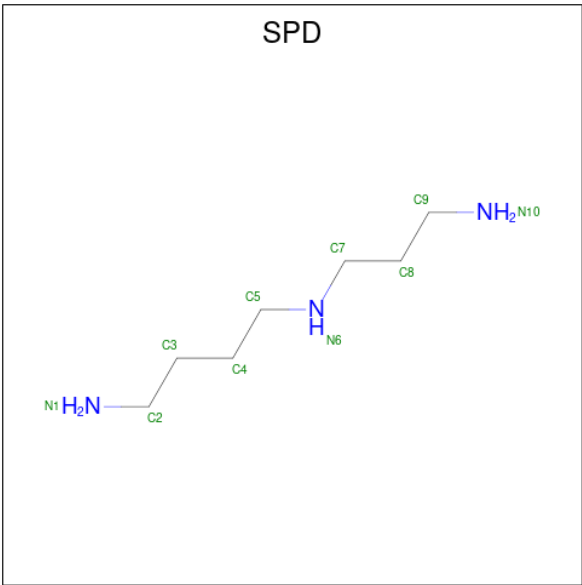
Mol	Chain	Residues	Atoms		AltConf
54	m	1	Total	Zn	0
			1	1	

- Molecule 55 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					AltConf
55	n	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 56 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



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

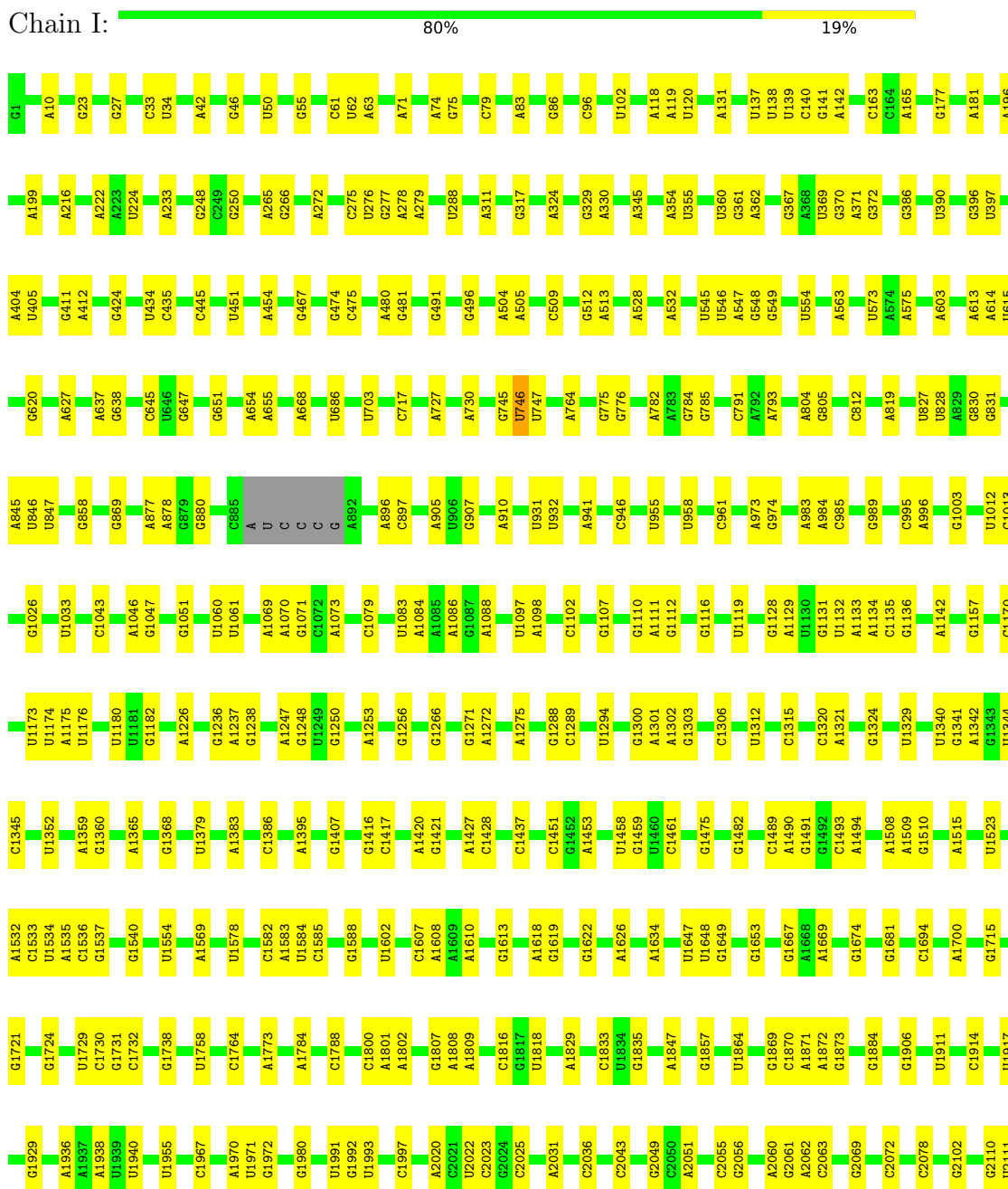
- Molecule 57 is water.

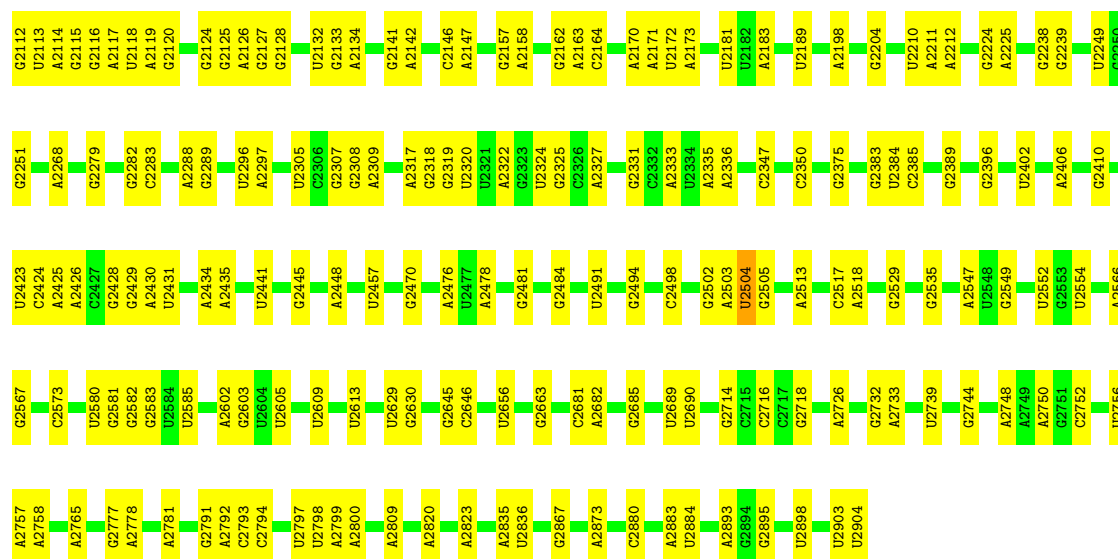
Mol	Chain	Residues	Atoms		AltConf
57	I	18	Total	O	0
			18	18	
57	z	10	Total	O	0
			10	10	

### 3 Residue-property plots

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.

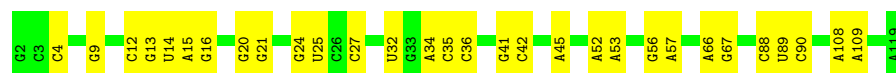
#### • Molecule 1: 23S ribosomal RNA





- Molecule 2: 5S ribosomal RNA

Chain J: 75% 25%



- Molecule 3: 50S ribosomal protein L2

Chain K: 98%



- Molecule 4: 50S ribosomal protein L3

Chain L: 97%



- Molecule 5: 50S ribosomal protein L4

Chain M: 98%



- Molecule 6: 50S ribosomal protein L6

Chain O: 96%





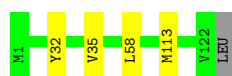
- Molecule 7: 50S ribosomal protein L13

Chain R: 96% .



- Molecule 8: 50S ribosomal protein L14

Chain S: 96% ..



- Molecule 9: 50S ribosomal protein L15

Chain T: 97% .



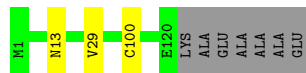
- Molecule 10: 50S ribosomal protein L16

Chain U: 99% .



- Molecule 11: 50S ribosomal protein L17

Chain V: 92% . 6%



- Molecule 12: 50S ribosomal protein L18

Chain W: 93% 6% .



- Molecule 13: 50S ribosomal protein L19

Chain X: 94% 5% .



- Molecule 14: 50S ribosomal protein L20

Chain Y: 97% ..



- Molecule 15: 50S ribosomal protein L21

Chain Z: 92% 8%



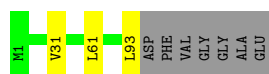
- Molecule 16: 50S ribosomal protein L22

Chain a: 97% .



- Molecule 17: 50S ribosomal protein L23

Chain b: 90% . 7%



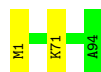
- Molecule 18: 50S ribosomal protein L24

Chain c: 95% ..



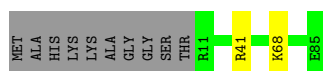
- Molecule 19: 50S ribosomal protein L25

Chain d: 98% .



- Molecule 20: 50S ribosomal protein L27

Chain e: 86% . 12%



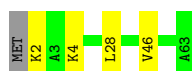
- Molecule 21: 50S ribosomal protein L28

Chain f: 99% .



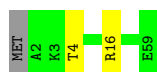
- Molecule 22: 50S ribosomal protein L29

Chain g: 92% 6% .



- Molecule 23: 50S ribosomal protein L30

Chain h: 95% . .



- Molecule 24: 50S ribosomal protein L32

Chain i: 91% 7% .



- Molecule 25: 50S ribosomal protein L33

Chain j: 87% . 9%



- Molecule 26: 50S ribosomal protein L34

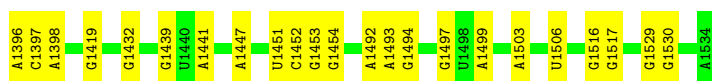
Chain k: 93% 7%



- Molecule 27: 50S ribosomal protein L35

Chain l: 92% 6% .





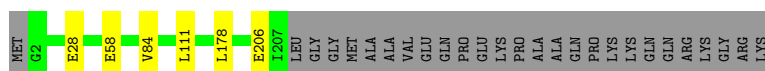
- Molecule 31: 30S ribosomal protein S2

Chain D: 89% 7%



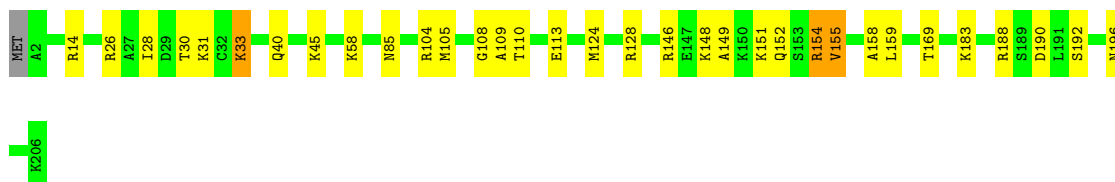
- Molecule 32: 30S ribosomal protein S3

Chain E: 86% 12%



- Molecule 33: 30S ribosomal protein S4

Chain F: 83% 15%



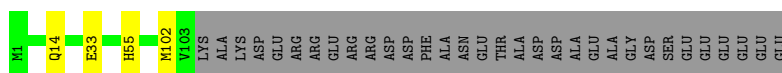
- Molecule 34: 30S ribosomal protein S5

Chain G: 92% 7%



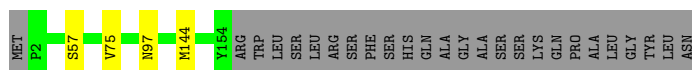
- Molecule 35: 30S ribosomal protein S6

Chain H: 73% 24%



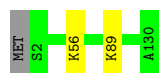
- Molecule 36: 30S ribosomal protein S7

Chain N: 83% 15%



- Molecule 37: 30S ribosomal protein S8

Chain P:  98% ..




- Molecule 38: 30S ribosomal protein S9

Chain Q:  95% ..




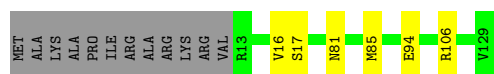
- Molecule 39: 30S ribosomal protein S10

Chain o:  88% 7% 5%



- Molecule 40: 30S ribosomal protein S11

Chain p:  86% 5% 9%



- Molecule 41: 30S ribosomal protein S12

Chain q:  94% 5% .



- Molecule 42: 30S ribosomal protein S13

Chain r:  93% . .



- Molecule 43: 30S ribosomal protein S14

Chain s:  97% ..



- Molecule 44: 30S ribosomal protein S15

Chain t:  96% ..




- Molecule 45: 30S ribosomal protein S16

Chain u:  95% ..



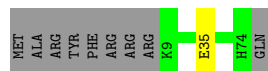
- Molecule 46: 30S ribosomal protein S17

Chain v:  88% 6% 6%




- Molecule 47: 30S ribosomal protein S18

Chain w:  87% 12%



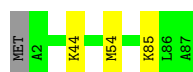
- Molecule 48: 30S ribosomal protein S19

Chain x:  88% 9%



- Molecule 49: 30S ribosomal protein S20

Chain y:  95% ..



- Molecule 50: 30S ribosomal protein S21

Chain 5:  93% 6%



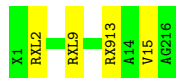
- Molecule 51: messenger RNA

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: Myxovalargin B

Chain z:  75% 25%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	376564	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 ( $e^-/\text{\AA}^2$ )	2.5	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (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: 2MG, 5MC, DAR, DHV, 2MA, SPD, OMU, FME, ALQ, 1MG, DAL, RXL, OMG, OMC, MG, IB9, DVA, AG2, PSU, 5MU, MAA, ZN, RX9

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	I	0.47	0/69266	0.74	0/108061
2	J	0.39	0/2828	0.76	0/4410
3	K	0.30	0/2121	0.58	0/2852
4	L	0.29	0/1586	0.52	0/2134
5	M	0.27	0/1571	0.52	0/2113
6	O	0.27	0/1343	0.53	0/1816
7	R	0.30	0/1152	0.53	0/1551
8	S	0.29	0/947	0.59	0/1268
9	T	0.30	0/1062	0.59	0/1413
10	U	0.30	0/1093	0.58	0/1460
11	V	0.29	0/973	0.58	0/1301
12	W	0.27	0/902	0.55	0/1209
13	X	0.29	0/929	0.57	0/1242
14	Y	0.30	0/960	0.57	0/1278
15	Z	0.28	0/829	0.55	0/1107
16	a	0.27	0/864	0.55	0/1156
17	b	0.27	0/744	0.51	0/994
18	c	0.29	0/787	0.52	0/1051
19	d	0.29	0/766	0.53	0/1025
20	e	0.29	0/576	0.56	0/762
21	f	0.27	0/635	0.59	0/848
22	g	0.26	0/502	0.55	0/667
23	h	0.25	0/453	0.56	0/605
24	i	0.29	0/450	0.59	0/599
25	j	0.31	0/416	0.51	0/554
26	k	0.27	0/380	0.68	0/498
27	l	0.29	0/513	0.56	0/676
28	m	0.31	0/303	0.62	0/397
29	n	0.78	0/1813	1.77	77/2825 (2.7%)
30	C	0.43	0/36502	0.82	0/56940
31	D	0.27	0/1784	0.50	0/2403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	E	0.26	0/1651	0.54	0/2225
33	F	0.28	0/1665	0.61	0/2227
34	G	0.28	0/1165	0.52	0/1568
35	H	0.28	0/858	0.52	0/1160
36	N	0.27	0/1219	0.56	0/1635
37	P	0.27	0/989	0.51	0/1326
38	Q	0.28	0/1034	0.61	0/1375
39	o	0.26	0/796	0.57	0/1077
40	p	0.27	0/893	0.56	0/1205
41	q	0.28	0/969	0.60	0/1300
42	r	0.26	0/900	0.58	0/1204
43	s	0.26	0/817	0.56	0/1088
44	t	0.26	0/722	0.56	0/964
45	u	0.27	0/653	0.59	0/877
46	v	0.27	0/650	0.54	0/871
47	w	0.31	0/553	0.56	0/742
48	x	0.25	0/685	0.53	0/922
49	y	0.25	0/676	0.48	0/895
50	5	0.29	0/597	0.60	0/792
51	6	0.60	0/72	0.85	0/110
52	z	0.20	0/10	0.57	0/11
All	All	0.42	0/152624	0.74	77/228789 (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
39	o	0	1
52	z	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	70	C	P-O3'-C3'	-11.99	105.31	119.70
29	n	64	G	P-O3'-C3'	-11.71	105.65	119.70
29	n	51	U	P-O3'-C3'	-11.40	106.02	119.70
29	n	12	G	P-O3'-C3'	-11.02	106.48	119.70
29	n	71	G	P-O3'-C3'	-10.70	106.86	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	o	38	GLY	Peptide
52	z	15	DHV	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	269/273 (98%)	255 (95%)	13 (5%)	1 (0%)	30	66
4	L	207/209 (99%)	194 (94%)	12 (6%)	1 (0%)	25	61
5	M	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	25	61
6	O	174/177 (98%)	164 (94%)	9 (5%)	1 (1%)	22	57
7	R	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
8	S	120/123 (98%)	109 (91%)	10 (8%)	1 (1%)	16	51
9	T	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
10	U	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	19	54
11	V	118/127 (93%)	107 (91%)	10 (8%)	1 (1%)	16	51
12	W	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
13	X	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
14	Y	115/118 (98%)	112 (97%)	2 (2%)	1 (1%)	14	49
15	Z	101/103 (98%)	85 (84%)	13 (13%)	3 (3%)	3	20
16	a	108/110 (98%)	99 (92%)	6 (6%)	3 (3%)	4	21
17	b	91/100 (91%)	87 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	c	100/104 (96%)	85 (85%)	15 (15%)	0	100	100
19	d	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
20	e	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
21	f	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
22	g	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	7	33
23	h	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	32
24	i	54/57 (95%)	51 (94%)	1 (2%)	2 (4%)	2	15
25	j	48/55 (87%)	44 (92%)	4 (8%)	0	100	100
26	k	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
27	l	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
28	m	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
31	D	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
32	E	204/233 (88%)	195 (96%)	8 (4%)	1 (0%)	25	61
33	F	203/206 (98%)	172 (85%)	20 (10%)	11 (5%)	1	9
34	G	154/167 (92%)	142 (92%)	11 (7%)	1 (1%)	22	57
35	H	101/135 (75%)	94 (93%)	6 (6%)	1 (1%)	13	46
36	N	151/179 (84%)	144 (95%)	7 (5%)	0	100	100
37	P	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
38	Q	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
39	o	96/103 (93%)	90 (94%)	4 (4%)	2 (2%)	5	28
40	p	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	14	49
41	q	121/124 (98%)	112 (93%)	7 (6%)	2 (2%)	7	33
42	r	113/118 (96%)	107 (95%)	5 (4%)	1 (1%)	14	49
43	s	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	13	46
44	t	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
45	u	79/82 (96%)	71 (90%)	7 (9%)	1 (1%)	10	39
46	v	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
47	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
48	x	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
49	y	84/87 (97%)	84 (100%)	0	0	100	100
50	5	68/71 (96%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	z	2/16 (12%)	0	2 (100%)	0	100	100
All	All	5216/5531 (94%)	4877 (94%)	299 (6%)	40 (1%)	19	51

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	a	64	ALA
33	F	151	LYS
33	F	154	ARG
35	H	33	GLU
33	F	28	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	
3	K	216/218 (99%)	214 (99%)	2 (1%)	75	89
4	L	164/164 (100%)	158 (96%)	6 (4%)	29	63
5	M	165/165 (100%)	162 (98%)	3 (2%)	54	80
6	O	137/138 (99%)	132 (96%)	5 (4%)	30	64
7	R	116/116 (100%)	111 (96%)	5 (4%)	25	58
8	S	103/104 (99%)	100 (97%)	3 (3%)	37	70
9	T	103/103 (100%)	99 (96%)	4 (4%)	27	61
10	U	109/109 (100%)	108 (99%)	1 (1%)	75	89
11	V	100/103 (97%)	98 (98%)	2 (2%)	50	78
12	W	86/87 (99%)	79 (92%)	7 (8%)	9	34
13	X	99/100 (99%)	93 (94%)	6 (6%)	15	46
14	Y	89/90 (99%)	88 (99%)	1 (1%)	70	87
15	Z	84/84 (100%)	79 (94%)	5 (6%)	16	47
16	a	93/93 (100%)	93 (100%)	0	100	100
17	b	80/84 (95%)	77 (96%)	3 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	c	83/85 (98%)	80 (96%)	3 (4%)	30	64
19	d	78/78 (100%)	76 (97%)	2 (3%)	41	72
20	e	56/63 (89%)	54 (96%)	2 (4%)	30	64
21	f	67/68 (98%)	67 (100%)	0	100	100
22	g	54/55 (98%)	51 (94%)	3 (6%)	17	49
23	h	48/49 (98%)	47 (98%)	1 (2%)	48	77
24	i	47/48 (98%)	45 (96%)	2 (4%)	25	58
25	j	45/49 (92%)	43 (96%)	2 (4%)	24	58
26	k	38/38 (100%)	35 (92%)	3 (8%)	10	35
27	l	51/52 (98%)	47 (92%)	4 (8%)	10	36
28	m	34/34 (100%)	33 (97%)	1 (3%)	37	70
31	D	186/199 (94%)	176 (95%)	10 (5%)	18	50
32	E	170/190 (90%)	165 (97%)	5 (3%)	37	70
33	F	172/173 (99%)	147 (86%)	25 (14%)	2	13
34	G	119/126 (94%)	117 (98%)	2 (2%)	56	81
35	H	90/116 (78%)	87 (97%)	3 (3%)	33	67
36	N	126/147 (86%)	122 (97%)	4 (3%)	34	67
37	P	104/105 (99%)	102 (98%)	2 (2%)	52	79
38	Q	105/107 (98%)	102 (97%)	3 (3%)	37	70
39	o	86/90 (96%)	82 (95%)	4 (5%)	22	56
40	p	90/99 (91%)	85 (94%)	5 (6%)	17	49
41	q	103/104 (99%)	99 (96%)	4 (4%)	27	61
42	r	93/96 (97%)	89 (96%)	4 (4%)	25	58
43	s	83/84 (99%)	82 (99%)	1 (1%)	67	86
44	t	76/77 (99%)	73 (96%)	3 (4%)	27	61
45	u	65/65 (100%)	63 (97%)	2 (3%)	35	68
46	v	73/78 (94%)	68 (93%)	5 (7%)	13	42
47	w	57/65 (88%)	56 (98%)	1 (2%)	54	80
48	x	72/79 (91%)	69 (96%)	3 (4%)	25	59
49	y	65/66 (98%)	62 (95%)	3 (5%)	23	56
50	5	60/61 (98%)	56 (93%)	4 (7%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	z	1/1 (100%)	1 (100%)	0	100	100
All	All	4341/4505 (96%)	4172 (96%)	169 (4%)	30	61

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	F	196	ASN
42	r	16	VAL
35	H	55	HIS
39	o	5	ARG
44	t	64	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2895/2904 (99%)	537 (18%)	60 (2%)
2	J	117/118 (99%)	28 (23%)	7 (5%)
29	n	75/76 (98%)	23 (30%)	0
30	C	1516/1533 (98%)	303 (19%)	39 (2%)
51	6	2/3 (66%)	0	0
All	All	4605/4634 (99%)	891 (19%)	106 (2%)

5 of 891 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	10	A
1	I	23	G
1	I	27	G
1	I	34	U
1	I	42	A

5 of 106 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	2797	U
30	C	408	A
30	C	1211	U

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Mol	Chain	Res	Type
1	I	2903	U
2	J	88	C

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

30 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$
1	OMU	I	2552	1	19,22,23	2.92	8 (42%)	26,31,34	1.74	4 (15%)
52	RXL	z	2	52	5,6,7	1.59	2 (40%)	5,7,9	1.55	2 (40%)
1	PSU	I	746	53,1	18,21,22	1.08	2 (11%)	22,30,33	1.72	3 (13%)
52	DHV	z	15	52	5,7,8	0.64	0	4,10,12	0.74	0
52	DVA	z	6	52	4,6,7	0.56	0	6,7,9	0.81	0
1	OMC	I	2498	1	19,22,23	0.67	0	26,31,34	0.65	0
1	PSU	I	1917	1	18,21,22	1.07	1 (5%)	22,30,33	1.77	5 (22%)
1	5MC	I	1962	1	18,22,23	0.65	0	26,32,35	0.63	0
52	IB9	z	7	52	12,12,13	0.27	0	12,15,17	0.54	0
1	PSU	I	2605	1	18,21,22	1.06	1 (5%)	22,30,33	1.71	2 (9%)
1	PSU	I	2580	1	18,21,22	1.12	2 (11%)	22,30,33	2.02	7 (31%)
1	PSU	I	2457	1	18,21,22	1.12	2 (11%)	22,30,33	2.03	6 (27%)
52	DVA	z	8	52	4,6,7	0.54	0	6,7,9	0.89	0
52	DAR	z	10	52	9,10,11	0.42	0	5,11,13	0.48	0
52	RX9	z	13	52	5,7,8	1.56	2 (40%)	2,8,10	2.52	2 (100%)
1	PSU	I	1911	1	18,21,22	1.07	2 (11%)	22,30,33	1.94	6 (27%)
1	OMG	I	2251	29,1	18,26,27	1.19	2 (11%)	19,38,41	0.84	1 (5%)
52	MAA	z	4	52	4,5,6	0.46	0	1,5,7	0.28	0
52	DVA	z	12	52	4,6,7	0.55	0	6,7,9	0.74	0
1	2MG	I	1835	1	18,26,27	1.16	2 (11%)	16,38,41	0.92	1 (6%)
1	PSU	I	955	1	18,21,22	1.06	1 (5%)	22,30,33	1.78	3 (13%)
1	PSU	I	2504	1	18,21,22	1.10	2 (11%)	22,30,33	1.84	6 (27%)
52	RXL	z	9	52	5,6,7	1.65	2 (40%)	5,7,9	1.75	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MU	I	747	1	19,22,23	0.59	0	28,32,35	0.49	0
1	2MG	I	2445	1	18,26,27	1.21	2 (11%)	16,38,41	0.89	1 (6%)
1	5MU	I	1939	1	19,22,23	0.51	0	28,32,35	0.46	0
52	DAL	z	14	52	3,4,5	0.65	0	2,4,6	0.93	0
1	1MG	I	745	1	18,26,27	2.77	6 (33%)	19,39,42	1.50	4 (21%)
52	DVA	z	5	52	4,6,7	0.54	0	6,7,9	0.84	0
1	2MA	I	2503	1	19,25,26	3.43	7 (36%)	21,37,40	2.04	4 (19%)

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
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
52	RXL	z	2	52	-	0/0/6/8	-
1	PSU	I	746	53,1	-	3/7/25/26	0/2/2/2
52	DHV	z	15	52	-	0/4/8/10	-
52	DVA	z	6	52	-	1/5/6/8	-
1	OMC	I	2498	1	-	1/9/27/28	0/2/2/2
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
52	IB9	z	7	52	-	0/7/7/8	0/1/1/1
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
52	DVA	z	8	52	-	0/5/6/8	-
52	DAR	z	10	52	-	3/8/9/11	-
52	RX9	z	13	52	-	0/2/8/10	-
1	PSU	I	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	I	2251	29,1	-	1/5/27/28	0/3/3/3
52	MAA	z	4	52	-	0/1/4/6	-
52	DVA	z	12	52	-	0/5/6/8	-
1	2MG	I	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
52	RXL	z	9	52	-	0/0/6/8	-
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	2MG	I	2445	1	-	0/5/27/28	0/3/3/3
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
52	DAL	z	14	52	-	0/0/2/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MG	I	745	1	-	0/3/25/26	0/3/3/3
52	DVA	z	5	52	-	0/5/6/8	-
1	2MA	I	2503	1	-	2/3/25/26	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C4-N3	9.40	1.50	1.35
1	I	2503	2MA	C2-N1	6.88	1.46	1.34
1	I	745	1MG	C2-N3	6.75	1.46	1.34
1	I	2552	OMU	C2-N1	6.73	1.49	1.38
1	I	2503	2MA	C2-N3	6.45	1.45	1.34

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2503	2MA	C2-N3-C4	6.75	121.00	115.52
1	I	2552	OMU	C4-N3-C2	-5.49	119.34	126.58
1	I	2457	PSU	C4-N3-C2	-5.15	118.91	126.34
1	I	2457	PSU	N1-C2-N3	5.12	120.93	115.13
1	I	2580	PSU	N1-C2-N3	4.81	120.58	115.13

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	746	PSU	C2'-C1'-C5-C4
1	I	2251	OMG	C1'-C2'-O2'-CM2
52	z	6	DVA	C-CA-CB-CG2
52	z	10	DAR	NH1-CZ-NE-CD
1	I	2504	PSU	O4'-C4'-C5'-O5'

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 241 ligands modelled in this entry, 238 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	SPD	C	1688	-	9,9,9	0.32	0	8,8,8	0.83	0
56	SPD	C	1689	-	9,9,9	0.36	0	8,8,8	0.67	0
55	FME	n	101	29	8,9,10	0.79	0	7,9,11	1.24	1 (14%)

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	SPD	C	1688	-	-	0/7/7/7	-
56	SPD	C	1689	-	-	1/7/7/7	-
55	FME	n	101	29	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	n	101	FME	C-CA-N	2.39	114.04	109.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	C	1689	SPD	C4-C5-N6-C7
55	n	101	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.