



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 05:44 pm GMT

PDB ID : 8A3L  
EMDB ID : EMD-15116  
Title : Structural insights into the binding of bS1 to the ribosome  
Authors : D'Urso, G.; Chat, S.; Gillet, R.; Giudice, E.  
Deposited on : 2022-06-08  
Resolution : 3.42 Å(reported)  
Based on initial models : 7NBU, 6BU8

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

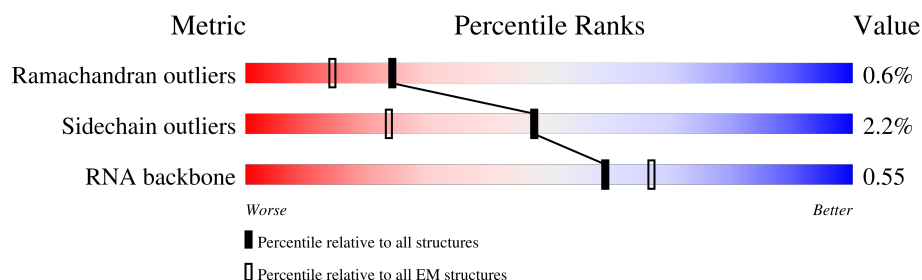
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.42 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.



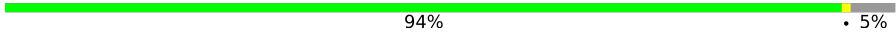

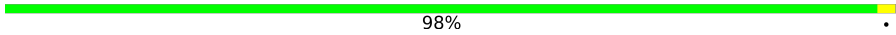
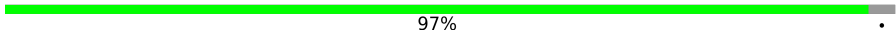
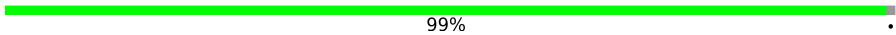
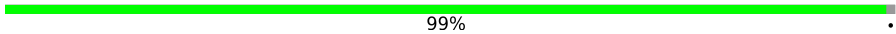
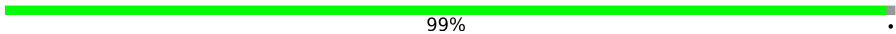
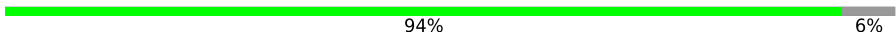


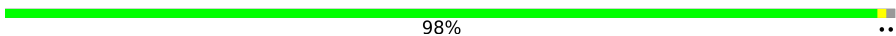


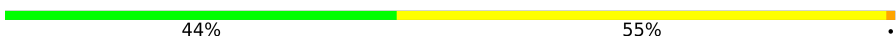




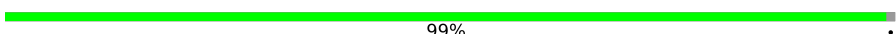
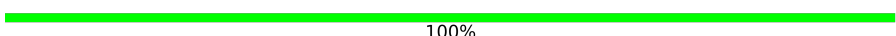
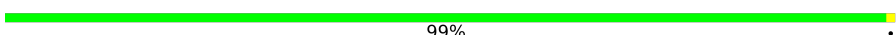
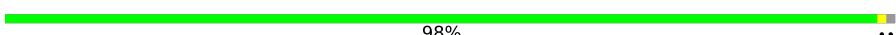
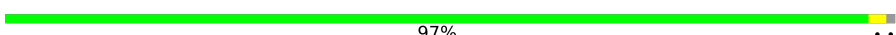
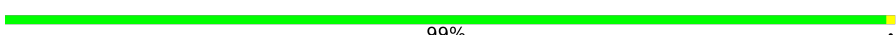
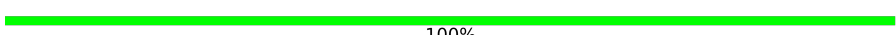
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	1539	
2	B	224	
3	C	206	
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	















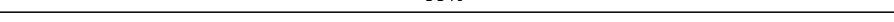
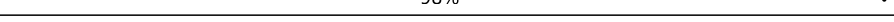
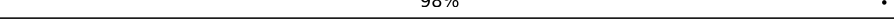
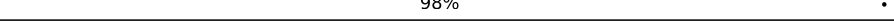

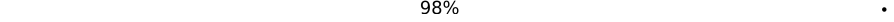
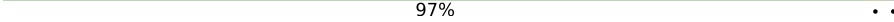
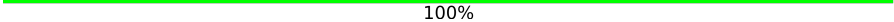
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Mol	Chain	Length	Quality of chain
10	J	103	 94% 5%
11	K	129	 89% 9%
12	L	124	 98% ..
13	M	118	 97% .
14	N	101	 99% .
15	O	89	 99% .
16	P	82	 99% .
17	Q	84	 94% 6%
18	R	75	 80% 7% 12%
19	S	92	 91% 9%
20	T	87	 98% ..
21	U	71	 69% 23% . .
22	V	77	 78% 21% .
23	W	77	 44% 55% .
24	X	38	 . 8% 5% 84%
25	Y	557	 18% 11% . 69%
26	a	2903	 80% 20%
27	b	120	 85% 15%
28	c	273	 99% .
29	d	209	 100%
30	e	201	 99% .
31	f	179	 98% ..
32	g	177	 97% ..
33	h	149	 99% .
34	i	142	 100%

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Mol	Chain	Length	Quality of chain
35	j	123	 100%
36	k	144	 100%
37	l	136	 99%
38	m	127	 93% 7%
39	n	117	 99%
40	o	115	 99%
41	p	118	 99%
42	q	103	 100%
43	r	110	 100%
44	s	100	 92% 7%
45	t	104	 98%
46	u	94	 100%
47	v	85	 99%
48	w	78	 99%
49	x	63	 98%
50	y	59	 98%
51	z	57	 98%
52	0	55	 93% 7%
53	1	46	 98%
54	2	65	 97%
55	3	38	 100%
56	4	70	 93% 6%

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 147640 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1539	Total	C	N	O	P	0	0
			33022	14736	6046	10702	1538		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	U	-	insertion	GB J01859
A	1002	A	G	conflict	GB J01859
A	1006	C	G	conflict	GB J01859
A	1010	C	U	conflict	GB J01859
A	1019	G	A	conflict	GB J01859
A	1020	A	G	conflict	GB J01859
A	1021	U	A	conflict	GB J01859
A	1022	U	A	conflict	GB J01859
A	1023	G	U	conflict	GB J01859
A	1038	U	C	conflict	GB J01859
A	1120	U	C	conflict	GB J01859

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	68	Total	C	N	O	S	0	0
			569	351	123	94	1		

- Molecule 22 is a RNA chain called P-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace	
22	V	77	Total	C	N	O	P	S	0	0
			1643	733	297	535	77	1		

- Molecule 23 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	6	Total	C	N	O	P	0	0
			136	60	30	40	6		

- Molecule 25 is a protein called 30S ribosomal protein S1.



Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	172	Total	C	N	O	0	0
			1332	840	230	262		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	2903	Total	C	N	O	P	0	0
			62337	27817	11469	20148	2903		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB NR_103073

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	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
1	137	MS6	MET	conflict	UNP P0ADY7

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	71	Total	Mg	0
			71	71	
57	a	234	Total	Mg	0
			234	234	
57	b	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
57	c	3	Total 3	Mg 3	0
57	d	1	Total 1	Mg 1	0
57	m	1	Total 1	Mg 1	0
57	z	1	Total 1	Mg 1	0

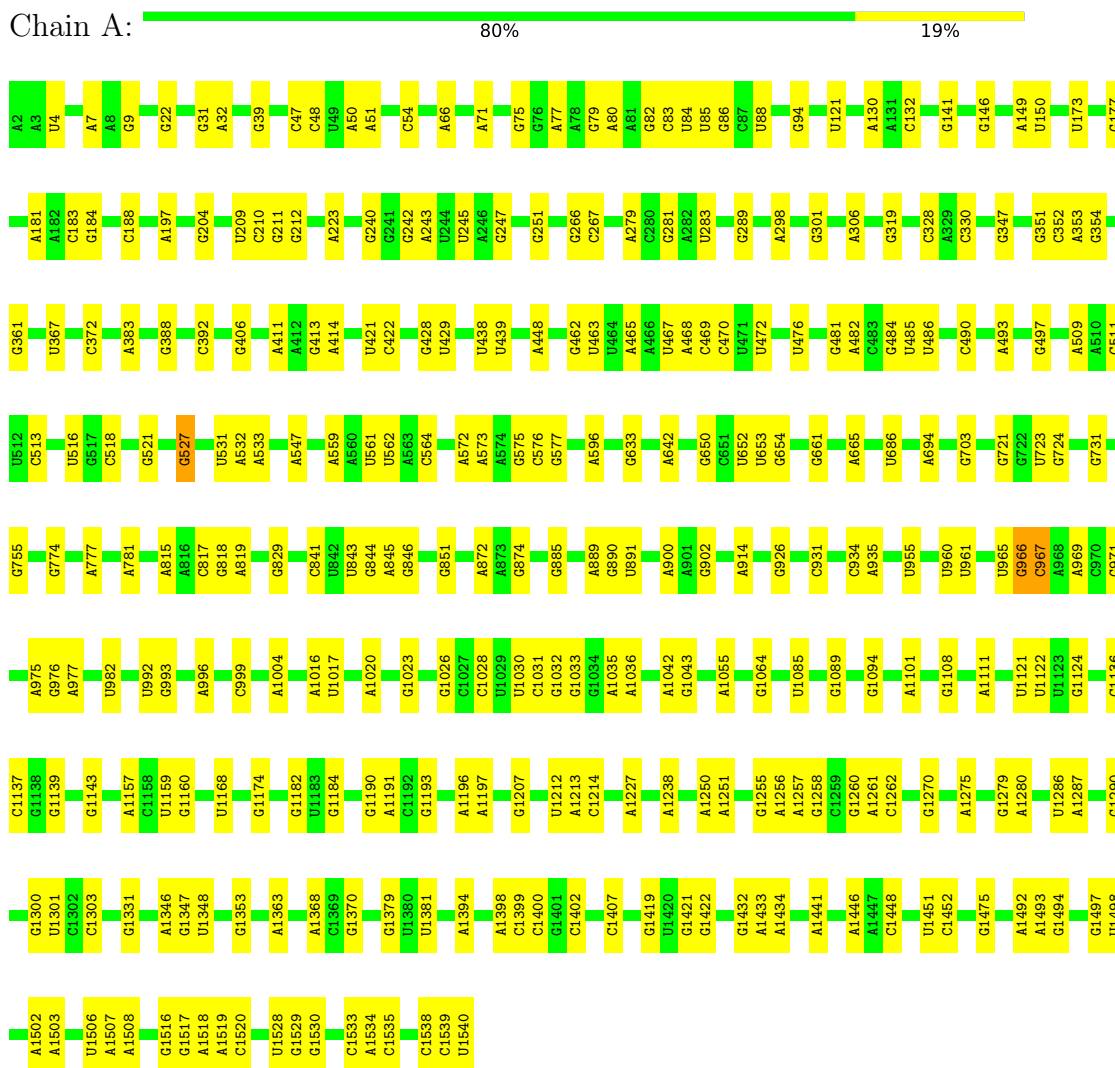
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

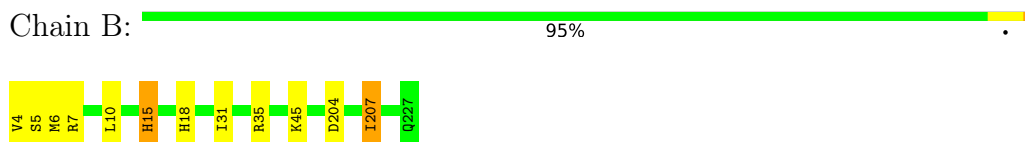
### 3 Residue-property plots

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: 16S ribosomal RNA



#### • Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

Chain C:  99%



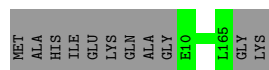
- Molecule 4: 30S ribosomal protein S4

Chain D:  99%




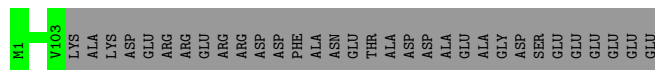
- Molecule 5: 30S ribosomal protein S5

Chain E:  93% 7%




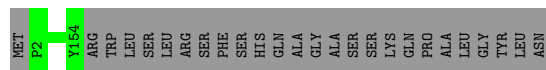
- Molecule 6: 30S ribosomal protein S6

Chain F:  76% 24%



- Molecule 7: 30S ribosomal protein S7

Chain G:  85% 15%



- Molecule 8: 30S ribosomal protein S8

Chain H:  99%



- Molecule 9: 30S ribosomal protein S9

Chain I:  97%



- Molecule 10: 30S ribosomal protein S10

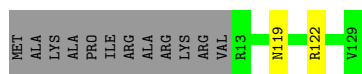


Chain J:  94% • 5%



- Molecule 11: 30S ribosomal protein S11

Chain K:  89% • 9%



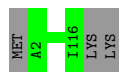
- Molecule 12: 30S ribosomal protein S12

Chain L:  98% ••



- Molecule 13: 30S ribosomal protein S13

Chain M:  97% •



- Molecule 14: 30S ribosomal protein S14

Chain N:  99% •



- Molecule 15: 30S ribosomal protein S15

Chain O:  99% •



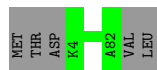
- Molecule 16: 30S ribosomal protein S16

Chain P:  99% •




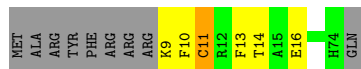
- Molecule 17: 30S ribosomal protein S17

Chain Q:  94% 6%




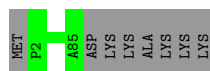
- Molecule 18: 30S ribosomal protein S18

Chain R:  80% 7% 12%



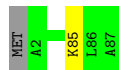
- Molecule 19: 30S ribosomal protein S19

Chain S:  91% 9%



- Molecule 20: 30S ribosomal protein S20

Chain T:  98% ..




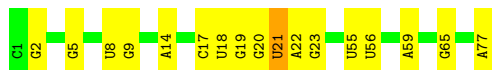
- Molecule 21: 30S ribosomal protein S21

Chain U:  69% 23% . .



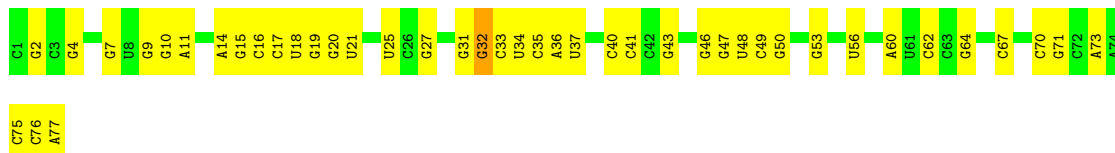
- Molecule 22: P-site fMet-tRNA(fMet)

Chain V:  78% 21% .



- Molecule 23: E-site tRNA

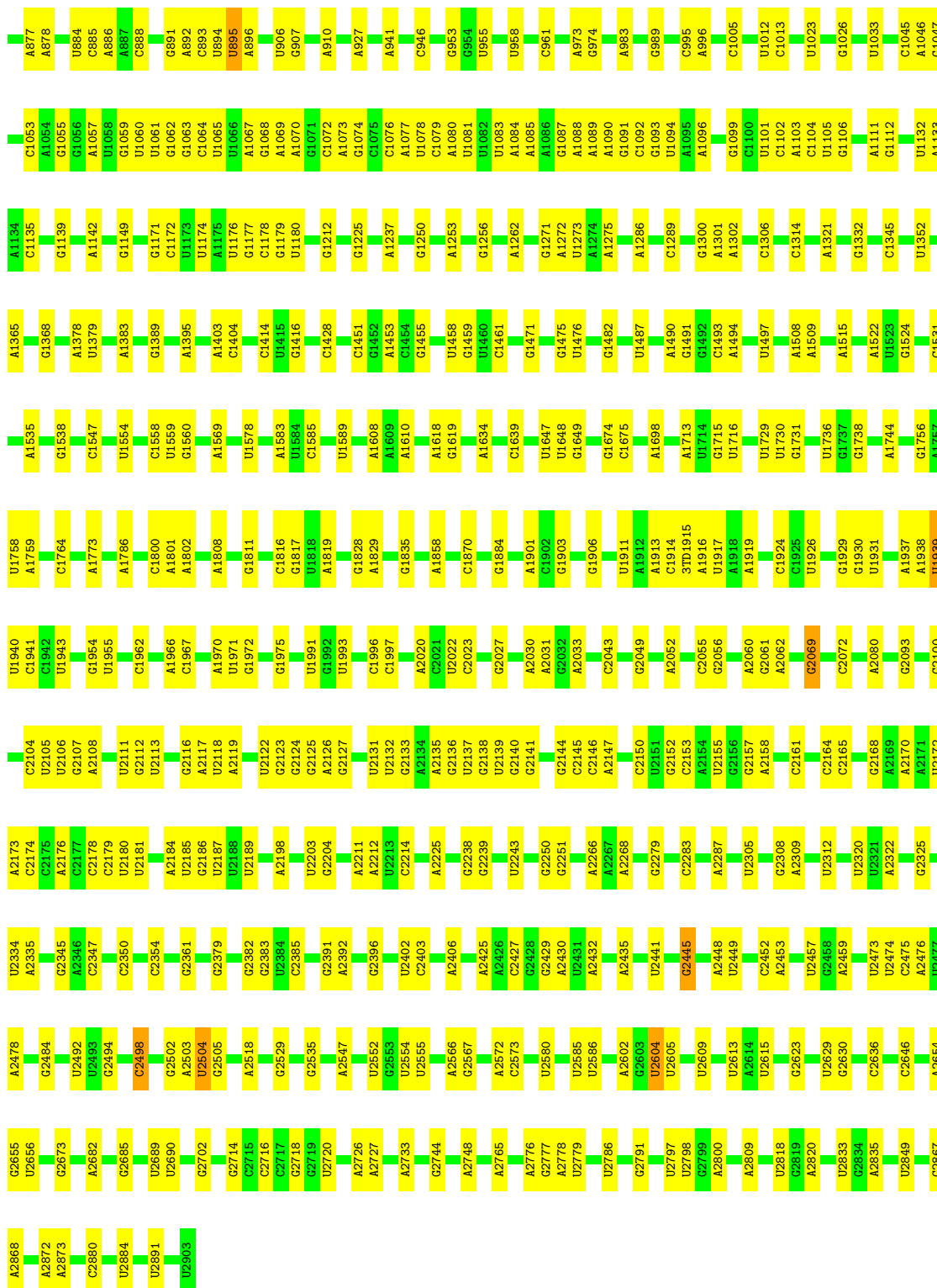
Chain W:  44% 55% .



G G G C U U U A A G U A U U A A1 G2 G3 A4 G5 G6 A A A A A A A U U U G C C A C A G G G A

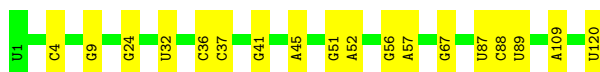
[illegible]

G645	G646	C436	C239	G1
G647	U448	U448	G242	A10
A655	C455	C455	U243	A14
G669	C456	C456	G248	G15
G678	C457	C457	C249	U34
A685	C458	C458	G250	G35
U686	U459	U459	A255	A42
G711	G481	G481	A255	G45
C717	A482	A482	A255	C46
G726	C490	C490	C275	U50
G729	G491	G491	U276	G51
G730	A501	A501	G277	G58
G737	A502	A502	A278	U59
G745	A503	A503	A279	G60
U746	A504	A504	U280	C61
A753	A505	A505	G285	U62
G764	G506	G506	U286	A63
C765	C509	C509	G301	A71
G775	C510	C510	A311	A74
A782	A513	A513	C323	G75
G783	G518	G518	G329	C96
G784	A528	A528	A330	A101
G785	A529	A529	A346	U102
A789	G530	G530	A346	A103
A792	C531	C531	U358	A118
G805	A532	A532	G361	A119
C812	U546	U546	A362	U120
A819	G548	G548	G372	U138
U827	G549	G549	U373	U139
U828	A556	A556	G386	C140
C846	A563	A563	U395	A160
U847	U573	U573	G396	A161
G858	A575	A575	U403	U162
U860	A603	A603	A404	A196
	A609	A609	U405	A199
	A613	A613	G411	G215
	A614	A614	A412	A216
	A627	A627	C417	A222
	A637	A637	A422	C229
			A423	A232



• Molecule 27: 5S ribosomal RNA

Chain b:



- Molecule 28: 50S ribosomal protein L2

Chain c:  99%



- Molecule 29: 50S ribosomal protein L3

Chain d:  100%



- Molecule 30: 50S ribosomal protein L4

Chain e:  99%



- Molecule 31: 50S ribosomal protein L5

Chain f:  98%



- Molecule 32: 50S ribosomal protein L6

Chain g:  97%



- Molecule 33: 50S ribosomal protein L9

Chain h:  99%



- Molecule 34: 50S ribosomal protein L13

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: 50S ribosomal protein L14

Chain j:  100%

There are no outlier residues recorded for this chain.

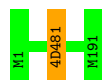
- Molecule 36: 50S ribosomal protein L15

Chain k:  100%

There are no outlier residues recorded for this chain.

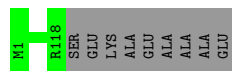
- Molecule 37: 50S ribosomal protein L16

Chain l:  99%



- Molecule 38: 50S ribosomal protein L17

Chain m:  93% 7%



- Molecule 39: 50S ribosomal protein L18

Chain n:  99%



- Molecule 40: 50S ribosomal protein L19

Chain o:  99%



- Molecule 41: 50S ribosomal protein L20

Chain p:  99%



- Molecule 42: 50S ribosomal protein L21

Chain q:  100%

There are no outlier residues recorded for this chain.

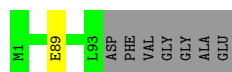
- Molecule 43: 50S ribosomal protein L22

Chain r:  100%

There are no outlier residues recorded for this chain.

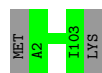
- Molecule 44: 50S ribosomal protein L23

Chain s:  92% • 7%



- Molecule 45: 50S ribosomal protein L24

Chain t:  98% •



- Molecule 46: 50S ribosomal protein L25

Chain u:  100%

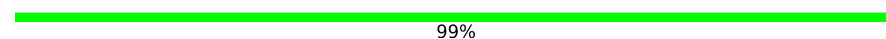
There are no outlier residues recorded for this chain.

- Molecule 47: 50S ribosomal protein L27

Chain v:  99% •



- Molecule 48: 50S ribosomal protein L28

Chain w:  99% •



- Molecule 49: 50S ribosomal protein L29

Chain x:  98% •



- Molecule 50: 50S ribosomal protein L30

Chain y:  98% •



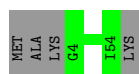
- Molecule 51: 50S ribosomal protein L32

Chain z: 98% .



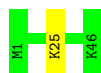
- Molecule 52: 50S ribosomal protein L33

Chain 0: 93% 7%



- Molecule 53: 50S ribosomal protein L34

Chain 1: 98% .



- Molecule 54: 50S ribosomal protein L35

Chain 2: 97% . .



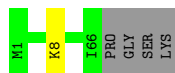
- Molecule 55: 50S ribosomal protein L36

Chain 3: 100%

There are no outlier residues recorded for this chain.

- Molecule 56: 50S ribosomal protein L31

Chain 4: 93% . 6%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16381	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (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: 4SU, 4D4, PSU, UR3, 4OC, OMU, ZN, 5MU, 5MC, H2U, 6MZ, MEQ, 3TD, OMG, 2MA, MG, 2MG, D2T, MA6, OMC, G7M, MS6, 1MG

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	A	0.67	0/36690	0.82	2/57230 (0.0%)
2	B	0.48	0/1784	0.64	1/2403 (0.0%)
3	C	0.34	0/1651	0.46	0/2225
4	D	0.37	0/1665	0.47	0/2227
5	E	0.37	0/1165	0.48	0/1568
6	F	0.38	0/858	0.50	0/1160
7	G	0.29	0/1219	0.43	0/1635
8	H	0.37	0/989	0.51	0/1326
9	I	0.34	0/1034	0.48	0/1375
10	J	0.33	0/796	0.54	0/1077
11	K	0.38	0/893	0.54	0/1205
12	L	0.36	0/960	0.50	0/1286
13	M	0.32	0/900	0.51	0/1204
14	N	0.34	0/817	0.44	0/1088
15	O	0.33	0/722	0.44	0/964
16	P	0.37	0/653	0.49	0/877
17	Q	0.36	0/650	0.48	0/871
18	R	0.56	0/553	0.66	0/742
19	S	0.33	0/685	0.49	0/922
20	T	0.31	0/676	0.43	0/895
21	U	0.52	0/576	0.78	1/763 (0.1%)
22	V	0.52	0/1746	0.81	0/2721
23	W	0.51	0/1832	0.85	1/2855 (0.0%)
24	X	0.68	0/153	1.75	4/238 (1.7%)
25	Y	0.63	0/1347	0.79	1/1817 (0.1%)
26	a	0.77	0/69244	0.83	1/108022 (0.0%)
27	b	0.62	0/2872	0.80	0/4478
28	c	0.41	0/2121	0.50	0/2852
29	d	0.42	0/1576	0.51	0/2119
30	e	0.41	0/1571	0.49	0/2113
31	f	0.34	0/1434	0.47	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	g	0.33	0/1343	0.49	0/1816
33	h	0.42	0/1122	0.65	0/1515
34	i	0.41	0/1152	0.47	0/1551
35	j	0.39	0/955	0.51	0/1279
36	k	0.38	0/1062	0.52	0/1413
37	l	0.38	0/1073	0.50	0/1433
38	m	0.40	0/958	0.47	0/1281
39	n	0.37	0/902	0.46	0/1209
40	o	0.39	0/929	0.49	0/1242
41	p	0.46	0/960	0.43	0/1278
42	q	0.42	0/829	0.51	0/1107
43	r	0.37	0/864	0.50	0/1156
44	s	0.38	0/744	0.48	0/994
45	t	0.37	0/787	0.50	0/1051
46	u	0.37	0/766	0.49	0/1025
47	v	0.40	0/642	0.45	0/848
48	w	0.38	0/635	0.47	0/848
49	x	0.31	0/502	0.43	0/667
50	y	0.37	0/453	0.54	0/605
51	z	0.39	0/450	0.47	0/599
52	0	0.38	0/424	0.48	0/565
53	1	0.39	0/380	0.47	0/498
54	2	0.41	0/513	0.53	0/676
55	3	0.37	0/303	0.46	0/397
56	4	0.36	0/531	0.48	0/709
All	All	0.65	0/159111	0.76	11/237946 (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
37	l	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	HIS	C-N-CA	-8.27	101.03	121.70
1	A	1528	U	P-O3'-C3'	7.75	129.00	119.70
24	X	4	A	N9-C4-C5	-6.79	103.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	2	G	C5-C6-O6	-6.30	124.82	128.60
1	A	1528	U	OP2-P-O3'	5.90	118.18	105.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	l	81	4D4	Mainchain

## 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	
2	B	222/224 (99%)	192 (86%)	27 (12%)	3 (1%)	9	32
3	C	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	13	40
4	D	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
5	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
6	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
7	G	151/179 (84%)	142 (94%)	9 (6%)	0	100	100
8	H	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
9	I	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
10	J	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	13	40
11	K	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
12	L	120/124 (97%)	108 (90%)	11 (9%)	1 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
14	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
17	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
18	R	64/75 (85%)	48 (75%)	13 (20%)	3 (5%)	2	12
19	S	82/92 (89%)	77 (94%)	5 (6%)	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	66/71 (93%)	51 (77%)	8 (12%)	7 (11%)	0	3
25	Y	170/557 (30%)	88 (52%)	68 (40%)	14 (8%)	1	4
28	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
29	d	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
30	e	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
31	f	175/179 (98%)	158 (90%)	17 (10%)	0	100	100
32	g	174/177 (98%)	158 (91%)	14 (8%)	2 (1%)	12	38
33	h	147/149 (99%)	110 (75%)	35 (24%)	2 (1%)	9	32
34	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
35	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
36	k	142/144 (99%)	132 (93%)	10 (7%)	0	100	100
37	l	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
38	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
39	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
40	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
41	p	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
42	q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
43	r	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
44	s	91/100 (91%)	83 (91%)	7 (8%)	1 (1%)	12	38
45	t	100/104 (96%)	83 (83%)	17 (17%)	0	100	100
46	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
47	v	82/85 (96%)	73 (89%)	9 (11%)	0	100	100
48	w	75/78 (96%)	72 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
50	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
51	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
52	0	49/55 (89%)	49 (100%)	0	0	100	100
53	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	8	29
55	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
56	4	64/70 (91%)	56 (88%)	8 (12%)	0	100	100
All	All	5773/6426 (90%)	5304 (92%)	432 (8%)	37 (1%)	24	51

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	18	HIS
12	L	16	VAL
21	U	57	ALA
21	U	62	ARG
21	U	65	ALA

### 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	
2	B	186/186 (100%)	176 (95%)	10 (5%)	18	44
3	C	170/170 (100%)	170 (100%)	0	100	100
4	D	172/173 (99%)	170 (99%)	2 (1%)	67	79
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	104 (99%)	1 (1%)	73	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	90/99 (91%)	88 (98%)	2 (2%)	47	68
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	53 (93%)	4 (7%)	12	37
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	64 (98%)	1 (2%)	60	76
21	U	58/61 (95%)	44 (76%)	14 (24%)	0	1
25	Y	144/461 (31%)	81 (56%)	63 (44%)	0	0
28	c	216/218 (99%)	216 (100%)	0	100	100
29	d	163/163 (100%)	163 (100%)	0	100	100
30	e	165/165 (100%)	163 (99%)	2 (1%)	67	79
31	f	148/150 (99%)	147 (99%)	1 (1%)	81	89
32	g	137/138 (99%)	135 (98%)	2 (2%)	60	76
33	h	114/114 (100%)	114 (100%)	0	100	100
34	i	116/116 (100%)	116 (100%)	0	100	100
35	j	104/104 (100%)	104 (100%)	0	100	100
36	k	103/103 (100%)	103 (100%)	0	100	100
37	l	107/107 (100%)	107 (100%)	0	100	100
38	m	98/103 (95%)	98 (100%)	0	100	100
39	n	86/87 (99%)	86 (100%)	0	100	100
40	o	99/100 (99%)	99 (100%)	0	100	100
41	p	89/90 (99%)	89 (100%)	0	100	100
42	q	84/84 (100%)	84 (100%)	0	100	100
43	r	93/93 (100%)	93 (100%)	0	100	100
44	s	80/84 (95%)	80 (100%)	0	100	100
45	t	83/85 (98%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	u	78/78 (100%)	78 (100%)	0	100	100
47	v	62/63 (98%)	62 (100%)	0	100	100
48	w	67/68 (98%)	67 (100%)	0	100	100
49	x	54/55 (98%)	54 (100%)	0	100	100
50	y	48/49 (98%)	48 (100%)	0	100	100
51	z	47/48 (98%)	47 (100%)	0	100	100
52	0	46/49 (94%)	46 (100%)	0	100	100
53	1	38/38 (100%)	37 (97%)	1 (3%)	41	64
54	2	51/52 (98%)	51 (100%)	0	100	100
55	3	34/34 (100%)	34 (100%)	0	100	100
56	4	59/62 (95%)	58 (98%)	1 (2%)	56	74
All	All	4805/5254 (92%)	4701 (98%)	104 (2%)	47	68

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Y	84	LEU
25	Y	117	LYS
31	f	30	ARG
25	Y	86	ARG
25	Y	103	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
29	d	36	GLN
29	d	49	GLN
54	2	31	HIS
32	g	38	ASN
9	I	37	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1535/1539 (99%)	279 (18%)	21 (1%)
22	V	76/77 (98%)	13 (17%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	W	76/77 (98%)	43 (56%)	3 (3%)
24	X	5/38 (13%)	4 (80%)	0
26	a	2898/2903 (99%)	578 (19%)	0
27	b	119/120 (99%)	18 (15%)	0
All	All	4709/4754 (99%)	935 (19%)	25 (0%)

5 of 935 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	A
1	A	9	G
1	A	22	G
1	A	31	G

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1256	A
1	A	1399	C
23	W	76	C
1	A	1347	G
1	A	1432	G

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

42 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	$\# Z  > 2$
22	H2U	V	21	22	18,21,22	2.91	5 (27%)	21,30,33	1.98	5 (23%)
1	MA6	A	1518	1	18,26,27	1.22	3 (16%)	19,38,41	2.21	7 (36%)
37	4D4	l	81	37	9,11,12	1.90	2 (22%)	8,13,15	1.85	2 (25%)
26	PSU	a	2580	26	18,21,22	1.44	2 (11%)	22,30,33	2.05	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	A	1516	1	18,26,27	1.16	2 (11%)	16,38,41	1.24	1 (6%)
1	PSU	A	516	57,1	18,21,22	1.49	2 (11%)	22,30,33	1.97	3 (13%)
26	PSU	a	1917	26	18,21,22	1.53	3 (16%)	22,30,33	1.92	5 (22%)
26	PSU	a	1911	26	18,21,22	1.09	2 (11%)	22,30,33	1.88	5 (22%)
26	H2U	a	2449	26	18,21,22	2.70	5 (27%)	21,30,33	2.11	5 (23%)
26	5MU	a	747	26	19,22,23	1.49	5 (26%)	28,32,35	2.13	10 (35%)
26	6MZ	a	1618	26	18,25,26	1.93	3 (16%)	16,36,39	2.25	4 (25%)
26	5MU	a	1939	26	19,22,23	1.51	6 (31%)	28,32,35	2.16	8 (28%)
26	2MG	a	2445	26	18,26,27	1.17	1 (5%)	16,38,41	1.32	3 (18%)
26	PSU	a	2504	26	18,21,22	1.55	2 (11%)	22,30,33	2.02	5 (22%)
22	4SU	V	8	22	18,21,22	3.71	7 (38%)	26,30,33	2.35	6 (23%)
26	5MC	a	1962	26	18,22,23	3.53	7 (38%)	26,32,35	1.12	1 (3%)
22	5MU	V	55	22	19,22,23	1.45	6 (31%)	28,32,35	1.74	8 (28%)
26	PSU	a	2605	26	18,21,22	1.45	3 (16%)	22,30,33	1.87	4 (18%)
26	2MG	a	1835	26	18,26,27	1.08	1 (5%)	16,38,41	1.14	2 (12%)
26	OMC	a	2498	57,26	19,22,23	3.12	8 (42%)	26,31,34	0.71	0
12	D2T	L	89	12	7,9,10	1.37	1 (14%)	6,11,13	2.60	4 (66%)
1	UR3	A	1498	1	19,22,23	2.77	7 (36%)	26,32,35	1.40	2 (7%)
1	5MC	A	967	1	18,22,23	3.59	7 (38%)	26,32,35	1.05	1 (3%)
26	PSU	a	746	26	18,21,22	1.33	2 (11%)	22,30,33	1.98	4 (18%)
22	PSU	V	56	22	18,21,22	1.46	3 (16%)	22,30,33	1.79	3 (13%)
26	6MZ	a	2030	26	18,25,26	1.99	3 (16%)	16,36,39	2.20	4 (25%)
26	PSU	a	2604	26	18,21,22	1.46	2 (11%)	22,30,33	2.00	4 (18%)
26	1MG	a	745	26	18,26,27	0.90	0	19,39,42	1.32	4 (21%)
1	2MG	A	966	1	18,26,27	1.08	1 (5%)	16,38,41	1.44	3 (18%)
1	MA6	A	1519	1	18,26,27	1.22	3 (16%)	19,38,41	1.83	7 (36%)
26	OMG	a	2251	26,22	18,26,27	1.10	2 (11%)	19,38,41	1.07	2 (10%)
26	PSU	a	2457	26	18,21,22	1.57	3 (16%)	22,30,33	1.93	5 (22%)
1	4OC	A	1402	1	20,23,24	3.03	8 (40%)	26,32,35	0.92	2 (7%)
26	PSU	a	955	26	18,21,22	1.11	2 (11%)	22,30,33	1.87	4 (18%)
26	2MA	a	2503	57,26	19,25,26	0.98	1 (5%)	21,37,40	2.35	5 (23%)
26	G7M	a	2069	26	20,26,27	1.25	2 (10%)	17,39,42	0.97	1 (5%)
1	2MG	A	1207	1	18,26,27	1.17	2 (11%)	16,38,41	1.19	2 (12%)
26	OMU	a	2552	57,26	19,22,23	2.81	8 (42%)	26,31,34	1.82	4 (15%)
1	5MC	A	1407	1	18,22,23	3.52	7 (38%)	26,32,35	1.00	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	3TD	a	1915	26	18,22,23	4.32	7 (38%)	22,32,35	1.73	4 (18%)
29	MEQ	d	150	29	8,9,10	0.95	0	5,10,12	1.13	1 (20%)
1	G7M	A	527	1	20,26,27	1.24	2 (10%)	17,39,42	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	H2U	V	21	22	-	7/7/38/39	0/2/2/2
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
37	4D4	l	81	37	-	2/11/12/14	-
26	PSU	a	2580	26	-	1/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
1	PSU	A	516	57,1	-	0/7/25/26	0/2/2/2
26	PSU	a	1917	26	-	0/7/25/26	0/2/2/2
26	PSU	a	1911	26	-	0/7/25/26	0/2/2/2
26	H2U	a	2449	26	-	0/7/38/39	0/2/2/2
26	5MU	a	747	26	-	1/7/25/26	0/2/2/2
26	6MZ	a	1618	26	-	4/5/27/28	0/3/3/3
26	5MU	a	1939	26	-	2/7/25/26	0/2/2/2
26	2MG	a	2445	26	-	2/5/27/28	0/3/3/3
26	PSU	a	2504	26	-	2/7/25/26	0/2/2/2
22	4SU	V	8	22	-	0/7/25/26	0/2/2/2
26	5MC	a	1962	26	-	2/7/25/26	0/2/2/2
22	5MU	V	55	22	-	0/7/25/26	0/2/2/2
26	PSU	a	2605	26	-	0/7/25/26	0/2/2/2
26	2MG	a	1835	26	-	2/5/27/28	0/3/3/3
26	OMC	a	2498	57,26	-	2/9/27/28	0/2/2/2
12	D2T	L	89	12	-	3/7/12/14	-
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
26	PSU	a	746	26	-	2/7/25/26	0/2/2/2
22	PSU	V	56	22	-	0/7/25/26	0/2/2/2
26	6MZ	a	2030	26	-	2/5/27/28	0/3/3/3
26	PSU	a	2604	26	-	2/7/25/26	0/2/2/2
26	1MG	a	745	26	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	966	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1519	1	-	5/7/29/30	0/3/3/3
26	OMG	a	2251	26,22	-	1/5/27/28	0/3/3/3
26	PSU	a	2457	26	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	1/9/29/30	0/2/2/2
26	PSU	a	955	26	-	0/7/25/26	0/2/2/2
26	2MA	a	2503	57,26	-	1/3/25/26	0/3/3/3
26	G7M	a	2069	26	-	2/3/25/26	0/3/3/3
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
26	OMU	a	2552	57,26	-	3/9/27/28	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
26	3TD	a	1915	26	-	6/7/25/26	0/2/2/2
29	MEQ	d	150	29	-	2/8/9/11	-
1	G7M	A	527	1	-	1/3/25/26	0/3/3/3

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	1915	3TD	C6-C5	12.35	1.49	1.35
1	A	1407	5MC	C6-C5	9.35	1.50	1.34
1	A	967	5MC	C6-C5	9.26	1.49	1.34
22	V	21	H2U	C2-N1	9.23	1.48	1.35
26	a	1915	3TD	C2-N1	9.13	1.49	1.37

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	8	4SU	C4-N3-C2	-7.94	119.62	127.34
26	a	2503	2MA	C2-N3-C4	7.93	121.97	115.52
26	a	2449	H2U	C4-N3-C2	-6.98	120.00	125.79
1	A	1518	MA6	N1-C6-N6	6.70	124.11	117.06
22	V	21	H2U	C4-N3-C2	-6.55	120.36	125.79

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1498	UR3	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	A	1498	UR3	O4'-C1'-N1-C2
1	A	1518	MA6	C5-C6-N6-C9

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 315 ligands modelled in this entry, 315 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.