



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 26, 2018 – 06:30 PM EST

PDB ID : 5IQR  
EMDB ID: : EMD-8107  
Title : Structure of RelA bound to the 70S ribosome  
Authors : Brown, A.; Fernandez, I.S.; Gordiyenko, Y.; Ramakrishnan, V.  
Deposited on : 2016-03-11  
Resolution : 3.00 Å(reported)  
Based on PDB ID : 4YBB

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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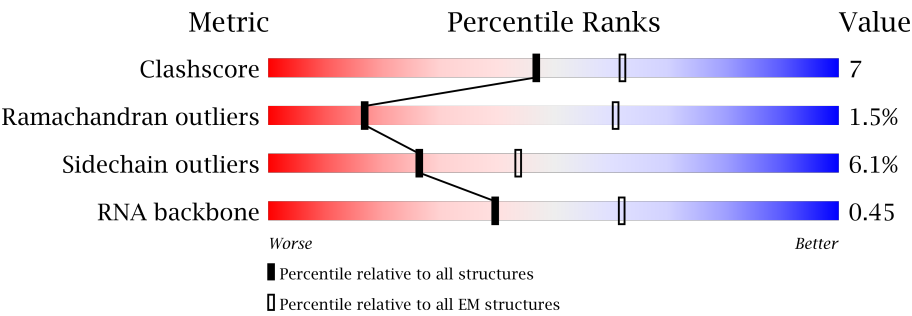
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

# 1 Overall quality at a glance i

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.









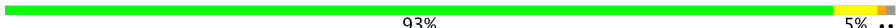











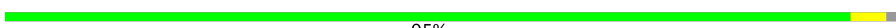






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	B	273	85% 14% ..
2	C	209	86% 14%
3	D	201	88% 11%
4	E	179	84% 13% ..
5	F	177	89% 11% .
6	G	149	95% . .
7	H	165	72% 7% . 21%
8	I	142	92% 8% .

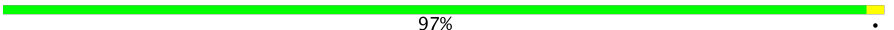







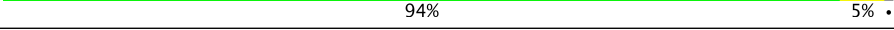

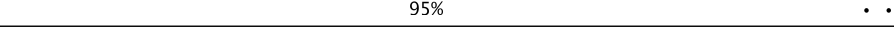
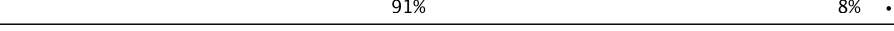







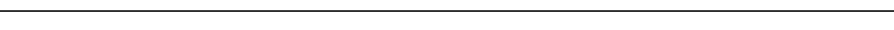

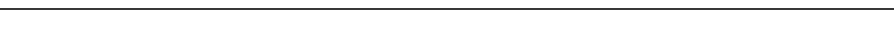
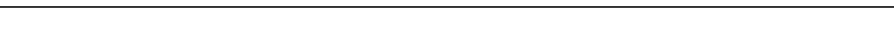


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Mol	Chain	Length	Quality of chain
9	J	142	 91% 8%
10	K	123	 90% 10%
11	L	144	 90% 10%
12	M	136	 92% 8%
13	N	127	 67% 24% 6%
14	O	117	 80% 17%
15	P	115	 93% 5%
16	Q	118	 80% 18%
17	R	103	 87% 12%
18	S	110	 85% 14%
19	T	100	 85% 8% 7%
20	U	104	 89% 8%
21	V	94	 87% 13%
22	W	85	 85% 6% 9%
23	X	78	 91% 8%
24	Y	63	 87% 10%
25	Z	59	 85% 14%
26	a	70	 91% 6%
27	b	57	 95%
28	c	55	 89% 9%
29	d	46	 87% 13%
30	e	65	 89% 9%
31	f	38	 89% 11%
32	g	241	 88% 5% 7%
33	h	233	 84% 5% 11%


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Mol	Chain	Length	Quality of chain
34	i	206	 97% .
35	j	167	 86% 8% 6%
36	k	135	 70% . 26%
37	l	179	 78% 6% . 16%
38	m	130	 92% 7% .
39	n	130	 90% 8% .
40	o	103	 84% 11% 5%
41	p	129	 84% 6% 9%
42	q	124	 94% 5% .
43	r	118	 90% 7% .
44	s	101	 95% . .
45	t	89	 91% 8% .
46	u	82	 88% 12%
47	v	84	 85% 11% 5%
48	w	75	 84% . 13%
49	x	92	 84% 5% 11%
50	y	87	 92% 7% .
51	z	71	 72% 7% 21%
52	1	2904	 52% 42% 7%
53	2	1533	 52% 43% 5%
54	3	118	 58% 38% .
55	4	76	 55% 36% 9%
56	5	78	 26% 44% 29% .
57	6	76	 21% 51% 25% .
58	7	10	 60% 40%

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Mol	Chain	Length	Quality of chain
59	8	744	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	H2U	6	16	X	-	-	-
57	H2U	6	20	X	-	-	-
57	PSU	6	32	X	-	-	-
57	6IA	6	37	X	-	-	-
57	PSU	6	55	X	-	-	-

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 154519 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.



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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	77	Total	C	N	O	S	0	0
			588	363	118	106	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is a protein called 30S ribosomal protein S2.

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

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	207	Total	C	N	O	S	0	0
			1628	1030	306	289	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	207	LEU	ILE	conflict	UNP P0A7V3
h	208	GLY	LEU	conflict	UNP P0A7V3

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

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

- Molecule 41 is a protein called 30S ribosomal protein S11.

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

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	65	Total	C	N	O	S	0	0
			539	341	100	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	15	GLU	ALA	conflict	UNP P0A7T7

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

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

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 52 is a RNA chain called LSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	2904	Total	C	N	O	P	0	0
			62356	27825	11472	20155	2904		

- Molecule 53 is a RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	1533	Total	C	N	O	P	0	0
			32907	14683	6036	10655	1533		

- Molecule 54 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 55 is a RNA chain called E-site tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 56 is a RNA chain called P-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	5	77	Total	C	N	O	P	S	0	0
			1639	734	294	534	76	1		

- Molecule 57 is a RNA chain called A/T tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
57	6	76	Total	C	N	O	P	S	0	0
			1637	734	290	536	76	1		

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	7	10	Total	C	N	O	P	0	0
			211	95	36	70	10		

- Molecule 59 is a protein called GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	8	615	Total	C	N	O	S	0	0
			4792	3010	875	885	22		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	2	64	Total	Mg	0
			64	64	
60	1	220	Total	Mg	0
			220	220	
60	B	1	Total	Mg	0
			1	1	

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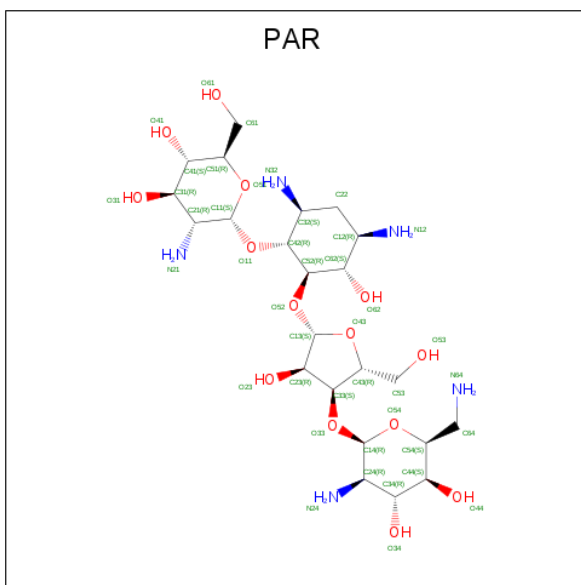
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Mol	Chain	Residues	Atoms		AltConf
60	C	1	Total 1	Mg 1	0
60	3	6	Total 6	Mg 6	0
60	N	1	Total 1	Mg 1	0
60	U	1	Total 1	Mg 1	0
60	8	1	Total 1	Mg 1	0
60	r	1	Total 1	Mg 1	0
60	L	2	Total 2	Mg 2	0
60	s	1	Total 1	Mg 1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

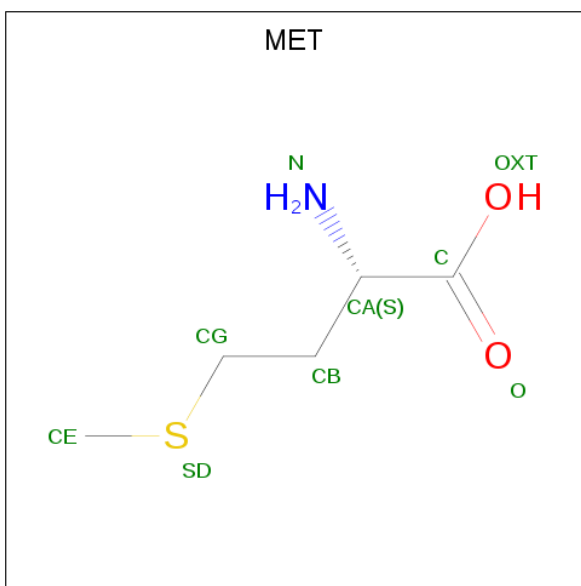
Mol	Chain	Residues	Atoms		AltConf
61	8	1	Total 1	Zn 1	0
61	a	1	Total 1	Zn 1	0
61	f	1	Total 1	Zn 1	0

- Molecule 62 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				AltConf
62	2	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 63 is METHIONINE (three-letter code: MET) (formula:  $\text{C}_5\text{H}_{11}\text{NO}_2\text{S}$ ).



Mol	Chain	Residues	Atoms					AltConf
63	5	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 64 is water.

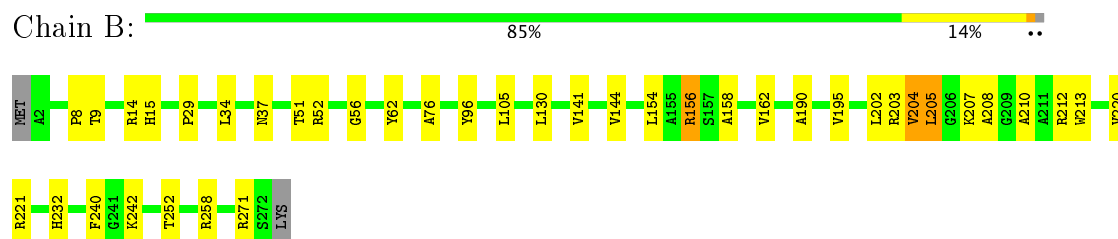


Mol	Chain	Residues	Atoms		AltConf
64	B	2	Total	O	0
			2	2	

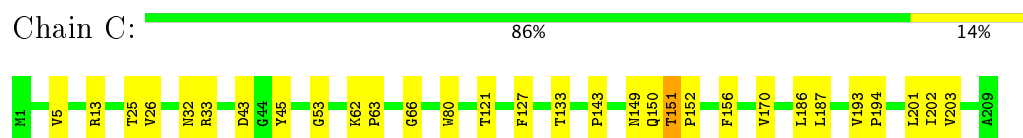
### 3 Residue-property plots

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

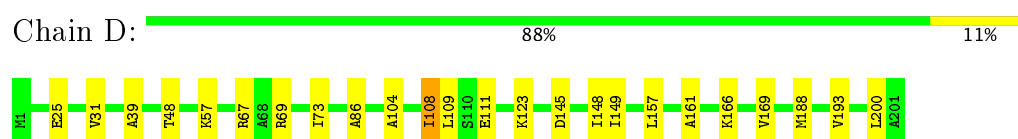
- Molecule 1: 50S ribosomal protein L2



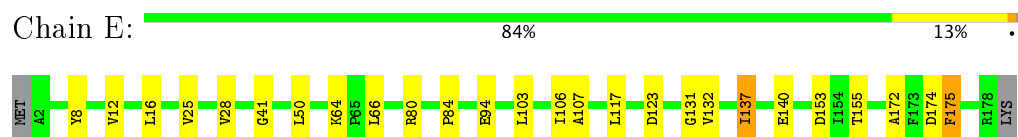
- Molecule 2: 50S ribosomal protein L3



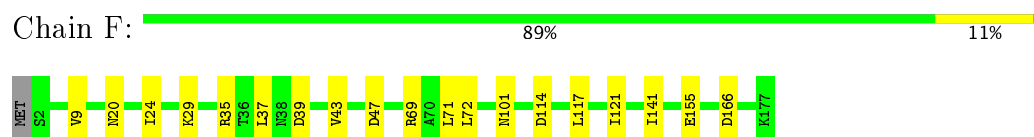
- Molecule 3: 50S ribosomal protein L4



- Molecule 4: 50S ribosomal protein L5



- Molecule 5: 50S ribosomal protein L6



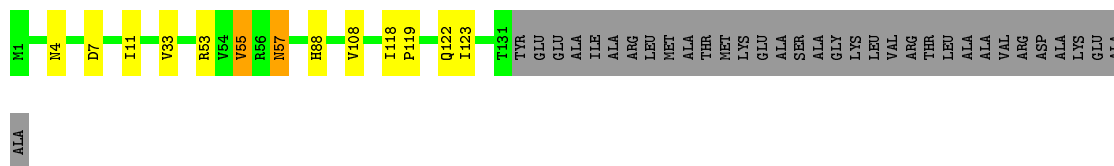
- Molecule 6: 50S ribosomal protein L9

Chain G:  95% ..




- Molecule 7: 50S ribosomal protein L10

Chain H:  72% 7% 21%




- Molecule 8: 50S ribosomal protein L11

Chain I:  92% 8%




- Molecule 9: 50S ribosomal protein L13

Chain J:  91% 8%




- Molecule 10: 50S ribosomal protein L14

Chain K:  90% 10%



- Molecule 11: 50S ribosomal protein L15

Chain L:  90% 10%



- Molecule 12: 50S ribosomal protein L16

Chain M:  92% 8%




- Molecule 13: 50S ribosomal protein L17

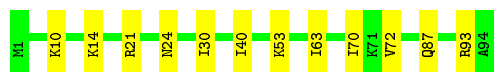


Chain U:  89% 8% ..




- Molecule 21: 50S ribosomal protein L25

Chain V:  87% 13%



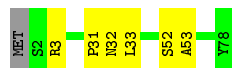
- Molecule 22: 50S ribosomal protein L27

Chain W:  85% 6% 9%




- Molecule 23: 50S ribosomal protein L28

Chain X:  91% 8%




- Molecule 24: 50S ribosomal protein L29

Chain Y:  87% 10% ..



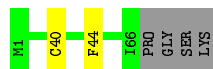
- Molecule 25: 50S ribosomal protein L30

Chain Z:  85% 14%



- Molecule 26: 50S ribosomal protein L31

Chain a:  91% 6%



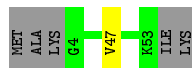
- Molecule 27: 50S ribosomal protein L32

Chain b:  95%



- Molecule 28: 50S ribosomal protein L33

Chain c: 89% 9%



- Molecule 29: 50S ribosomal protein L34

Chain d: 87% 13%



- Molecule 30: 50S ribosomal protein L35

Chain e: 89% 9%



- Molecule 31: 50S ribosomal protein L36

Chain f: 89% 11%



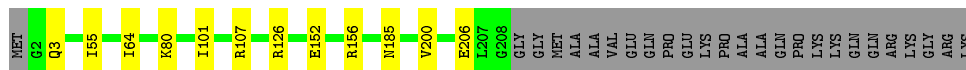
- Molecule 32: 30S ribosomal protein S2

Chain g: 88% 5% 7%



- Molecule 33: 30S ribosomal protein S3

Chain h: 84% 5% 11%




- Molecule 34: 30S ribosomal protein S4

Chain i: 97%



- Molecule 35: 30S ribosomal protein S5

Chain j:  86% 8% 6%




- Molecule 36: 30S ribosomal protein S6

Chain k:  70% 26%



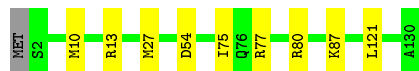
- Molecule 37: 30S ribosomal protein S7

Chain l:  78% 6% 16%



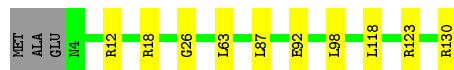
- Molecule 38: 30S ribosomal protein S8

Chain m:  92% 7%




- Molecule 39: 30S ribosomal protein S9

Chain n:  90% 8%




- Molecule 40: 30S ribosomal protein S10

Chain o:  84% 11% 5%



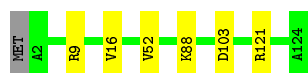
- Molecule 41: 30S ribosomal protein S11

Chain p:  84% 6% 9%




- Molecule 42: 30S ribosomal protein S12

Chain q:  94% 5%



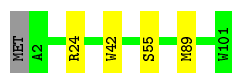
- Molecule 43: 30S ribosomal protein S13

Chain r:  90% 7%



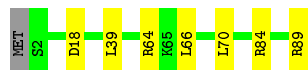
- Molecule 44: 30S ribosomal protein S14

Chain s:  95%




- Molecule 45: 30S ribosomal protein S15

Chain t:  91% 8%




- Molecule 46: 30S ribosomal protein S16

Chain u:  88% 12%




- Molecule 47: 30S ribosomal protein S17

Chain v:  85% 11% 5%




- Molecule 48: 30S ribosomal protein S18

Chain w:  84% 13%



- Molecule 49: 30S ribosomal protein S19

Chain x:  84% 5% 11%





- Molecule 50: 30S ribosomal protein S20

Chain v:  92% 7%



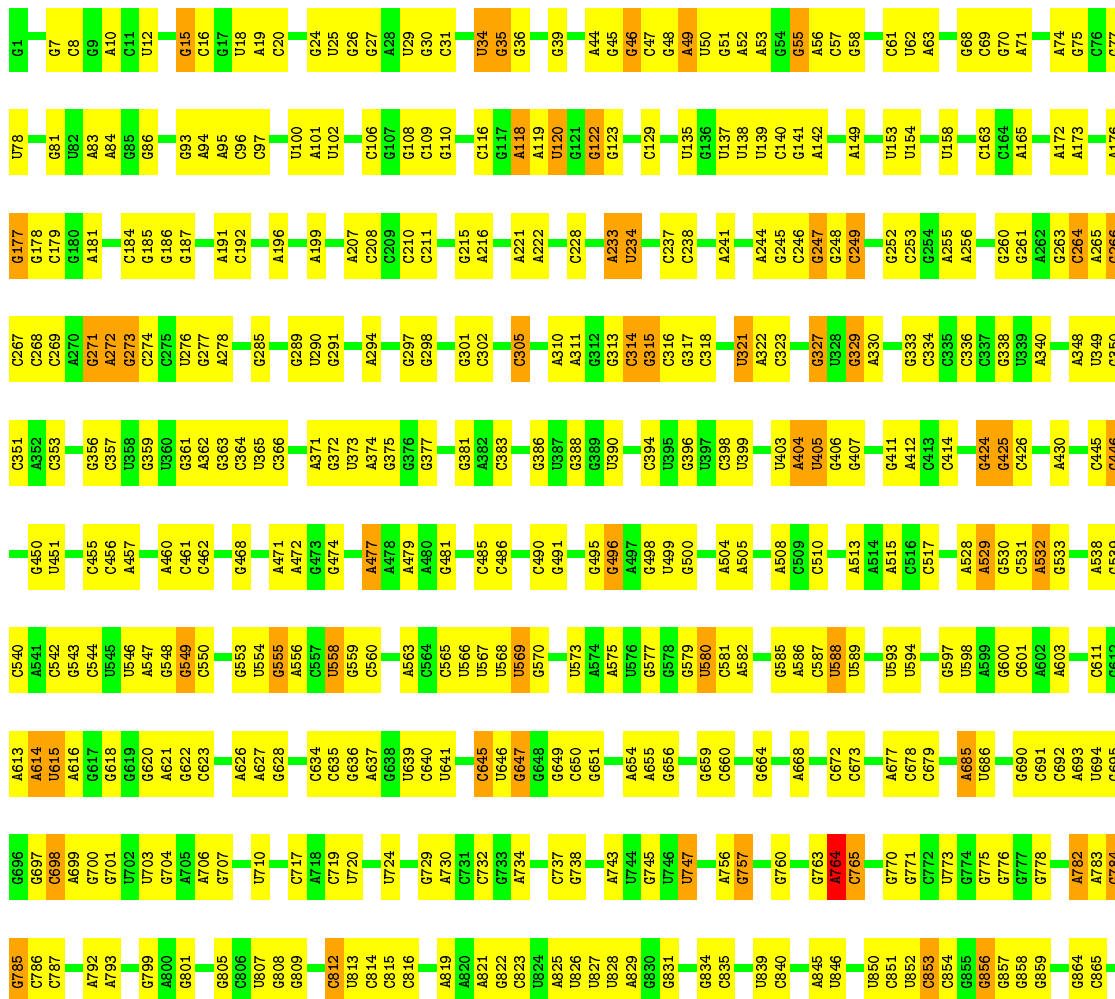
- Molecule 51: 30S ribosomal protein S21

Chain z:  72% 7% 21%

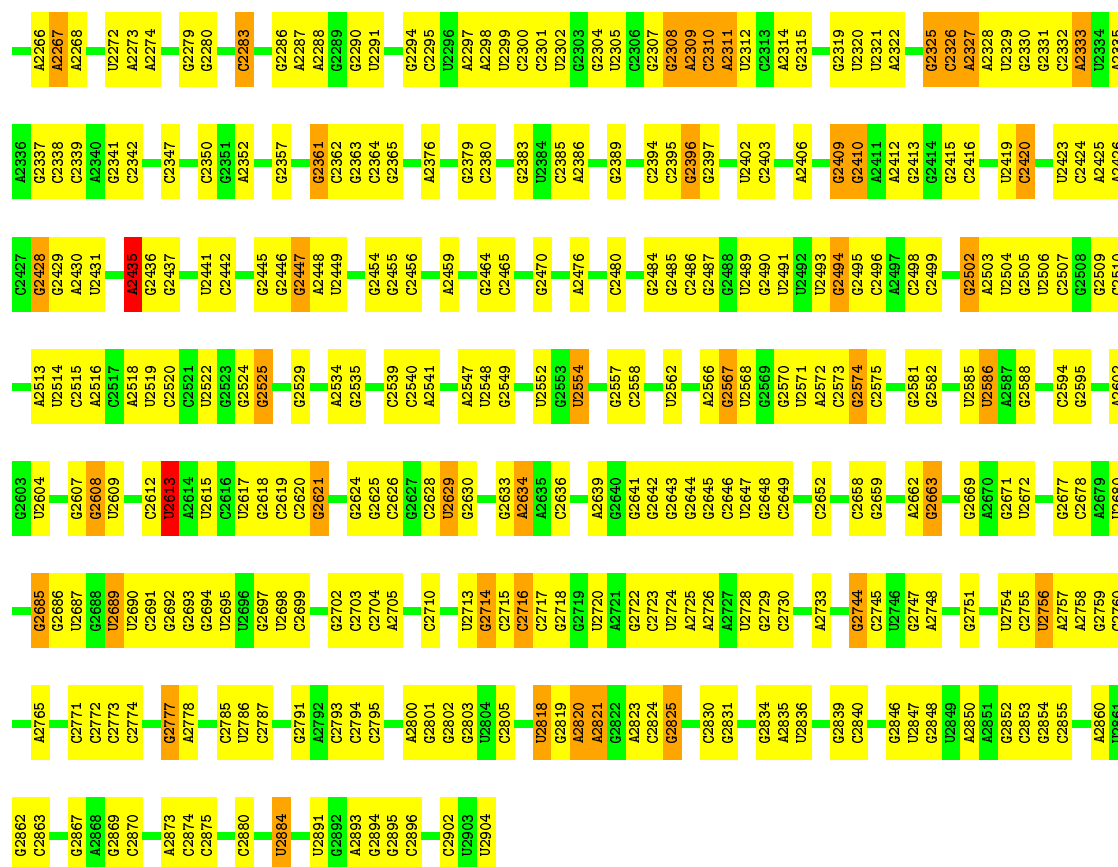


- Molecule 52: LSU rRNA

Chain 1:  52% 42% 7%

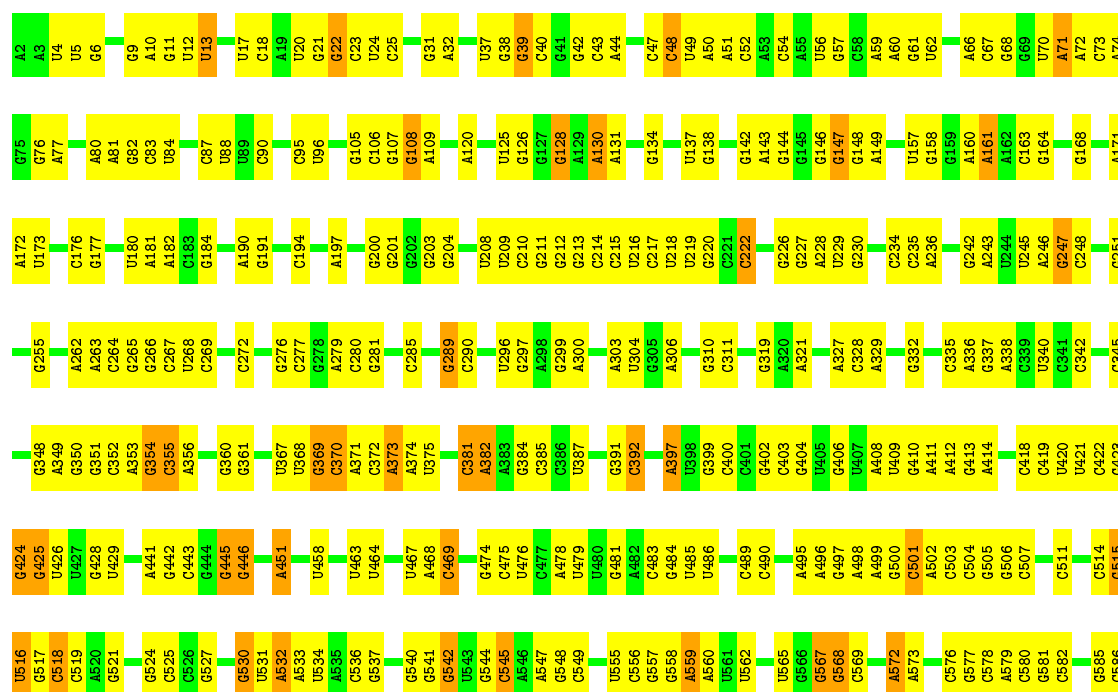


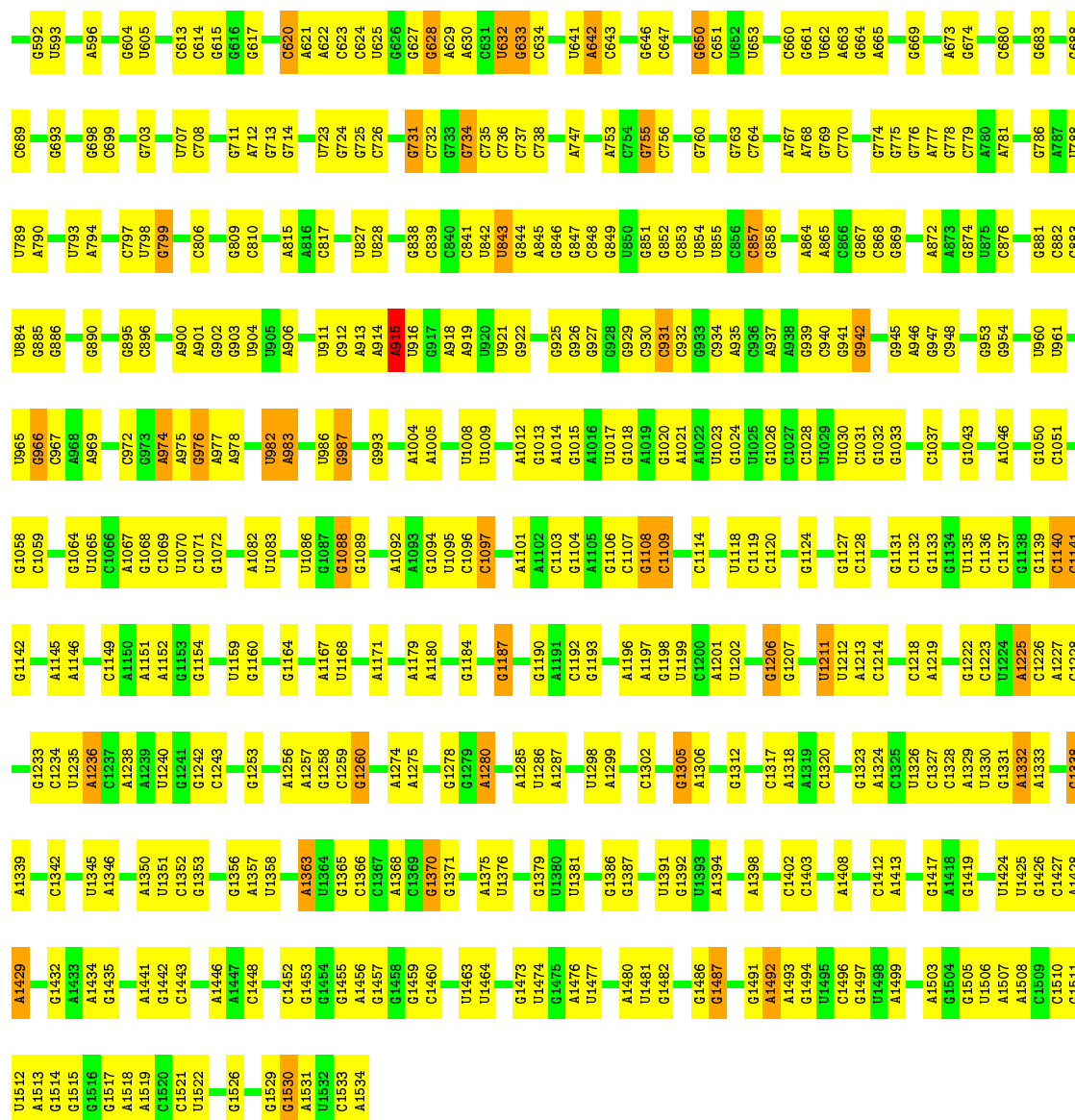
G2162	A2169	G1619	A1515	A1433	A1359	A1268	G1186	C1117	C951	G869
A2163	C1999	G1718	U1520	A1434	G1360	A1269	G1187	C1118	G952	G870
C2164	C2300	G1719	G1521	G1435	G1361	C1270	U1119	U1119	G953	U871
C2165	C2001	U1720	G1521	G1436	C1362	C1271	G1192	U1033	G954	U872
A2169	A1918	G1721	G1529	C1437	C1363	A1272	G1193	G1036	A959	G875
G2170	G1828	G1627	G1529	U1443	G1364	U1273	A1194	G1037	A960	
U2085	G1829	U1628	U1532	U1444	A1365	A1274	G1195	G1038	A961	A876
U2086	C1830	A1630	C1533	G1445	G1369	A1275	C1196	A1039		
G2087	G1831	A1635	G1533	C1446	C1370	A1276	U1201	G1042	C964	G882
U2092	C1832	A1639	U1534	G1449	C1371	C1277	U1127	C1043	C965	G883
A2094	C1833	C1639	A1535	G1450	U1374	G1278	G1128	G1046	G966	U884
A2095	C1837	G1643	G1536	C1451	C1376	C1289	A1204	A1047		C885
A2099	G1842	C1644	G1540	G1452	G1377	C1290	A1205		A972	A886
G2102	C1843	U1647	C1541	A1453	C1378	C1291	U1320	C1053	A973	A887
A2108	G1846	U1648	U1542	G1454	U1379	G1292	G1131		G974	C888
U2109	C1847	G1740	G1542	G1455	C1380	U1293	A1132	A1057		C889
G2110	G1850	C1741	A1544	G1458	G1381	U1294	A1133		G977	C890
U2111	U1851	A1745	G1555	U1458	G1382	C1295	G1136	G1062	G978	G891
G2112	U1852	A1746	C1556	G1459	U1383	G1296	A1213	G1063		A892
A2114	U1859	U1747	C1557	U1460	A1384	C1297	G1137	G1064	A983	C893
G2116	U1862	A1759	G1558	C1461	A1385		G1138	U1065	A984	U894
A2117	G1862	C1764	U1559	G1462	C1386	A1301	G1139	U1066	C985	U895
U2118	U1863	C1767	G1560	C1463	A1387	A1302	U1141	G1067	C986	A896
G2120	U1864	U1779	C1561	A1469	A1392		G1220	A1067	C987	C897
G2121	G1868	U1775	U1562	U1470	A1393	C1306	G1221	A1068	A988	C898
U2122	C1870	G1776	C1563	G1471	U1394		U1222	A1069	G989	
G2123	G1871	U1777	U1566	A1477	A1395	G1317	G1223	A1070	C990	C903
A2211	C1872	U1779	C1574	G1478	U1400	U1318	G1224	A1071	C991	G907
A2212	G1873	U1782	C1575	U1479	G1401	C1319	G1225	G1072	C992	C908
G2218	C1874	A1783	U1578	C1493	U1402	G1320	A1226	A1073		A909
G2221	G1878	U1784	U1583	A1494	G1403	G1321	G1227	G1074	C995	U909
C2222	U1880	C1784	U1584	A1495	U1404	A1322	G1228	G1075	A996	A910
A2225	A1889	U1791	C1585	A1496	U1405	C1323	C1229	A1076	G997	A911
C2226	A1890	G1792	U1588	U1497	U1406		G1232	A1077	C998	
A2227	G1891	C1793	G1589	C1498	G1407	U1326	G1233	U1083	U999	G914
G2228	C1892	U1794	U1593	A1502	G1408	A1327	U1234		A1000	C915
U2229	C1893	U1795	U1594	A1503	A1413	C1328	U1235	G1087	C1005	C922
G2236	C1894	G1796	C1595	A1504	C1414	U1329	G1236	A1088	G1006	G923
C2237	C1895	C1800	U1596	A1505	U1415	G1330	A1237	A1089	C1007	G924
A2241	G1896	A1801	U1597	U1506	G1416	G1331	G1238	A1090	A1008	
G2242	C1897	U1808	U1598	A1507	U1417	G1332	U1239	G1091	A1009	A927
U2243	G1904	U1809	U1599	U1508	C1418	G1333	U1240	C1092	A1010	A928
A2244	C1905	C1704	U1600	A1509	G1419	C1334	G1248	A1095	G1011	U929
U2245	G1906	G1707	A1608	G1510	A1419	C1335	U1249	A1096	U1012	G930
G2246	C1907	C1708	U1610	G1511	G1420	A1342	G1250	A1097	C1013	U931
U2247	G1908	U1815	A1616	U1512	G1421	G1343	G1253	A1098	G1017	A933
G2250	C1909	G1817	U1617	U1513	G1422	U1344	A1254	G1099	U1018	
C2261	U1913	U1817	U1715	U1514	G1423	C1345	U1255	C1100	U1019	G939
					U1424	G1346	G1256	G1107	A1020	G940
					G1425	C1347	U1257		A1021	A941
					U1426	C1350	C1257	G1178	G1022	G942
					A1427	G1351	U1263	C1179	U1023	
					G1428	U1352	U1264	U1180	U1024	C946
					U1429	C1353	A1265	U1181	G1025	A947
					G1430	U1354	U1266	A1111	G1026	C948
					U1431	C1355	G1267	G1112	U1027	G949
					U1432	U1356	U1268	U1113	A1027	
					U1433	U1357	U1269	G1116	A1028	G950



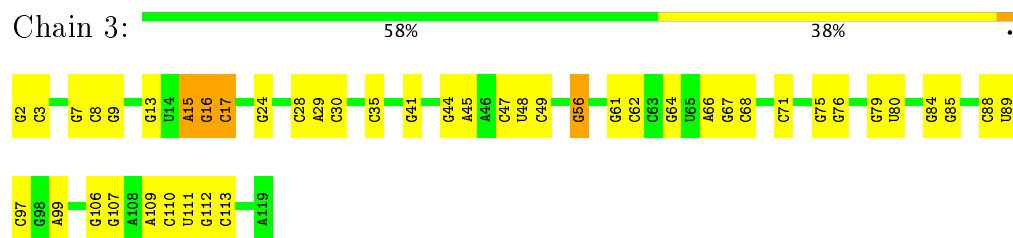
- Molecule 53: SSU rRNA

Chain 2:  52% 43% 5%

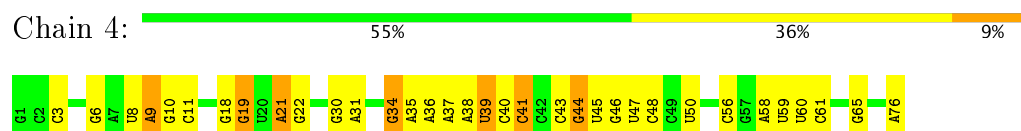




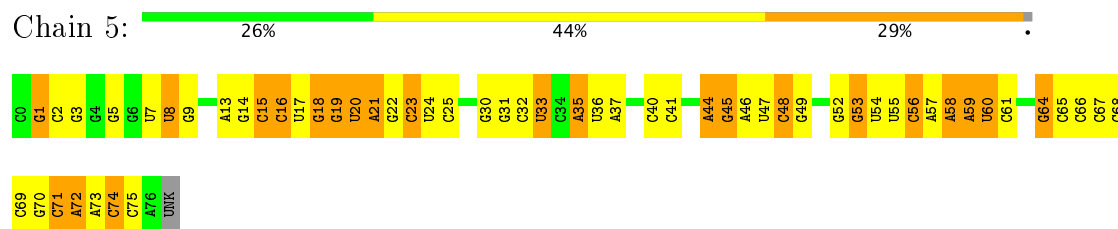
- Molecule 54: 5S rRNA



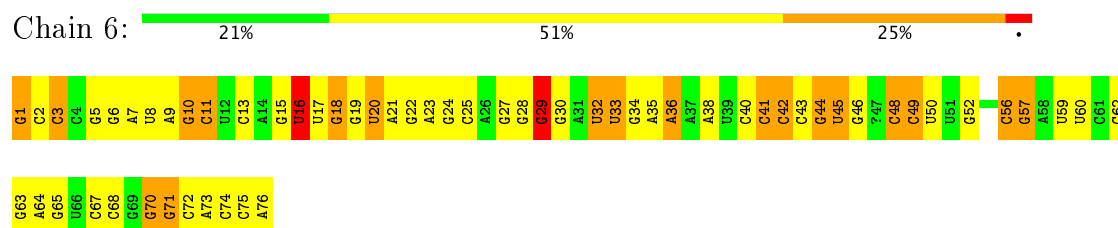
- Molecule 55: E-site tRNA(Phe)



- Molecule 56: P-site fMet-tRNA(fMet)



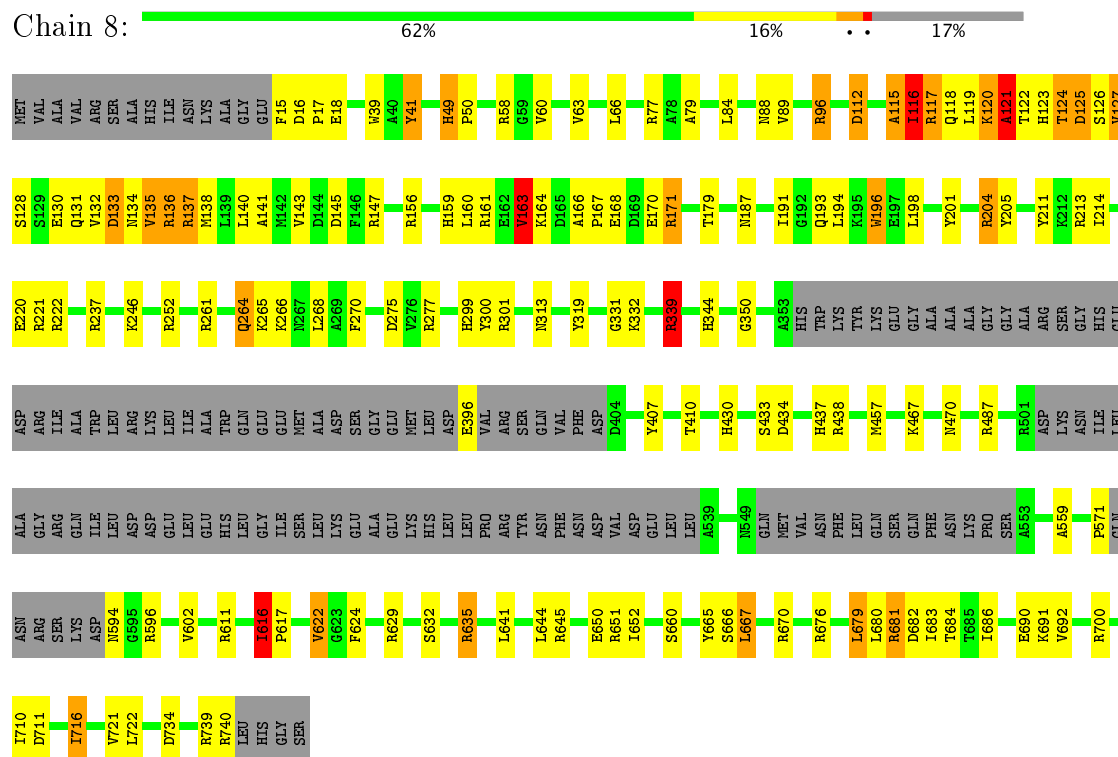
- Molecule 57: A/T tRNA(Phe)



- Molecule 58: mRNA



- Molecule 59: GTP pyrophosphokinase



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	98498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	104478	Depositor
Image detector	OTHER	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, MA6, 2MA, 2MG, 1MG, 3TD, G7M, D2T, 3AU, UR3, 7MG, 5MU, ZN, 6IA, 5MC, 6MZ, OMC, MG, OMG, H2U, OMU, 4OC, 4SU, PSU

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  >2	RMSZ	# Z  >2
1	B	0.35	0/2121	0.70	0/2852
10	K	0.35	0/955	0.72	0/1279
11	L	0.38	0/1062	0.74	0/1413
12	M	0.41	0/1093	0.72	0/1460
13	N	0.49	0/973	0.82	0/1301
14	O	0.47	0/902	0.81	0/1209
15	P	0.36	0/929	0.69	0/1242
16	Q	0.55	0/960	0.93	0/1278
17	R	0.33	0/829	0.66	0/1107
18	S	0.42	0/864	0.78	0/1156
19	T	0.41	0/744	0.68	0/994
2	C	0.35	0/1586	0.65	0/2134
20	U	0.35	0/787	0.61	0/1051
21	V	0.39	0/766	0.64	0/1025
22	W	0.34	0/595	0.64	0/787
23	X	0.42	0/635	0.75	0/848
24	Y	0.53	0/502	0.83	0/667
25	Z	0.44	0/453	0.71	0/605
26	a	0.43	0/531	0.66	0/709
27	b	0.41	0/450	0.73	0/599
28	c	0.34	0/416	0.62	0/554
29	d	0.52	0/380	0.95	0/498
3	D	0.43	0/1571	0.74	1/2113 (0.0%)
30	e	0.42	0/513	0.81	0/676
31	f	0.34	0/303	0.71	0/397
32	g	0.47	0/1784	0.71	0/2403
33	h	0.43	0/1655	0.72	0/2230
34	i	0.45	0/1665	0.72	0/2227
35	j	0.43	0/1169	0.76	0/1573
36	k	0.42	0/835	0.72	0/1128
37	l	0.48	0/1195	0.78	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	m	0.41	0/989	0.71	0/1326
39	n	0.43	0/1034	0.77	0/1375
4	E	0.45	0/1434	0.73	0/1926
40	o	0.42	0/796	0.74	0/1077
41	p	0.40	0/893	0.71	0/1205
42	q	0.35	0/960	0.72	0/1286
43	r	0.46	0/892	0.86	0/1193
44	s	0.47	0/817	0.78	0/1088
45	t	0.54	0/722	0.85	0/964
46	u	0.44	0/659	0.75	0/884
47	v	0.35	0/657	0.64	0/881
48	w	0.45	0/548	0.73	0/736
49	x	0.41	0/675	0.70	0/908
5	F	0.39	0/1343	0.65	0/1816
50	y	0.58	0/676	0.88	0/895
51	z	0.51	0/472	0.89	0/627
52	1	0.34	11/69300 (0.0%)	0.74	21/108089 (0.0%)
53	2	0.27	2/36561 (0.0%)	0.72	2/57019 (0.0%)
54	3	0.24	0/2828	0.70	0/4410
55	4	0.25	0/1808	0.70	0/2815
56	5	0.35	0/1716	0.83	0/2672
57	6	0.42	1/1606 (0.1%)	0.80	1/2497 (0.0%)
58	7	0.31	0/235	0.71	0/363
59	8	0.62	0/4878	1.14	30/6606 (0.5%)
6	G	0.42	0/1122	0.63	0/1515
7	H	0.46	0/1001	0.66	0/1350
8	I	0.42	0/1046	0.62	0/1410
9	J	0.44	0/1152	0.72	0/1551
All	All	0.36	14/166043 (0.0%)	0.75	55/247601 (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
52	1	0	9
53	2	0	2
57	6	8	3
59	8	0	19
All	All	8	33

The worst 5 of 14 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	2244	U	C2-N3	19.23	1.51	1.37
52	1	2244	U	N3-C4	17.42	1.54	1.38
52	1	2435	A	C6-N1	-15.77	1.24	1.35
52	1	2244	U	N1-C2	13.64	1.50	1.38
52	1	1775	U	C2-N3	12.29	1.46	1.37

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1	2244	U	C2-N3-C4	-18.02	116.19	127.00
52	1	2435	A	N1-C6-N6	-14.25	110.05	118.60
52	1	2244	U	C2-N1-C1'	13.09	133.41	117.70
52	1	2244	U	C6-N1-C1'	-11.39	105.26	121.20
52	1	2244	U	C5-C4-O4	-10.87	119.38	125.90

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	6	16	H2U	C2',C3',C1'
57	6	20	H2U	C2',C1'
57	6	32	PSU	C1'
57	6	37	6IA	C3'
57	6	55	PSU	C1'

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	1	1319	C	Sidechain
52	1	1335	C	Sidechain
52	1	305	C	Sidechain
52	1	314	C	Sidechain
52	1	764	A	Sidechain

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2082	0	2154	29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1565	0	1616	25	0
3	D	1552	0	1619	9	0
4	E	1410	0	1444	11	0
5	F	1323	0	1371	6	0
6	G	1111	0	1148	2	0
7	H	988	0	1025	2	0
8	I	1032	0	1088	1	0
9	J	1129	0	1162	9	0
10	K	946	0	1023	4	0
11	L	1053	0	1129	6	0
12	M	1074	0	1157	6	0
13	N	960	0	1000	21	0
14	O	892	0	923	10	0
15	P	917	0	962	5	0
16	Q	947	0	1019	13	0
17	R	816	0	839	6	0
18	S	857	0	922	9	0
19	T	738	0	807	1	0
20	U	779	0	831	3	0
21	V	753	0	780	5	0
22	W	588	0	604	4	0
23	X	625	0	652	4	0
24	Y	501	0	531	2	0
25	Z	449	0	488	4	0
26	a	522	0	521	0	0
27	b	444	0	458	0	0
28	c	409	0	440	0	0
29	d	377	0	418	0	0
30	e	504	0	572	0	0
31	f	302	0	342	0	0
32	g	1753	0	1780	0	0
33	h	1628	0	1699	0	0
34	i	1643	0	1707	0	0
35	j	1156	0	1199	0	0
36	k	817	0	808	0	0
37	l	1181	0	1238	0	0
38	m	979	0	1031	0	0
39	n	1022	0	1070	0	0
40	o	786	0	828	0	0
41	p	877	0	887	0	0
42	q	957	0	1017	0	0
43	r	883	0	941	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	s	805	0	844	0	0
45	t	714	0	734	0	0
46	u	649	0	666	0	0
47	v	648	0	691	0	0
48	w	539	0	553	0	0
49	x	658	0	683	0	0
50	y	670	0	719	0	0
51	z	465	0	491	0	0
52	1	62356	0	31391	951	0
53	2	32907	0	16580	469	0
54	3	2529	0	1281	37	0
55	4	1619	0	823	32	0
56	5	1639	0	843	42	0
57	6	1637	0	840	43	0
58	7	211	0	107	14	0
59	8	4792	0	4726	40	0
60	1	220	0	0	0	0
60	2	64	0	0	0	0
60	3	6	0	0	0	0
60	8	1	0	0	0	0
60	B	1	0	0	0	0
60	C	1	0	0	0	0
60	L	2	0	0	0	0
60	N	1	0	0	0	0
60	U	1	0	0	0	0
60	r	1	0	0	0	0
60	s	1	0	0	0	0
61	8	1	0	0	0	0
61	a	1	0	0	0	0
61	f	1	0	0	0	0
62	2	42	0	45	1	0
63	5	8	0	8	1	0
64	B	2	0	0	0	0
All	All	154519	0	105275	1739	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1739 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:2244:U:N3	52:1:2435:A:C6	1.94	1.32
53:2:13:U:N3	53:2:915:A:N6	1.76	1.31
52:1:2244:U:N3	52:1:2435:A:N6	1.79	1.29
52:1:1067:A:N3	57:6:56:C:N3	1.85	1.23
55:4:31:A:N1	55:4:39:U:O4	1.75	1.19

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	269/273 (98%)	249 (93%)	18 (7%)	2 (1%)	25	67
2	C	207/209 (99%)	190 (92%)	16 (8%)	1 (0%)	32	74
3	D	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	32	74
4	E	175/179 (98%)	158 (90%)	13 (7%)	4 (2%)	7	35
5	F	174/177 (98%)	156 (90%)	17 (10%)	1 (1%)	28	70
6	G	147/149 (99%)	126 (86%)	17 (12%)	4 (3%)	6	30
7	H	129/165 (78%)	103 (80%)	18 (14%)	8 (6%)	2	10
8	I	139/142 (98%)	113 (81%)	20 (14%)	6 (4%)	3	18
9	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
10	K	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
11	L	142/144 (99%)	131 (92%)	9 (6%)	2 (1%)	13	49
12	M	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
13	N	118/127 (93%)	107 (91%)	10 (8%)	1 (1%)	22	64
14	O	114/117 (97%)	103 (90%)	9 (8%)	2 (2%)	10	43
15	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
16	Q	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	20	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	101/103 (98%)	90 (89%)	9 (9%)	2 (2%)	9	39
18	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
19	T	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
20	U	100/104 (96%)	91 (91%)	7 (7%)	2 (2%)	9	39
21	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
22	W	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
23	X	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
24	Y	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	11	44
25	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
26	a	64/70 (91%)	51 (80%)	12 (19%)	1 (2%)	11	46
27	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	c	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
29	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	e	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	11	46
31	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	g	222/241 (92%)	200 (90%)	15 (7%)	7 (3%)	5	26
33	h	205/233 (88%)	185 (90%)	18 (9%)	2 (1%)	18	59
34	i	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
35	j	155/167 (93%)	142 (92%)	10 (6%)	3 (2%)	9	41
36	k	98/135 (73%)	88 (90%)	9 (9%)	1 (1%)	18	59
37	l	149/179 (83%)	140 (94%)	7 (5%)	2 (1%)	14	51
38	m	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	22	64
39	n	125/130 (96%)	113 (90%)	10 (8%)	2 (2%)	11	46
40	o	96/103 (93%)	82 (85%)	11 (12%)	3 (3%)	5	26
41	p	115/129 (89%)	98 (85%)	15 (13%)	2 (2%)	11	44
42	q	120/124 (97%)	109 (91%)	10 (8%)	1 (1%)	22	64
43	r	112/118 (95%)	106 (95%)	6 (5%)	0	100	100
44	s	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
45	t	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	u	80/82 (98%)	69 (86%)	7 (9%)	4 (5%)	2	15
47	v	78/84 (93%)	72 (92%)	4 (5%)	2 (3%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	w	63/75 (84%)	60 (95%)	3 (5%)	0	100	100
49	x	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	6	32
50	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
51	z	54/71 (76%)	52 (96%)	1 (2%)	1 (2%)	9	41
59	8	604/744 (81%)	528 (87%)	55 (9%)	21 (4%)	4	23
All	All	6455/6964 (93%)	5874 (91%)	487 (8%)	94 (2%)	17	48

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	175	PHE
7	H	4	ASN
7	H	123	ILE
11	L	99	ASN
17	R	51	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	216/218 (99%)	205 (95%)	11 (5%)	28	66
2	C	164/164 (100%)	159 (97%)	5 (3%)	46	81
3	D	165/165 (100%)	156 (94%)	9 (6%)	25	63
4	E	148/150 (99%)	138 (93%)	10 (7%)	18	54
5	F	137/138 (99%)	129 (94%)	8 (6%)	23	61
6	G	114/114 (100%)	114 (100%)	0	100	100
7	H	100/123 (81%)	97 (97%)	3 (3%)	46	81
8	I	109/110 (99%)	106 (97%)	3 (3%)	49	82
9	J	116/116 (100%)	114 (98%)	2 (2%)	66	89
10	K	104/104 (100%)	99 (95%)	5 (5%)	30	69
11	L	103/103 (100%)	98 (95%)	5 (5%)	29	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	109/109 (100%)	106 (97%)	3 (3%)	49	82
13	N	100/103 (97%)	96 (96%)	4 (4%)	36	74
14	O	86/87 (99%)	79 (92%)	7 (8%)	14	45
15	P	99/100 (99%)	96 (97%)	3 (3%)	46	81
16	Q	89/90 (99%)	82 (92%)	7 (8%)	14	46
17	R	84/84 (100%)	80 (95%)	4 (5%)	30	69
18	S	93/93 (100%)	87 (94%)	6 (6%)	20	56
19	T	80/84 (95%)	74 (92%)	6 (8%)	16	49
20	U	83/85 (98%)	80 (96%)	3 (4%)	40	77
21	V	78/78 (100%)	73 (94%)	5 (6%)	20	57
22	W	59/63 (94%)	59 (100%)	0	100	100
23	X	67/68 (98%)	67 (100%)	0	100	100
24	Y	54/55 (98%)	50 (93%)	4 (7%)	16	49
25	Z	48/49 (98%)	45 (94%)	3 (6%)	21	57
26	a	59/62 (95%)	58 (98%)	1 (2%)	66	89
27	b	47/48 (98%)	45 (96%)	2 (4%)	33	72
28	c	45/49 (92%)	44 (98%)	1 (2%)	57	86
29	d	38/38 (100%)	32 (84%)	6 (16%)	3	14
30	e	51/52 (98%)	46 (90%)	5 (10%)	9	34
31	f	34/34 (100%)	30 (88%)	4 (12%)	6	25
32	g	186/199 (94%)	179 (96%)	7 (4%)	38	75
33	h	170/189 (90%)	160 (94%)	10 (6%)	23	60
34	i	172/173 (99%)	167 (97%)	5 (3%)	48	82
35	j	119/126 (94%)	108 (91%)	11 (9%)	11	38
36	k	87/116 (75%)	82 (94%)	5 (6%)	24	62
37	l	124/147 (84%)	113 (91%)	11 (9%)	11	40
38	m	104/105 (99%)	96 (92%)	8 (8%)	15	48
39	n	105/107 (98%)	97 (92%)	8 (8%)	15	48
40	o	86/90 (96%)	78 (91%)	8 (9%)	10	38
41	p	90/99 (91%)	84 (93%)	6 (7%)	19	54
42	q	102/103 (99%)	97 (95%)	5 (5%)	29	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	r	92/96 (96%)	84 (91%)	8 (9%)	12	41
44	s	83/84 (99%)	79 (95%)	4 (5%)	30	69
45	t	76/77 (99%)	69 (91%)	7 (9%)	11	38
46	u	65/65 (100%)	59 (91%)	6 (9%)	11	38
47	v	74/78 (95%)	67 (90%)	7 (10%)	10	36
48	w	57/66 (86%)	55 (96%)	2 (4%)	41	78
49	x	72/79 (91%)	69 (96%)	3 (4%)	34	73
50	y	65/66 (98%)	59 (91%)	6 (9%)	11	38
51	z	48/61 (79%)	44 (92%)	4 (8%)	13	44
59	8	500/629 (80%)	438 (88%)	62 (12%)	5	23
All	All	5356/5691 (94%)	5028 (94%)	328 (6%)	26	59

5 of 328 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	h	156	ARG
37	l	130	ASN
59	8	457	MET
34	i	26	ARG
35	j	138	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
21	V	24	ASN
23	X	16	ASN
50	y	21	ASN
4	E	37	ASN
45	t	46	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	1	2891/2904 (99%)	610 (21%)	61 (2%)
53	2	1524/1533 (99%)	324 (21%)	24 (1%)
54	3	117/118 (99%)	19 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	4	74/76 (97%)	22 (29%)	0
56	5	75/78 (96%)	37 (49%)	14 (18%)
57	6	73/76 (96%)	42 (57%)	11 (15%)
58	7	9/10 (90%)	0	0
All	All	4763/4795 (99%)	1054 (22%)	110 (2%)

5 of 1054 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	1	10	A
52	1	15	G
52	1	34	U
52	1	35	G
52	1	39	G

5 of 110 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	1	2308	G
53	2	73	C
57	6	17	U
52	1	2319	G
52	1	2581	G

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

48 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	$\# Z  > 2$
52	6MZ	1	1618	52	18,25,26	0.58	0	16,36,39	1.19	1 (6%)
52	2MG	1	1835	52	19,26,27	1.08	1 (5%)	20,38,41	2.26	4 (20%)
52	PSU	1	1911	52	16,21,22	1.05	1 (6%)	20,30,33	4.94	5 (25%)
52	3TD	1	1915	52	16,22,23	0.89	1 (6%)	19,32,35	1.29	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	PSU	1	1917	52	16,21,22	1.04	1 (6%)	20,30,33	5.03	4 (20%)
52	5MU	1	1939	52	14,22,23	1.05	2 (14%)	16,32,35	3.62	2 (12%)
52	5MC	1	1962	52	15,22,23	0.73	1 (6%)	17,32,35	0.48	0
52	6MZ	1	2030	52	18,25,26	0.65	0	16,36,39	1.36	2 (12%)
52	G7M	1	2069	52	19,26,27	1.16	2 (10%)	19,39,42	2.51	3 (15%)
52	OMG	1	2251	56,52	18,26,27	1.07	1 (5%)	22,38,41	2.20	3 (13%)
52	2MG	1	2445	52	19,26,27	1.10	1 (5%)	20,38,41	2.29	5 (25%)
52	PSU	1	2457	52	16,21,22	1.09	1 (6%)	20,30,33	4.95	5 (25%)
52	OMC	1	2498	60,52	15,22,23	0.72	0	19,31,34	0.69	0
52	2MA	1	2503	60,52	18,25,26	1.06	2 (11%)	17,37,40	1.41	2 (11%)
52	PSU	1	2504	52	16,21,22	1.05	1 (6%)	20,30,33	5.01	6 (30%)
52	OMU	1	2552	60,52	14,22,23	1.00	1 (7%)	18,31,34	3.17	2 (11%)
52	PSU	1	2580	52	16,21,22	1.02	1 (6%)	20,30,33	4.96	5 (25%)
52	PSU	1	2605	52	16,21,22	1.05	1 (6%)	20,30,33	4.97	6 (30%)
52	1MG	1	745	52	18,26,27	0.84	1 (5%)	18,39,42	0.93	1 (5%)
52	PSU	1	746	60,52	16,21,22	1.07	1 (6%)	20,30,33	4.91	5 (25%)
52	5MU	1	747	52	14,22,23	1.01	2 (14%)	16,32,35	3.71	2 (12%)
52	PSU	1	955	52	16,21,22	1.06	1 (6%)	20,30,33	4.92	5 (25%)
53	2MG	2	1207	53	19,26,27	1.12	1 (5%)	20,38,41	2.32	5 (25%)
53	4OC	2	1402	53	16,23,24	0.68	0	19,32,35	0.82	0
53	5MC	2	1407	53	15,22,23	0.72	1 (6%)	17,32,35	0.71	0
53	UR3	2	1498	53	14,22,23	0.76	0	16,32,35	0.49	0
53	2MG	2	1516	53	19,26,27	1.14	1 (5%)	20,38,41	2.17	4 (20%)
53	MA6	2	1518	53	16,26,27	0.57	0	18,38,41	1.18	2 (11%)
53	MA6	2	1519	53	16,26,27	0.63	0	18,38,41	1.09	1 (5%)
53	PSU	2	516	53	16,21,22	1.04	1 (6%)	20,30,33	5.02	6 (30%)
53	G7M	2	527	53	19,26,27	1.17	2 (10%)	19,39,42	2.43	3 (15%)
53	2MG	2	966	53	19,26,27	1.13	1 (5%)	20,38,41	2.27	5 (25%)
53	5MC	2	967	53	15,22,23	0.76	1 (6%)	17,32,35	0.52	0
56	H2U	5	20	56	17,21,22	0.53	0	21,30,33	0.71	0
56	4OC	5	32	56	16,23,24	0.66	0	19,32,35	0.61	0
56	5MU	5	54	56	14,22,23	1.00	1 (7%)	16,32,35	3.85	3 (18%)
56	PSU	5	55	56	16,21,22	1.04	1 (6%)	20,30,33	4.89	5 (25%)
56	4SU	5	8	56	14,21,22	1.03	1 (7%)	15,30,33	1.84	2 (13%)
57	H2U	6	16	57	17,21,22	0.57	0	21,30,33	2.47	7 (33%)
57	H2U	6	20	57	17,21,22	0.63	0	21,30,33	1.65	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	PSU	6	32	57	16,21,22	1.20	1 (6%)	20,30,33	5.61	9 (45%)
57	6IA	6	37	57,58	21,29,30	0.56	0	21,41,44	1.90	5 (23%)
57	7MG	6	46	57	20,26,27	1.01	1 (5%)	22,39,42	2.11	3 (13%)
57	3AU	6	47	57	13,28,29	0.95	1 (7%)	13,40,43	0.47	0
57	5MU	6	54	57	14,22,23	1.03	2 (14%)	16,32,35	3.72	2 (12%)
57	PSU	6	55	57	16,21,22	1.22	1 (6%)	20,30,33	5.65	10 (50%)
57	4SU	6	8	57	14,21,22	1.03	1 (7%)	15,30,33	1.67	2 (13%)
42	D2T	q	89	42	5,9,10	1.46	1 (20%)	3,11,13	1.75	1 (33%)

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
52	6MZ	1	1618	52	-	0/5/27/28	0/3/3/3
52	2MG	1	1835	52	-	0/5/27/28	0/3/3/3
52	PSU	1	1911	52	-	0/7/25/26	0/2/2/2
52	3TD	1	1915	52	-	0/7/25/26	0/2/2/2
52	PSU	1	1917	52	-	0/7/25/26	0/2/2/2
52	5MU	1	1939	52	-	0/3/25/26	0/2/2/2
52	5MC	1	1962	52	-	0/3/25/26	0/2/2/2
52	6MZ	1	2030	52	-	0/5/27/28	0/3/3/3
52	G7M	1	2069	52	-	0/3/25/26	0/3/3/3
52	OMG	1	2251	56,52	-	0/5/27/28	0/3/3/3
52	2MG	1	2445	52	-	0/5/27/28	0/3/3/3
52	PSU	1	2457	52	-	0/7/25/26	0/2/2/2
52	OMC	1	2498	60,52	-	0/5/27/28	0/2/2/2
52	2MA	1	2503	60,52	-	0/3/25/26	0/3/3/3
52	PSU	1	2504	52	-	0/7/25/26	0/2/2/2
52	OMU	1	2552	60,52	-	0/5/27/28	0/2/2/2
52	PSU	1	2580	52	-	0/7/25/26	0/2/2/2
52	PSU	1	2605	52	-	0/7/25/26	0/2/2/2
52	1MG	1	745	52	-	0/3/25/26	0/3/3/3
52	PSU	1	746	60,52	-	0/7/25/26	0/2/2/2
52	5MU	1	747	52	-	0/3/25/26	0/2/2/2
52	PSU	1	955	52	-	0/7/25/26	0/2/2/2
53	2MG	2	1207	53	-	0/5/27/28	0/3/3/3
53	4OC	2	1402	53	-	0/7/29/30	0/2/2/2
53	5MC	2	1407	53	-	0/3/25/26	0/2/2/2
53	UR3	2	1498	53	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	2MG	2	1516	53	-	0/5/27/28	0/3/3/3
53	MA6	2	1518	53	-	0/7/29/30	0/3/3/3
53	MA6	2	1519	53	-	0/7/29/30	0/3/3/3
53	PSU	2	516	53	-	0/7/25/26	0/2/2/2
53	G7M	2	527	53	-	0/3/25/26	0/3/3/3
53	2MG	2	966	53	-	0/5/27/28	0/3/3/3
53	5MC	2	967	53	-	0/3/25/26	0/2/2/2
56	H2U	5	20	56	-	0/7/38/39	0/2/2/2
56	4OC	5	32	56	-	0/7/29/30	0/2/2/2
56	5MU	5	54	56	-	0/3/25/26	0/2/2/2
56	PSU	5	55	56	-	0/7/25/26	0/2/2/2
56	4SU	5	8	56	-	0/3/25/26	0/2/2/2
57	H2U	6	16	57	3/3/8/9	0/7/38/39	0/2/2/2
57	H2U	6	20	57	2/2/8/9	0/7/38/39	0/2/2/2
57	PSU	6	32	57	1/1/5/5	0/7/25/26	0/2/2/2
57	6IA	6	37	57,58	1/1/6/7	0/9/31/32	0/3/3/3
57	7MG	6	46	57	-	0/7/37/38	0/3/3/3
57	3AU	6	47	57	-	0/8/34/35	0/2/2/2
57	5MU	6	54	57	-	0/3/25/26	0/2/2/2
57	PSU	6	55	57	1/1/5/5	0/7/25/26	0/2/2/2
57	4SU	6	8	57	-	0/3/25/26	0/2/2/2
42	D2T	q	89	42	-	0/2/12/14	0/0/0/0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	967	5MC	C6-C5	-2.08	1.34	1.40
52	1	747	5MU	C6-C5	-2.08	1.34	1.40
52	1	1962	5MC	C6-C5	-2.08	1.34	1.40
52	1	1939	5MU	C6-C5	-2.05	1.34	1.40
53	2	1407	5MC	C6-C5	-2.02	1.34	1.40

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1	1917	PSU	N1-C2-N3	-17.09	116.11	128.40
52	1	955	PSU	N1-C2-N3	-16.99	116.18	128.40
57	6	32	PSU	N1-C2-N3	-16.98	116.19	128.40
52	1	2605	PSU	N1-C2-N3	-16.96	116.20	128.40
52	1	2504	PSU	N1-C2-N3	-16.87	116.27	128.40

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	6	16	H2U	C2'
57	6	16	H2U	C3'
57	6	16	H2U	C1'
57	6	55	PSU	C1'
57	6	32	PSU	C1'

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	1	1915	3TD	1	0
52	1	1939	5MU	1	0
52	1	2030	6MZ	3	0
52	1	2445	2MG	2	0
52	1	2498	OMC	1	0
52	1	2503	2MA	2	0
52	1	2552	OMU	1	0
52	1	745	1MG	1	0
52	1	747	5MU	1	0
53	2	1207	2MG	1	0
53	2	1402	4OC	1	0
53	2	1518	MA6	1	0
53	2	1519	MA6	1	0
53	2	516	PSU	1	0
53	2	966	2MG	2	0
53	2	967	5MC	2	0
56	5	20	H2U	3	0
56	5	32	4OC	1	0
56	5	54	5MU	2	0
56	5	8	4SU	1	0
57	6	16	H2U	1	0
57	6	32	PSU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 304 ligands modelled in this entry, 302 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
62	PAR	2	1665	-	45,45,45	0.82	2 (4%)	60,67,67	0.67	1 (1%)
63	MET	5	101	-	7,7,8	0.98	1 (14%)	5,7,9	0.91	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
62	PAR	2	1665	-	-	0/18/94/94	0/4/4/4
63	MET	5	101	-	-	0/4/6/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	2	1665	PAR	O51-C11	-3.85	1.32	1.41
62	2	1665	PAR	C14-C24	-2.13	1.48	1.52
63	5	101	MET	CA-C	2.24	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	2	1665	PAR	O51-C11-C21	2.36	115.36	110.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	2	1665	PAR	1	0
63	5	101	MET	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	1	8
53	2	4
55	4	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1588:G	O3'	1589:U	P	4.95
1	4	1:G	O3'	2:C	P	4.28
1	1	2098:U	O3'	2099:U	P	3.58
1	2	480:U	O3'	481:G	P	3.44
1	1	1408:G	O3'	1409:U	P	3.41