



## wwPDB EM Map/Model Validation Report ⓘ

Sep 20, 2016 – 09:13 PM EDT

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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

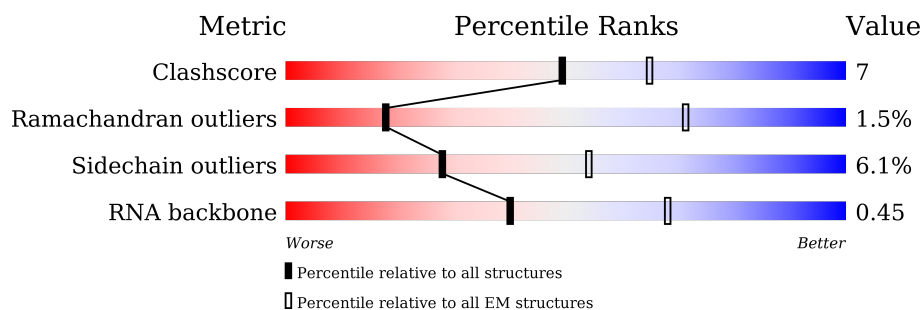
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





















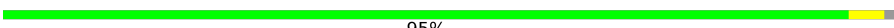






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	
2	C	209	
3	D	201	
4	E	179	
5	F	177	
6	G	149	
7	H	165	
8	I	142	

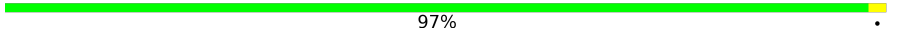






















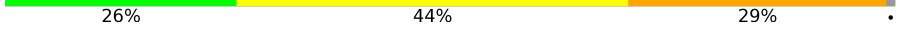
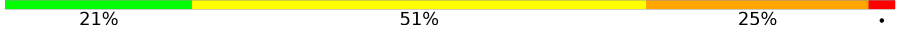
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Mol	Chain	Length	Quality of chain
9	J	142	 91% 8%
10	K	123	 90% 10%
11	L	144	 90% 10%
12	M	136	 92% 8%
13	N	127	 67% 24% 6%
14	O	117	 80% 17% ..
15	P	115	 93% 5% ..
16	Q	118	 80% 18% ..
17	R	103	 87% 12% .
18	S	110	 85% 14% .
19	T	100	 85% 8% 7%
20	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 [i](#)

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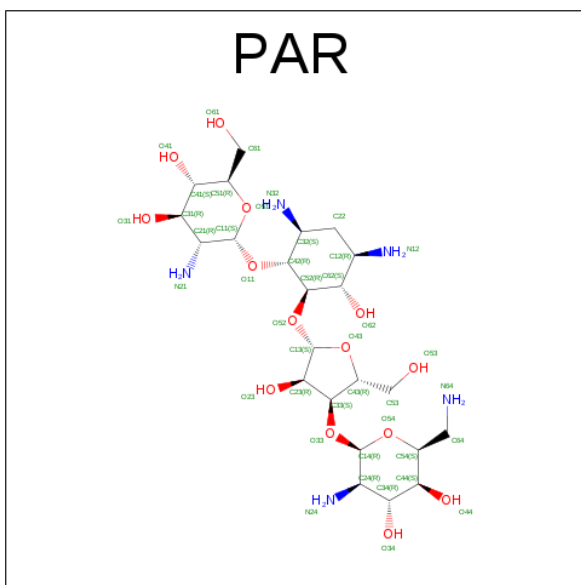
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Mol	Chain	Residues	Atoms		AltConf
60	C	1	Total 1	Mg 1	0
60	3	6	Total 6	Mg 6	0
60	N	1	Total 1	Mg 1	0
60	U	1	Total 1	Mg 1	0
60	8	1	Total 1	Mg 1	0
60	r	1	Total 1	Mg 1	0
60	L	2	Total 2	Mg 2	0
60	s	1	Total 1	Mg 1	0

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

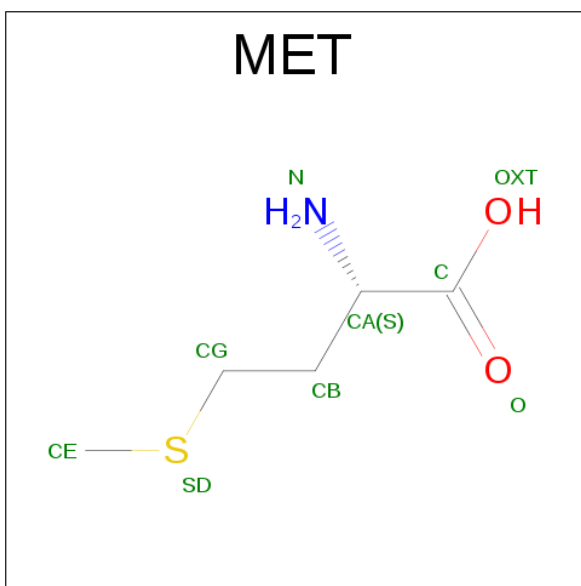
Mol	Chain	Residues	Atoms		AltConf
61	8	1	Total 1	Zn 1	0
61	a	1	Total 1	Zn 1	0
61	f	1	Total 1	Zn 1	0

- 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.

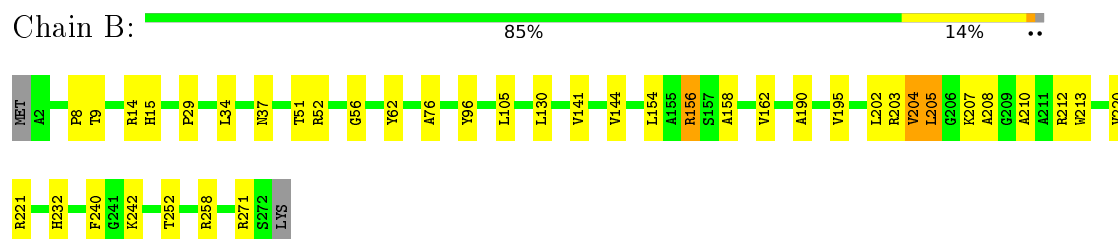


Mol	Chain	Residues	Atoms		AltConf
64	B	2	Total	O	0
			2	2	

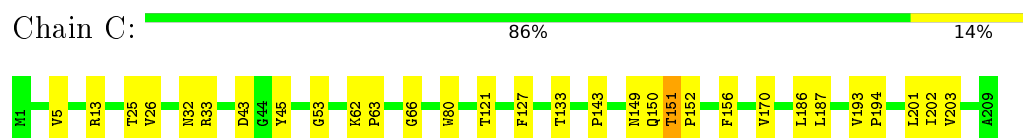
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

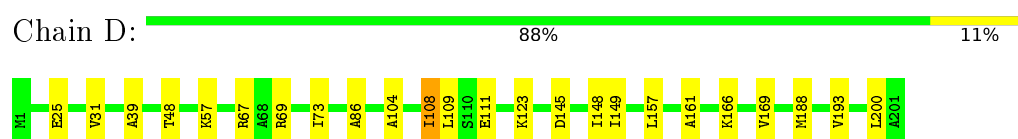
- Molecule 1: 50S ribosomal protein L2



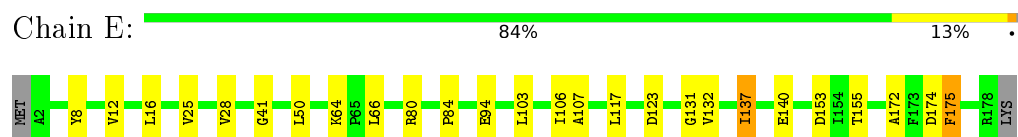
- Molecule 2: 50S ribosomal protein L3



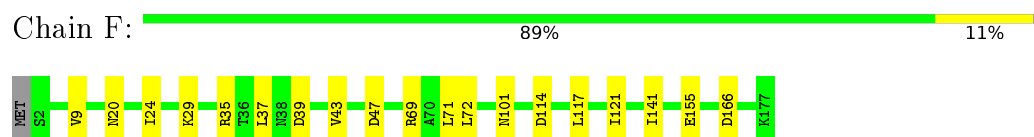
- Molecule 3: 50S ribosomal protein L4



- Molecule 4: 50S ribosomal protein L5



- Molecule 5: 50S ribosomal protein L6



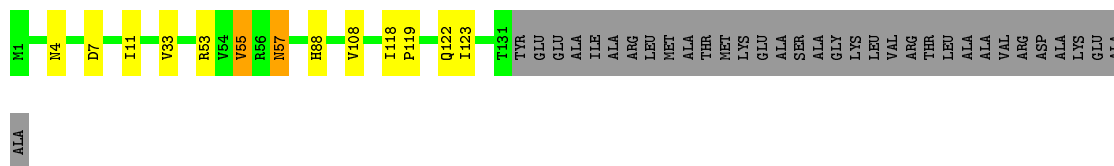
- Molecule 6: 50S ribosomal protein L9

Chain G:  95% ..




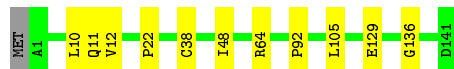
- Molecule 7: 50S ribosomal protein L10

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%

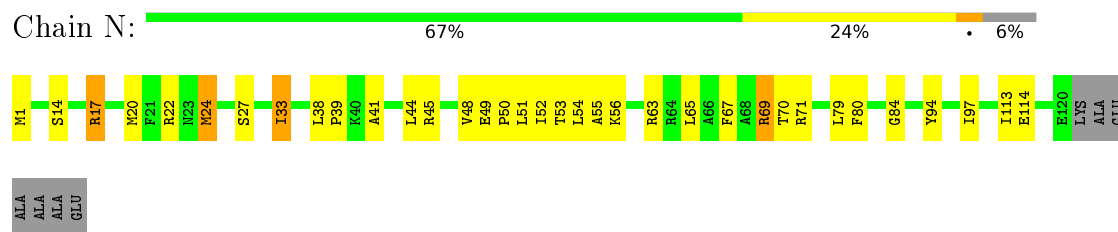


- Molecule 12: 50S ribosomal protein L16

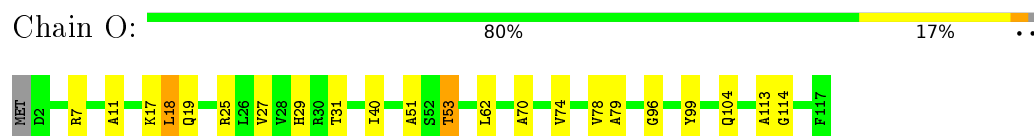
Chain M:  92% 8%



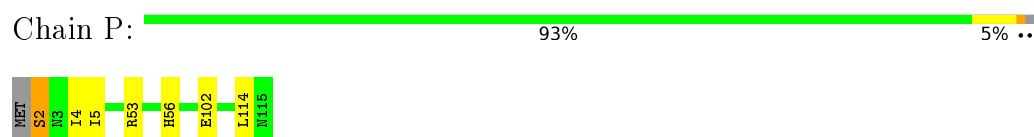
- Molecule 13: 50S ribosomal protein L17



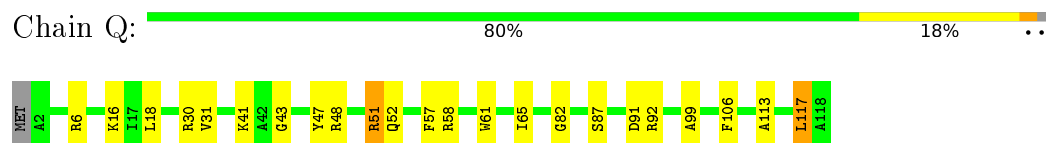
- Molecule 14: 50S ribosomal protein L18



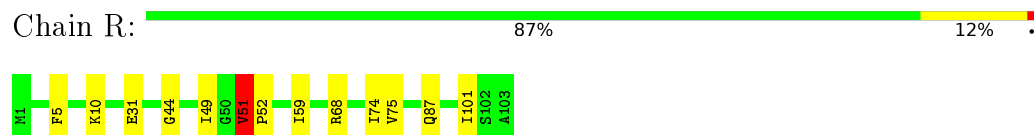
- Molecule 15: 50S ribosomal protein L19



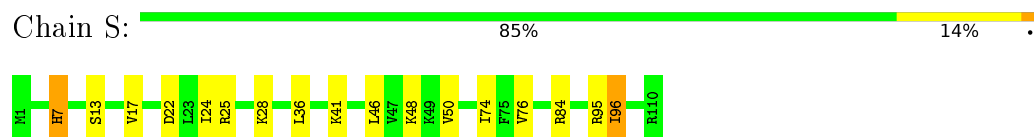
- Molecule 16: 50S ribosomal protein L20



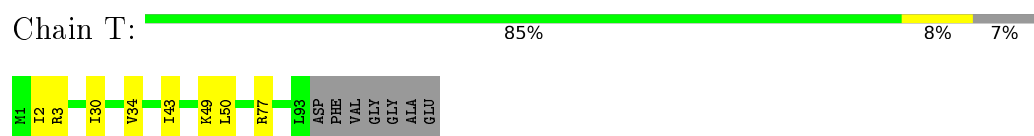
- Molecule 17: 50S ribosomal protein L21




- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23




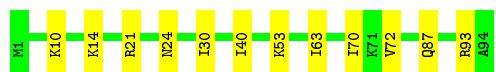
- Molecule 20: 50S ribosomal protein L24

Chain U:  89% 8% ..



- Molecule 21: 50S ribosomal protein L25

Chain V:  87% 13%



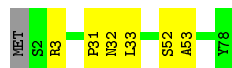
- Molecule 22: 50S ribosomal protein L27

Chain W:  85% 6% 9%



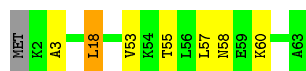
- Molecule 23: 50S ribosomal protein L28

Chain X:  91% 8% .




- Molecule 24: 50S ribosomal protein L29

Chain Y:  87% 10% ..




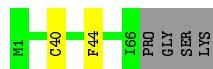
- Molecule 25: 50S ribosomal protein L30

Chain Z:  85% 14% .



- Molecule 26: 50S ribosomal protein L31

Chain a:  91% . 6%



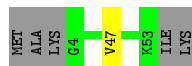
- Molecule 27: 50S ribosomal protein L32

Chain b:  95% ..



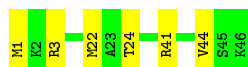
- Molecule 28: 50S ribosomal protein L33

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%



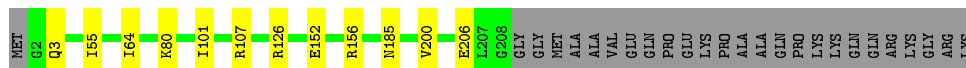
- Molecule 32: 30S ribosomal protein S2

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%



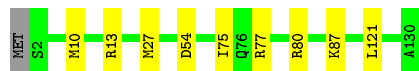
- Molecule 37: 30S ribosomal protein S7

Chain l:  78% 6% 16%




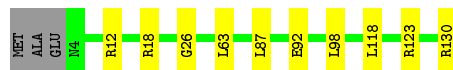
- Molecule 38: 30S ribosomal protein S8

Chain m:  92% 7%




- Molecule 39: 30S ribosomal protein S9

Chain n:  90% 8%




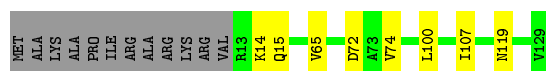
- Molecule 40: 30S ribosomal protein S10

Chain o:  84% 11% 5%



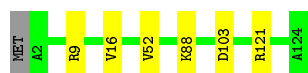
- Molecule 41: 30S ribosomal protein S11

Chain p:  84% 6% 9%




- Molecule 42: 30S ribosomal protein S12

Chain q:  94% 5%



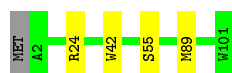
- Molecule 43: 30S ribosomal protein S13

Chain r:  90% 7%




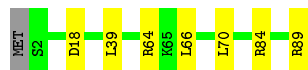
- Molecule 44: 30S ribosomal protein S14

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%



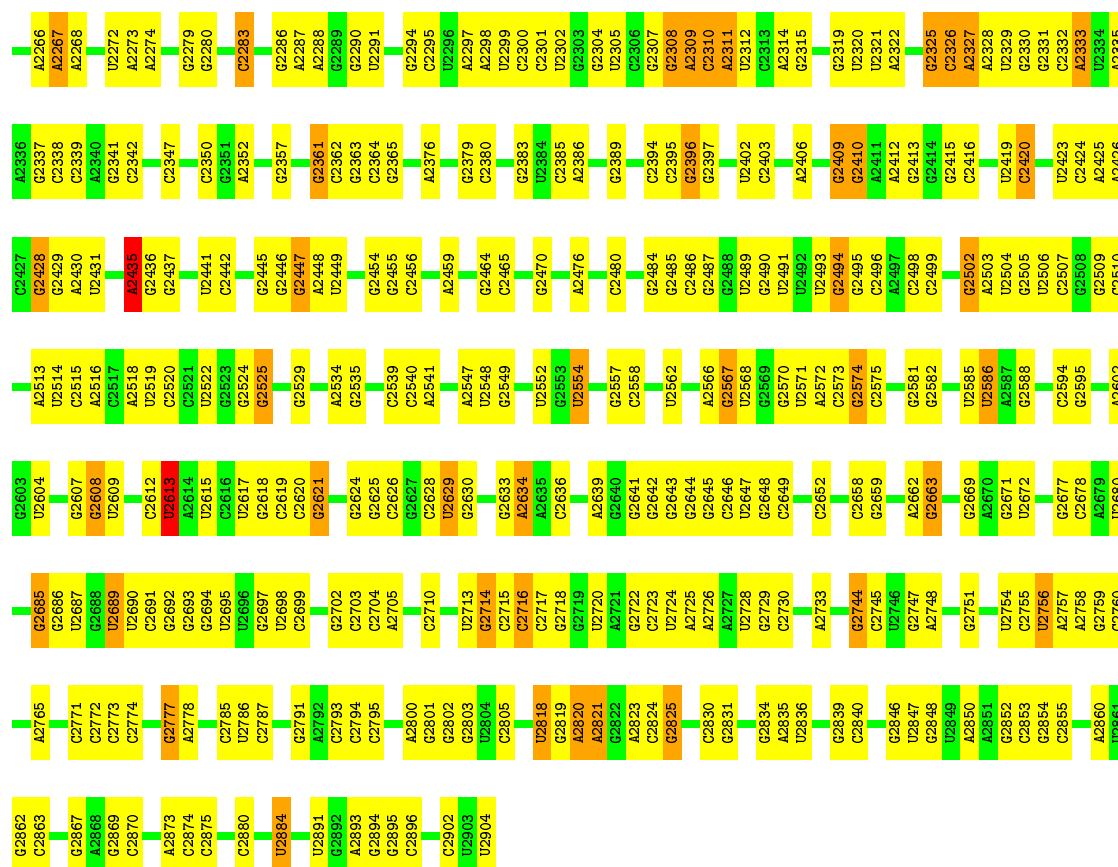
- Molecule 49: 30S ribosomal protein S19

Chain x:  84% 5% 11%



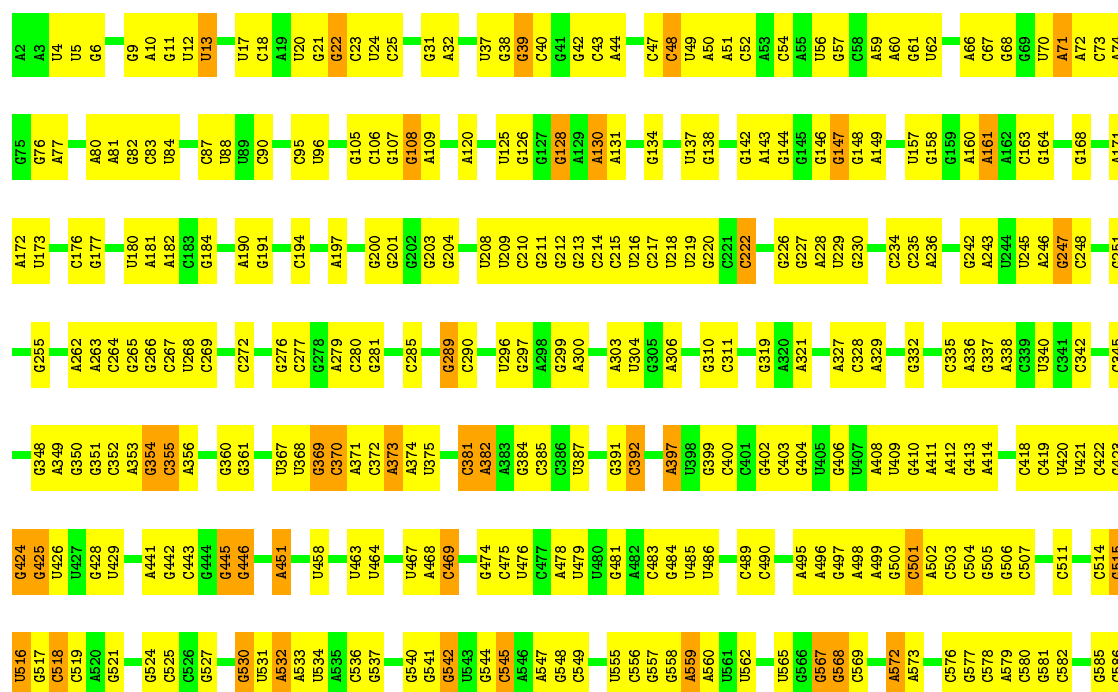


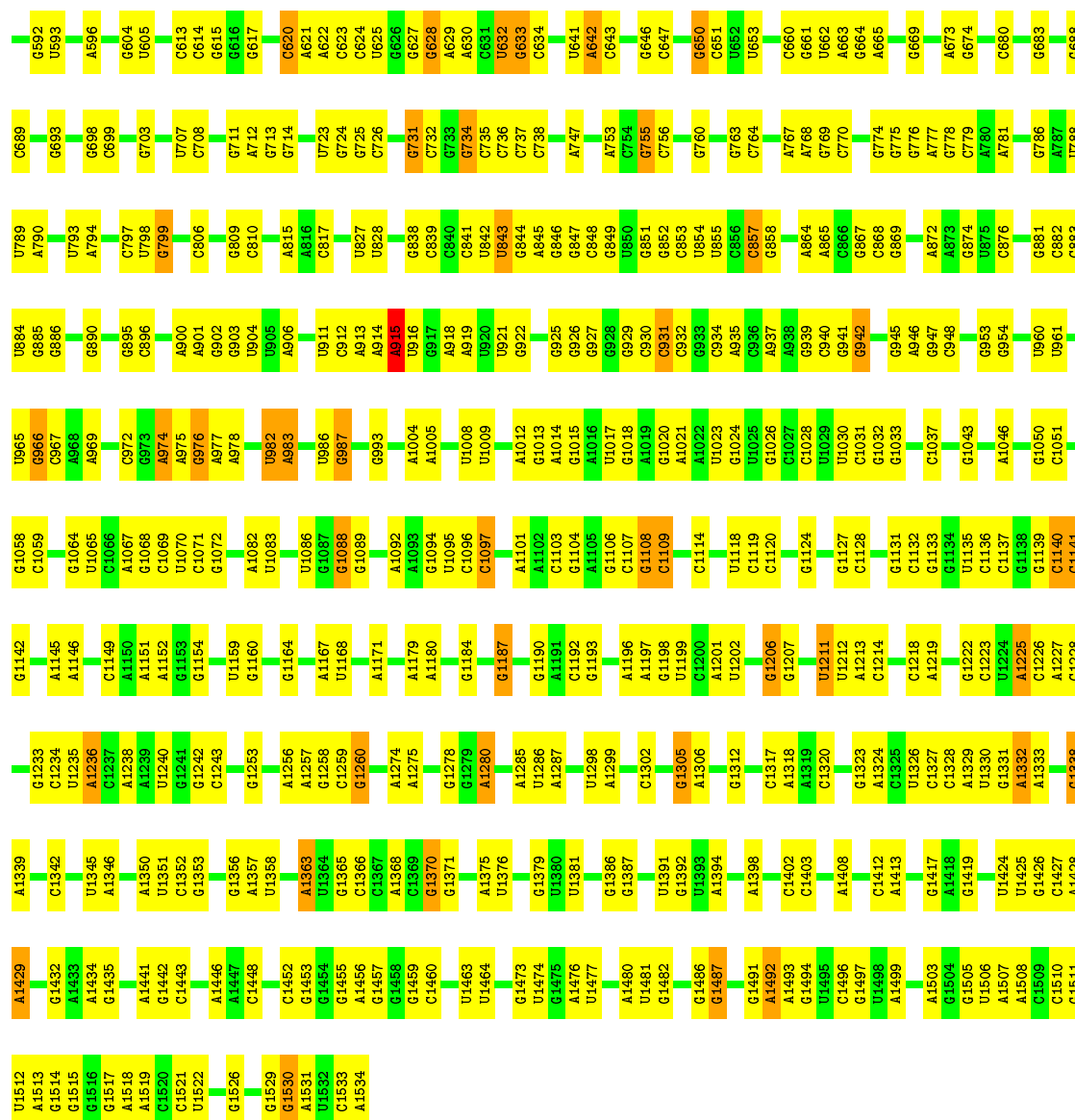
G2162	A1998	C1914	U1818	A1717	G1619	A1515	A1433	A1359	A1268	G1186	C1117	C951	G869
A2163	C1999	G1915	G1824	G1718	G1623	U1520	A1434	G1360	A1269	G1187	C1118	G952	U870
C2164	C2000	A1916	G1919	G1719	G1623	U1521	G1435	G1361	C1270	U1119	U1033	G953	U871
C2165	C2001	U1917	G1920	G1720	G1627	G1529	C1437	C1363	A1272	G1192	U1035	G954	U872
A2169	C2002	A1918	G1921	G1721	G1628	G1530	U1443	C1364	U1273	G1193	G1036	A959	G875
G2170	C2006	A1919	G1922	G1722	U1629	U1532	U1444	A1365	A1274	A1194	G1037	A960	G876
U2171	G2010	C1924	C1830	C1728	A1630	C1533	G1445	G1369	A1275	G1195	G1038	A961	A878
U2172	A2013	A1927	C1831	U1729	A1635	C1534	C1446	C1370	G1277	U1201	G1042	C964	G882
U2182	C2093	A1928	G1731	G1730	C1639	A1536	G1449	G1374	G1278	G1127	C1043	G965	G883
A2183	A2014	G1929	G1732	G1733	C1643	G1537	G1450	U1375	A1204	A1129	G1046	G966	U884
U2189	A2019	G1930	G1734	G1734	C1644	G1540	G1451	C1376	A1205	U1130	A1047	A972	C885
G2190	A2020	U1931	G1738	G1738	C1644	C1541	G1452	G1377	G1207	G1131	G1053	A973	A887
A2191	C2021	A1932	U1739	U1739	U1647	U1542	A1463	A1378	C1208	U1132	C1053	G974	C888
U2192	U2022	G1933	G1740	G1740	U1648	G1543	G1464	U1379	G1209	A1133	A1067	C889	C890
G2193	C2023	C1934	C1741	C1741	G1649	A1544	G1465	G1380	G1210	A1134	A1067	G977	C890
U2194	G2024	G1935	G1745	G1745	A1650	A1544	U1468	G1381	U1294	G1136	A1067	G978	G891
U2195	C2025	A1936	U1746	U1746	G1651	G1555	G1469	G1382	C1295	A1213	G1062	A983	G892
A2198	U2030	U1937	A1746	A1746	G1652	C1557	U1470	A1383	G1296	G1137	G1063	A984	C893
G2201	A2031	A1938	U1747	U1747	G1659	C1557	C1461	A1384	C1297	G1138	C1064	C985	U894
U2202	C2032	U1939	U1747	U1747	G1660	C1558	C1462	C1386	G1300	G1139	U1065	C985	U895
U2203	A2033	G1949	A1759	A1759	G1661	U1559	C1463	A1387	A1301	U1141	U1066	C986	A896
G2204	G2037	U1955	C1764	C1764	U1662	G1560	A1469	A1392	A1302	G1221	G1068	C987	C897
U2205	C2038	U1956	U1764	U1764	G1663	C1561	A1470	A1393	C1306	U1222	A1069	A988	C898
C2207	U2039	C1957	G1767	G1767	U1664	U1563	G1471	U1394	A1306	G1223	A1070	G989	C903
U2210	G2043	U1958	G1773	A1773	G1666	A1566	A1477	A1395	G1317	G1225	G1072	C992	G907
A2211	C2044	C1961	C1774	C1774	A1669	U1569	G1478	U1400	U1318	A1226	A1073	C995	C908
A2212	C2045	C1962	U1775	U1775	G1674	A1570	G1479	G1401	C1319	G1227	G1074	C996	A909
G2218	C2046	U1963	G1776	G1776	G1677	A1571	U1481	C1404	A1321	G1228	G1075	A996	A910
U2221	C2047	G1964	U1779	U1779	A1677	G1572	U1482	U1405	C1322	C1229	A1076	G997	A911
G2222	G2048	C1965	A1779	A1779	A1678	G1573	G1483	U1406	G1323	G1232	A1077	C998	G914
A2225	C2049	A1966	U1782	U1782	A1679	C1574	G1484	U1407	U1326	U1234	U1083	U999	C915
C2226	A2051	C1967	U1783	U1783	G1682	C1575	A1490	G1408	A1327	G1235	G1087	C1005	C922
A2227	C2052	U1971	A1784	A1784	U1683	U1578	C1493	G1409	A1328	G1236	A1088	G1006	G923
G2228	C2055	G1972	U1789	U1789	U1684	A1583	A1494	C1414	U1329	A1237	A1089	C1007	G924
U2229	C2056	C1973	C1790	C1790	C1685	U1584	A1495	U1415	G1330	G1238	A1090	A1008	A927
U2236	C2057	C1974	A1791	A1791	U1688	U1585	A1496	G1416	G1331	G1239	A1091	A1009	A928
G2237	A2058	A1989	G1792	G1792	U1689	C1586	U1497	C1417	G1332	U1240	G1092	A1010	U929
C2238	C2059	A1890	C1793	C1793	G1695	G1588	C1498	G1418	G1333	G1248	A1095	G1011	G930
G2239	A2060	G1891	A1794	A1794	A1698	U1593	A1502	A1419	C1335	U1249	A1096	U1012	U931
C2240	C2061	C1892	C1795	C1795	G1699	U1594	A1504	G1421	A1342	G1250	A1098	C1013	U932
U2241	A2062	C1893	G1797	G1797	A1700	C1595	A1505	G1422	U1343	A1254	G1099	G1017	A933
A2242	G2069	G1894	C1800	C1800	G1703	U1596	A1506	G1423	U1344	U1255	C1100	U1018	G939
G2243	A2070	C1895	A1801	A1801	C1704	A1597	C1507	G1424	G1345	G1256	G1107	A1020	G940
U2244	C2071	G1896	G1808	G1808	G1707	U1598	A1508	G1425	C1350	C1257	G1178	A1021	A941
A2247	C2072	G1904	A1809	A1809	C1704	U1609	A1509	G1426	G1351	U1180	U1023	G1022	G942
G2250	C2073	C1905	G1809	G1809	G1707	A1608	G1510	A1427	U1352	U1181	G1110	U1024	C946
U2257	U2074	G1906	G1814	G1814	C1708	A1610	G1511	G1429	G1356	U1263	A1111	G1025	A947
G2259	C1907	G1907	A1815	A1815	G1715	U1616	U1512	A1430	C1357	A1264	G1112	G1026	C948
C2261	C1908	C1908	G1816	G1816	G1715	A1616	U1513	A1431	G1358	G1266	U1113	A1027	G949
	A1913	C1997	U1817	U1817	U1716		G1514	G1432	G1358	U1267	G1116	A1028	G950



# • Molecule 53: SSU rRNA

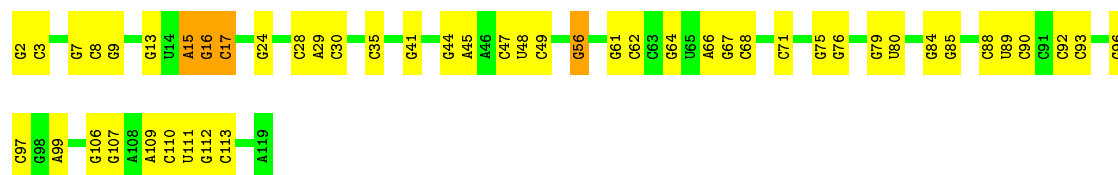
Chain 2: 52% 43% 5%





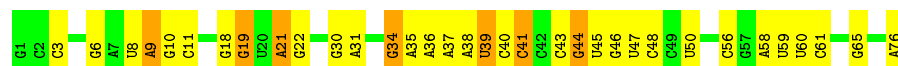
### • Molecule 54: 5S rRNA

Chain 3: 58% 38%

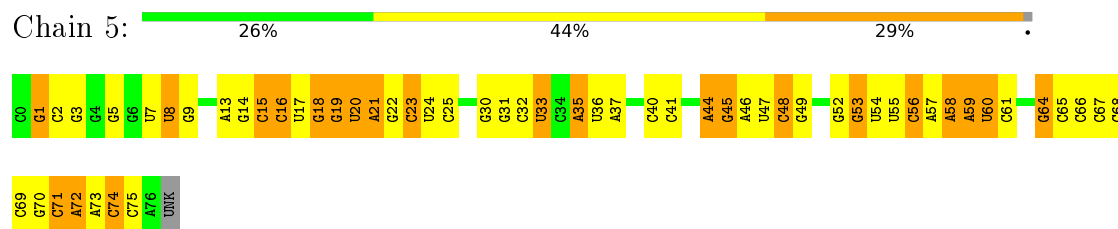


### • Molecule 55: E-site tRNA(Phe)

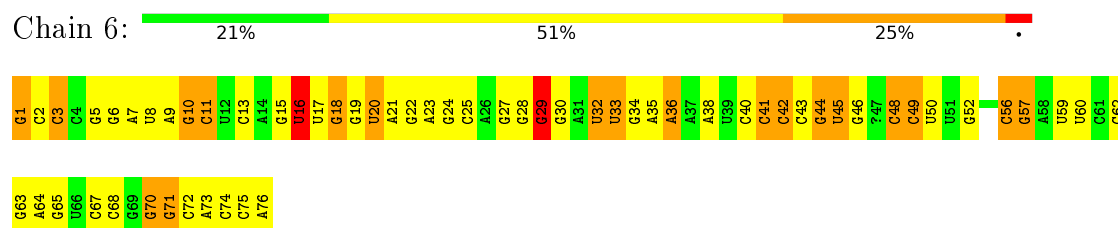
Chain 4: 55% 36% 9%



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



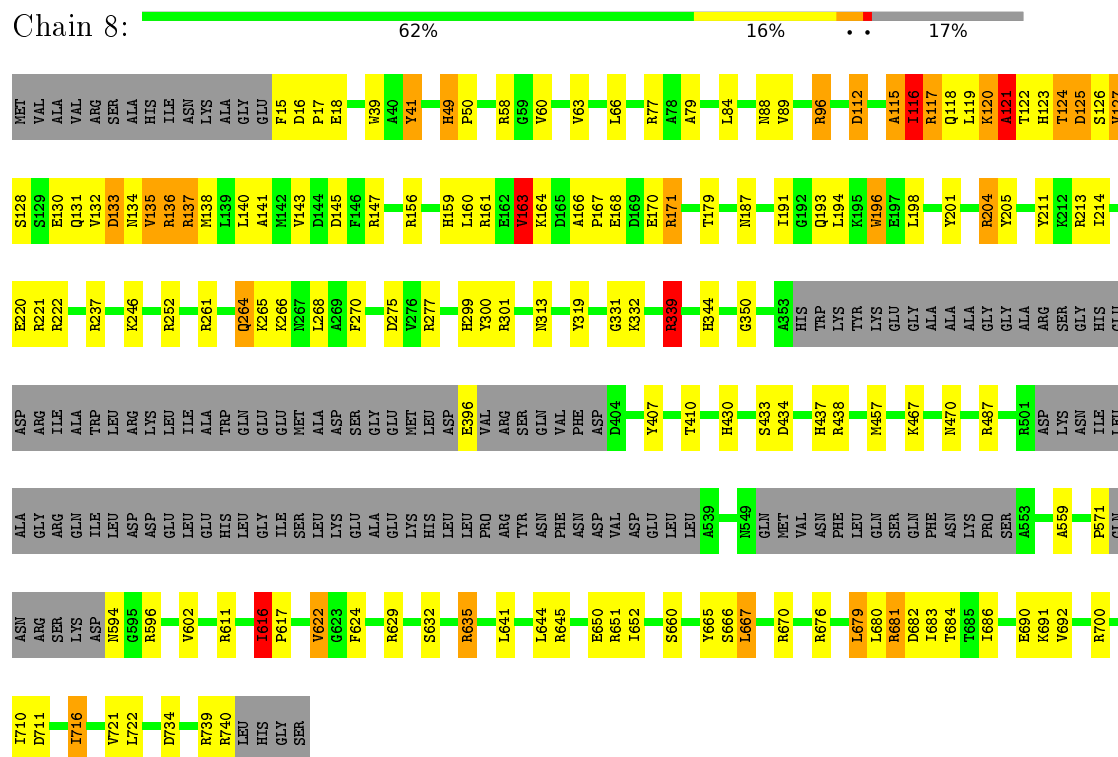
- Molecule 57: A/T tRNA(Phe)



- 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	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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

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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	952	0
53	2	32907	0	16580	469	0
54	3	2529	0	1281	37	0
55	4	1619	0	823	31	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%)	26	70
2	C	207/209 (99%)	190 (92%)	16 (8%)	1 (0%)	34	76
3	D	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	34	76
4	E	175/179 (98%)	158 (90%)	13 (7%)	4 (2%)	8	36
5	F	174/177 (98%)	156 (90%)	17 (10%)	1 (1%)	30	72
6	G	147/149 (99%)	126 (86%)	17 (12%)	4 (3%)	6	32
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	19
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%)	14	51
12	M	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
13	N	118/127 (93%)	107 (91%)	10 (8%)	1 (1%)	24	66
14	O	114/117 (97%)	103 (90%)	9 (8%)	2 (2%)	11	45
15	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
16	Q	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	21	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	101/103 (98%)	90 (89%)	9 (9%)	2 (2%)	9	41
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	41
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	46
25	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
26	a	64/70 (91%)	51 (80%)	12 (19%)	1 (2%)	12	48
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%)	12	48
31	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	g	222/241 (92%)	200 (90%)	15 (7%)	7 (3%)	5	27
33	h	205/233 (88%)	185 (90%)	18 (9%)	2 (1%)	19	61
34	i	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
35	j	155/167 (93%)	142 (92%)	10 (6%)	3 (2%)	10	43
36	k	98/135 (73%)	88 (90%)	9 (9%)	1 (1%)	19	61
37	l	149/179 (83%)	140 (94%)	7 (5%)	2 (1%)	15	53
38	m	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	24	66
39	n	125/130 (96%)	113 (90%)	10 (8%)	2 (2%)	12	48
40	o	96/103 (93%)	82 (85%)	11 (12%)	3 (3%)	5	28
41	p	115/129 (89%)	98 (85%)	15 (13%)	2 (2%)	11	46
42	q	120/124 (97%)	109 (91%)	10 (8%)	1 (1%)	24	66
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%)	3	15
47	v	78/84 (93%)	72 (92%)	4 (5%)	2 (3%)	7	33

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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%)	7	34
50	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
51	z	54/71 (76%)	52 (96%)	1 (2%)	1 (2%)	10	43
59	8	604/744 (81%)	528 (87%)	55 (9%)	21 (4%)	4	24
All	All	6455/6964 (93%)	5874 (91%)	487 (8%)	94 (2%)	18	50

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%)	29	69
2	C	164/164 (100%)	159 (97%)	5 (3%)	48	83
3	D	165/165 (100%)	156 (94%)	9 (6%)	27	65
4	E	148/150 (99%)	138 (93%)	10 (7%)	20	56
5	F	137/138 (99%)	129 (94%)	8 (6%)	25	63
6	G	114/114 (100%)	114 (100%)	0	100	100
7	H	100/123 (81%)	97 (97%)	3 (3%)	48	83
8	I	109/110 (99%)	106 (97%)	3 (3%)	51	84
9	J	116/116 (100%)	114 (98%)	2 (2%)	68	91
10	K	104/104 (100%)	99 (95%)	5 (5%)	31	71
11	L	103/103 (100%)	98 (95%)	5 (5%)	31	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	109/109 (100%)	106 (97%)	3 (3%)	51	84
13	N	100/103 (97%)	96 (96%)	4 (4%)	38	77
14	O	86/87 (99%)	79 (92%)	7 (8%)	15	47
15	P	99/100 (99%)	96 (97%)	3 (3%)	48	83
16	Q	89/90 (99%)	82 (92%)	7 (8%)	15	48
17	R	84/84 (100%)	80 (95%)	4 (5%)	31	71
18	S	93/93 (100%)	87 (94%)	6 (6%)	21	58
19	T	80/84 (95%)	74 (92%)	6 (8%)	17	51
20	U	83/85 (98%)	80 (96%)	3 (4%)	42	79
21	V	78/78 (100%)	73 (94%)	5 (6%)	22	59
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%)	17	52
25	Z	48/49 (98%)	45 (94%)	3 (6%)	22	60
26	a	59/62 (95%)	58 (98%)	1 (2%)	68	91
27	b	47/48 (98%)	45 (96%)	2 (4%)	35	75
28	c	45/49 (92%)	44 (98%)	1 (2%)	60	88
29	d	38/38 (100%)	32 (84%)	6 (16%)	3	15
30	e	51/52 (98%)	46 (90%)	5 (10%)	10	36
31	f	34/34 (100%)	30 (88%)	4 (12%)	6	26
32	g	186/199 (94%)	179 (96%)	7 (4%)	40	78
33	h	170/189 (90%)	160 (94%)	10 (6%)	24	63
34	i	172/173 (99%)	167 (97%)	5 (3%)	50	84
35	j	119/126 (94%)	108 (91%)	11 (9%)	11	40
36	k	87/116 (75%)	82 (94%)	5 (6%)	25	64
37	l	124/147 (84%)	113 (91%)	11 (9%)	12	42
38	m	104/105 (99%)	96 (92%)	8 (8%)	16	50
39	n	105/107 (98%)	97 (92%)	8 (8%)	16	51
40	o	86/90 (96%)	78 (91%)	8 (9%)	11	39
41	p	90/99 (91%)	84 (93%)	6 (7%)	20	57
42	q	102/103 (99%)	97 (95%)	5 (5%)	31	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	r	92/96 (96%)	84 (91%)	8 (9%)	13	43
44	s	83/84 (99%)	79 (95%)	4 (5%)	31	71
45	t	76/77 (99%)	69 (91%)	7 (9%)	11	40
46	u	65/65 (100%)	59 (91%)	6 (9%)	11	40
47	v	74/78 (95%)	67 (90%)	7 (10%)	11	38
48	w	57/66 (86%)	55 (96%)	2 (4%)	43	80
49	x	72/79 (91%)	69 (96%)	3 (4%)	36	76
50	y	65/66 (98%)	59 (91%)	6 (9%)	11	40
51	z	48/61 (79%)	44 (92%)	4 (8%)	14	46
59	8	500/629 (80%)	438 (88%)	62 (12%)	6	24
All	All	5356/5691 (94%)	5028 (94%)	328 (6%)	28	61

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	17,25,26	0.57	0	15,36,39	1.15	2 (13%)
52	2MG	1	1835	52	18,26,27	1.09	1 (5%)	21,38,41	2.44	5 (23%)
52	PSU	1	1911	52	15,21,22	1.07	1 (6%)	16,30,33	2.66	1 (6%)
52	3TD	1	1915	52	15,22,23	0.89	1 (6%)	17,32,35	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	PSU	1	1917	52	15,21,22	1.06	1 (6%)	16,30,33	2.75	1 (6%)
52	5MU	1	1939	52	13,22,23	1.08	2 (15%)	16,32,35	4.14	2 (12%)
52	5MC	1	1962	52	14,22,23	0.73	1 (7%)	17,32,35	0.47	0
52	6MZ	1	2030	52	17,25,26	0.62	0	15,36,39	1.21	1 (6%)
52	G7M	1	2069	52	18,26,27	1.18	2 (11%)	21,39,42	2.70	3 (14%)
52	OMG	1	2251	56,52	18,26,27	1.06	1 (5%)	21,38,41	2.56	3 (14%)
52	2MG	1	2445	52	18,26,27	1.10	1 (5%)	21,38,41	2.48	5 (23%)
52	PSU	1	2457	52	15,21,22	1.10	1 (6%)	16,30,33	2.69	2 (12%)
52	OMC	1	2498	60,52	15,22,23	0.69	0	20,31,34	0.89	1 (5%)
52	2MA	1	2503	60,52	17,25,26	1.08	2 (11%)	18,37,40	2.17	2 (11%)
52	PSU	1	2504	52	15,21,22	1.05	1 (6%)	16,30,33	2.77	3 (18%)
52	OMU	1	2552	60,52	14,22,23	1.00	1 (7%)	19,31,34	2.57	2 (10%)
52	PSU	1	2580	52	15,21,22	1.03	1 (6%)	16,30,33	2.75	1 (6%)
52	PSU	1	2605	52	15,21,22	1.06	1 (6%)	16,30,33	2.72	2 (12%)
52	1MG	1	745	52	17,26,27	0.85	1 (5%)	19,39,42	0.85	1 (5%)
52	PSU	1	746	60,52	15,21,22	1.08	1 (6%)	16,30,33	2.64	1 (6%)
52	5MU	1	747	52	13,22,23	1.04	2 (15%)	16,32,35	4.26	2 (12%)
52	PSU	1	955	52	15,21,22	1.07	1 (6%)	16,30,33	2.62	1 (6%)
53	2MG	2	1207	53	18,26,27	1.12	1 (5%)	21,38,41	2.52	5 (23%)
53	4OC	2	1402	53	15,23,24	0.69	0	21,32,35	1.25	2 (9%)
53	5MC	2	1407	53	14,22,23	0.71	0	17,32,35	0.70	0
53	UR3	2	1498	53	13,22,23	0.76	0	18,32,35	0.54	0
53	2MG	2	1516	53	18,26,27	1.14	1 (5%)	21,38,41	2.37	3 (14%)
53	MA6	2	1518	53	18,26,27	0.55	0	15,38,41	1.20	2 (13%)
53	MA6	2	1519	53	18,26,27	0.60	0	15,38,41	1.16	2 (13%)
53	PSU	2	516	53	15,21,22	1.07	1 (6%)	16,30,33	2.89	2 (12%)
53	G7M	2	527	53	18,26,27	1.20	2 (11%)	21,39,42	2.61	3 (14%)
53	2MG	2	966	53	18,26,27	1.13	1 (5%)	21,38,41	2.47	5 (23%)
53	5MC	2	967	53	14,22,23	0.74	1 (7%)	17,32,35	0.52	0
56	H2U	5	20	56	17,21,22	0.56	0	23,30,33	0.77	0
56	4OC	5	32	56	15,23,24	0.67	0	21,32,35	1.11	2 (9%)
56	5MU	5	54	56	13,22,23	1.03	1 (7%)	16,32,35	4.38	2 (12%)
56	PSU	5	55	56	15,21,22	1.07	1 (6%)	16,30,33	2.63	2 (12%)
56	4SU	5	8	56	12,21,22	1.04	1 (8%)	15,30,33	1.80	2 (13%)
57	H2U	6	16	57	17,21,22	0.57	0	23,30,33	2.30	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	H2U	6	20	57	17,21,22	0.62	0	23,30,33	1.56	4 (17%)
57	PSU	6	32	57	15,21,22	1.23	1 (6%)	16,30,33	3.55	5 (31%)
57	6IA	6	37	57,58	20,29,30	0.55	0	22,41,44	1.85	5 (22%)
57	7MG	6	46	57	20,26,27	1.03	1 (5%)	23,39,42	2.33	4 (17%)
57	3AU	6	47	57	16,28,29	0.86	1 (6%)	16,40,43	0.55	0
57	5MU	6	54	57	13,22,23	1.06	1 (7%)	16,32,35	4.24	2 (12%)
57	PSU	6	55	57	15,21,22	1.26	1 (6%)	16,30,33	3.61	5 (31%)
57	4SU	6	8	57	12,21,22	1.05	1 (8%)	15,30,33	1.54	1 (6%)
42	D2T	q	89	42	4,9,10	0.54	0	4,11,13	2.13	2 (50%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	UR3	2	1498	53	-	0/3/25/26	0/2/2/2
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 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	747	5MU	C6-C5	-2.05	1.34	1.40
53	2	967	5MC	C6-C5	-2.05	1.34	1.40
52	1	1962	5MC	C6-C5	-2.04	1.34	1.40
52	1	1939	5MU	C6-C5	-2.02	1.34	1.40
52	1	2069	G7M	C8-N9	2.27	1.37	1.33

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1	747	5MU	C5-C4-N3	-11.50	115.70	125.35
56	5	54	5MU	C5-C4-N3	-11.43	115.75	125.35
57	6	54	5MU	C5-C4-N3	-11.04	116.08	125.35
52	1	1939	5MU	C5-C4-N3	-10.90	116.20	125.35
52	1	2069	G7M	C5-C6-N1	-8.57	112.32	123.52

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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	-	5,7,8	0.42	0	4,7,9	0.96	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	2	1665	PAR	O51-C11	-3.72	1.32	1.41
62	2	1665	PAR	C14-C24	-2.27	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	2	1665	PAR	O51-C11-C21	2.40	115.36	109.88

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