



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

Dec 8, 2019 – 08:24 PM EST

PDB ID : 5A2Q  
EMDB ID: : EMD-3019  
Title : Structure of the HCV IRES bound to the human ribosome  
Authors : Quade, N.; Leiundgut, M.; Boehringer, D.; Heuvel, J.v.d.; Ban, N.  
Deposited on : 2015-05-21  
Resolution : 3.90 Å(reported)  
Based on PDB ID : 4W23

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

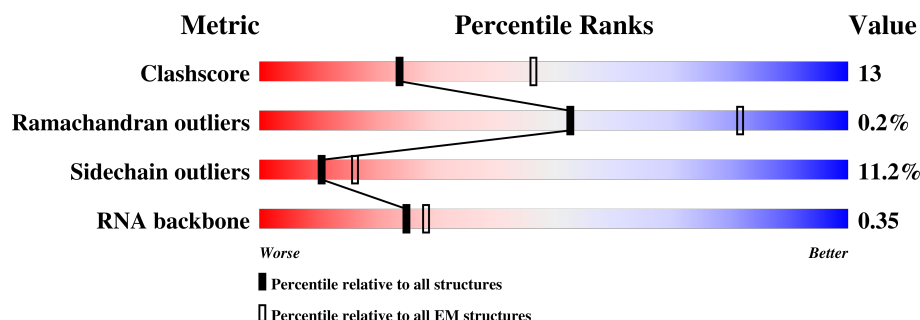
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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.







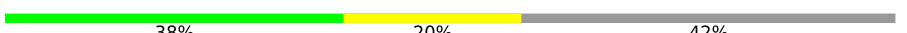
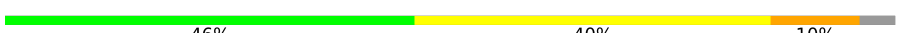





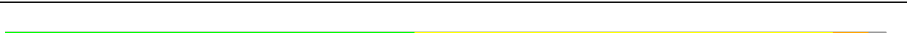











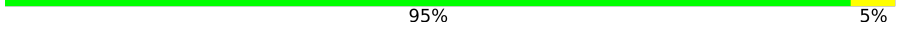
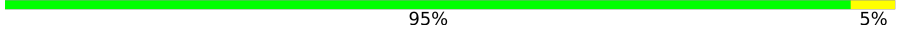
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	2	1868	<div> <div>32%</div> <div>36%</div> <div>17%</div> <div>•</div> <div>11%</div> </div>
2	3	257	<div> <div>32%</div> <div>39%</div> <div>27%</div> <div>•</div> </div>
3	A	295	<div> <div>46%</div> <div>25%</div> <div>•</div> <div>27%</div> </div>
4	B	264	<div> <div>51%</div> <div>26%</div> <div>•</div> <div>19%</div> </div>
5	C	293	<div> <div>42%</div> <div>25%</div> <div>7%</div> <div>26%</div> </div>
6	D	243	<div> <div>63%</div> <div>27%</div> <div>•</div> <div>7%</div> </div>
7	E	263	<div> <div>54%</div> <div>37%</div> <div>8%</div> </div>
8	F	204	<div> <div>69%</div> <div>23%</div> <div>7%</div> </div>

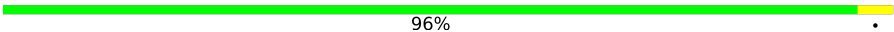
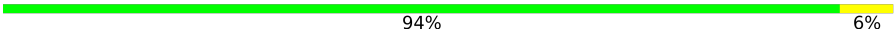


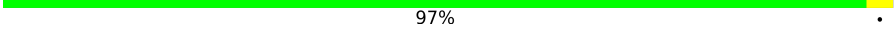
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Mol	Chain	Length	Quality of chain
9	G	249	
10	H	194	
11	I	208	
12	J	194	
13	K	165	
14	L	158	
15	M	132	
16	N	151	
17	O	151	
18	P	145	
19	Q	146	
20	R	135	
21	S	152	
22	T	146	
23	U	119	
24	V	83	
25	W	130	
26	X	143	
27	Y	130	
28	Z	125	
29	a	101	
30	b	82	
31	c	61	
32	d	55	
33	e	56	

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Mol	Chain	Length	Quality of chain
34	f	72	 96% .
35	g	315	 94% 6%
36	h	24	 88% 13%
37	r	13	 92% 8%
38	w	62	 97% .

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 80749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1665	Total	C	N	O	P	0	0
			35552	15869	6385	11633	1665		

- Molecule 2 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	257	Total	C	N	O	P	0	0
			5485	2444	979	1805	257		

- Molecule 3 is a protein called RIBOSOMAL PROTEIN US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 4 is a protein called RIBOSOMAL PROTEIN ES1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called RIBOSOMAL PROTEIN US5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 6 is a protein called RIBOSOMAL PROTEIN US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 7 is a protein called RIBOSOMAL PROTEIN ES4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 8 is a protein called RIBOSOMAL PROTEIN US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 9 is a protein called RIBOSOMAL PROTEIN ES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	230	Total	C	N	O	S	0	0
			1864	1164	373	320	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	221	ARG	LYS	conflict	UNP P62753

- Molecule 10 is a protein called RIBOSOMAL PROTEIN ES7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 11 is a protein called RIBOSOMAL PROTEIN ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 12 is a protein called RIBOSOMAL PROTEIN US4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 13 is a protein called RIBOSOMAL PROTEIN ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 14 is a protein called RIBOSOMAL PROTEIN US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 15 is a protein called RIBOSOMAL PROTEIN ES12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 16 is a protein called RIBOSOMAL PROTEIN US15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 17 is a protein called RIBOSOMAL PROTEIN US11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 18 is a protein called RIBOSOMAL PROTEIN US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 19 is a protein called RIBOSOMAL PROTEIN US9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 20 is a protein called RIBOSOMAL PROTEIN ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 21 is a protein called RIBOSOMAL PROTEIN US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 22 is a protein called RIBOSOMAL PROTEIN ES19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	145	Total	C	N	O	S	0	0
			1128	706	218	201	3		

- Molecule 23 is a protein called RIBOSOMAL PROTEIN US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 24 is a protein called RIBOSOMAL PROTEIN ES21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 25 is a protein called RIBOSOMAL PROTEIN US8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 26 is a protein called RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 27 is a protein called RIBOSOMAL PROTEIN ES24.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 28 is a protein called RIBOSOMAL PROTEIN ES25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 29 is a protein called RIBOSOMAL PROTEIN ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	101	Total	C	N	O	S	0	0
			816	509	170	132	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	78	VAL	ALA	conflict	UNP P62854

- Molecule 30 is a protein called RIBOSOMAL PROTEIN ES27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 31 is a protein called RIBOSOMAL PROTEIN ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 32 is a protein called RIBOSOMAL PROTEIN US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 33 is a protein called RIBOSOMAL PROTEIN ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	56	Total	C	N	O	S	0	0
			442	273	96	72	1		

- Molecule 34 is a protein called RIBOSOMAL PROTEIN ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	72	Total	C	N	O	S	0	0
			585	366	114	97	8		

- Molecule 35 is a protein called RIBOSOMAL PROTEIN RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 36 is a protein called RIBOSOMAL PROTEIN EL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	24	Total	C	N	O	S	0	0
			231	140	63	26	2		

- Molecule 37 is a protein called RIBOSOMAL PROTEIN EL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	r	13	Total	C	N	O	0	0
			118	68	31	19		

- Molecule 38 is a protein called RIBOSOMAL PROTEIN EL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	62	Total	C	N	O	S	0	0
			452	279	92	80	1		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	2	98	Total	Mg	0
			98	98	

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	a	1	Total 1	Zn 1	0
40	d	1	Total 1	Zn 1	0
40	f	1	Total 1	Zn 1	0

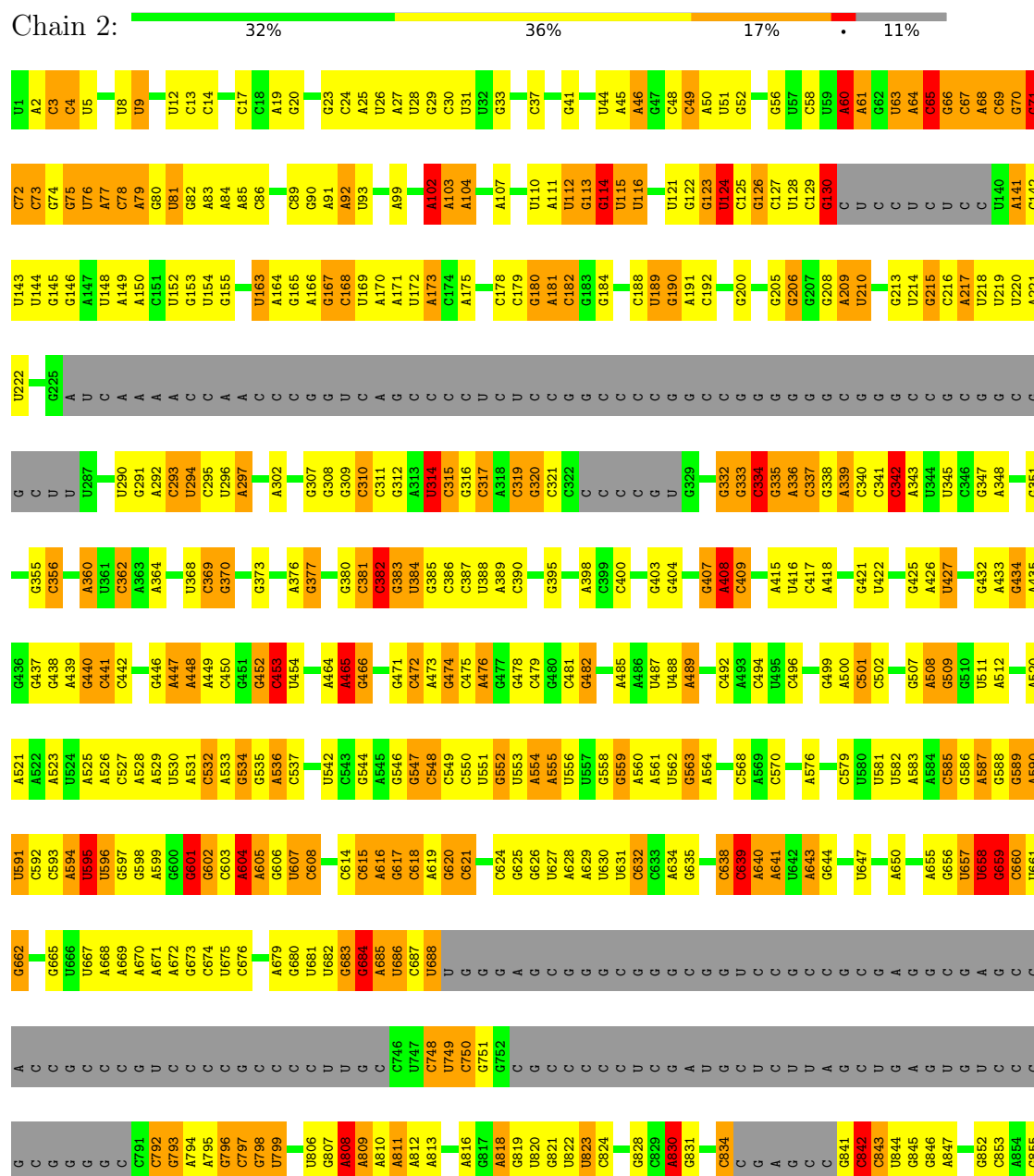
- Molecule 41 is water.

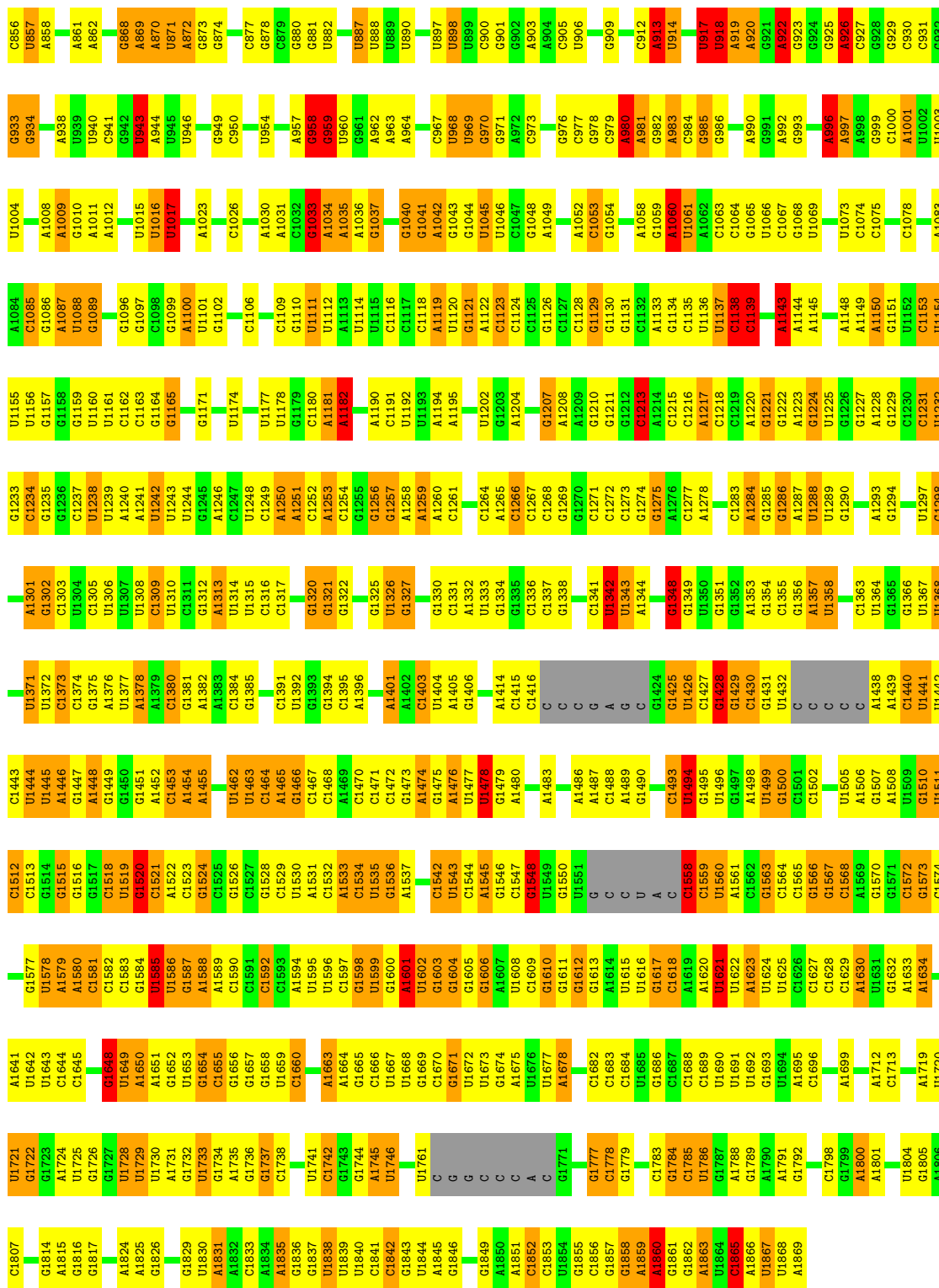
Mol	Chain	Residues	Atoms		AltConf
41	2	141	Total 141	O 141	0
41	C	2	Total 2	O 2	0
41	e	1	Total 1	O 1	0

### 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: 18S RRNA

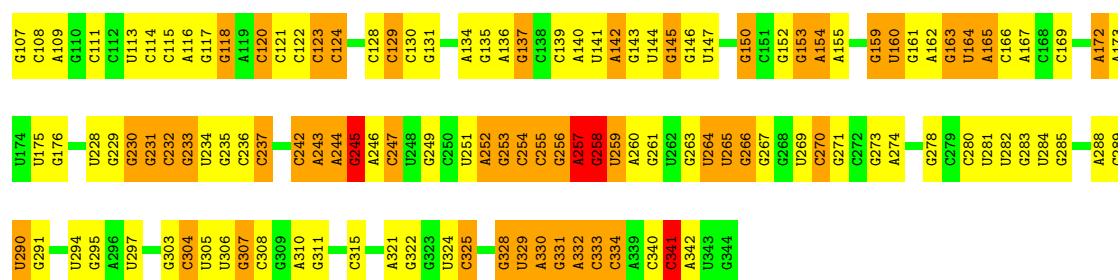




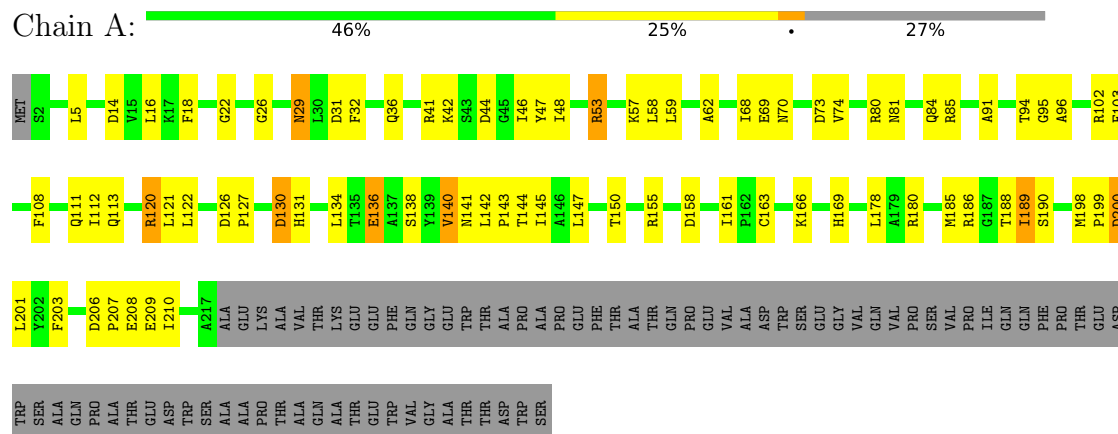
- Molecule 2: HCV IRES

Chain 3:  32% 39% 27% .

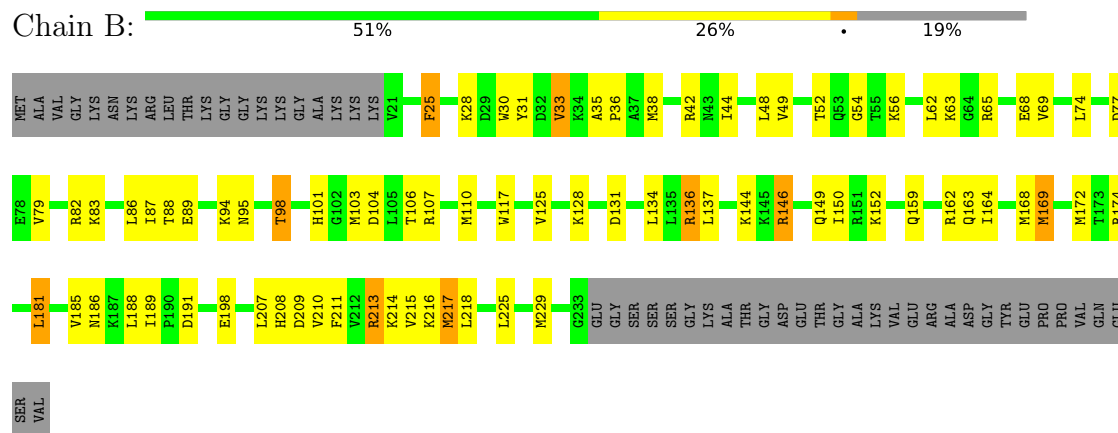




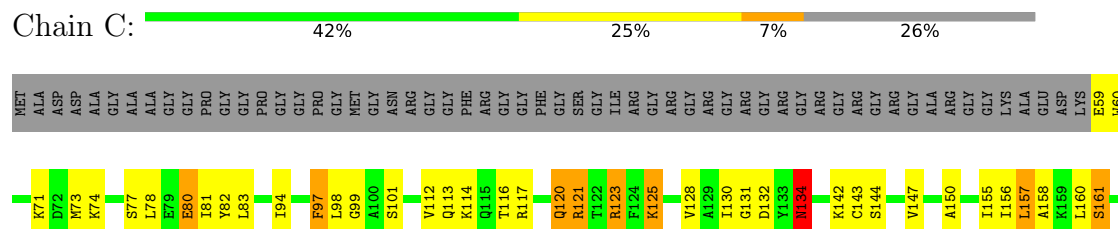
### • Molecule 3: RIBOSOMAL PROTEIN US2

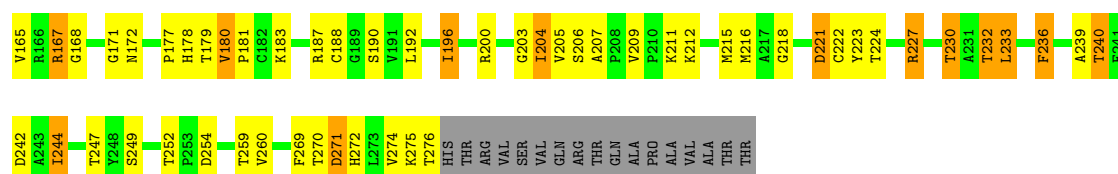


### • Molecule 4: RIBOSOMAL PROTEIN ES1



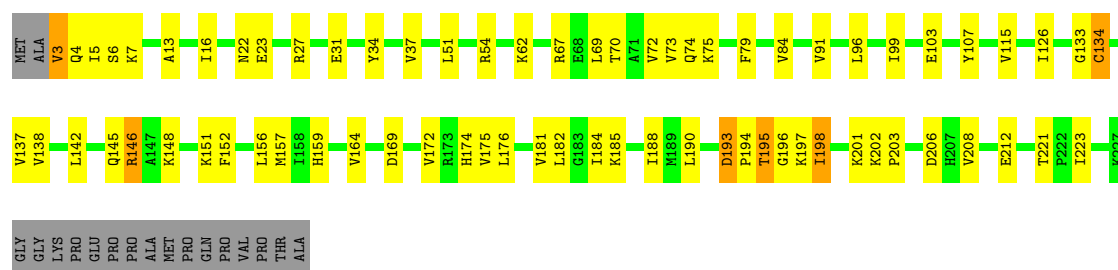
### • Molecule 5: RIBOSOMAL PROTEIN US5





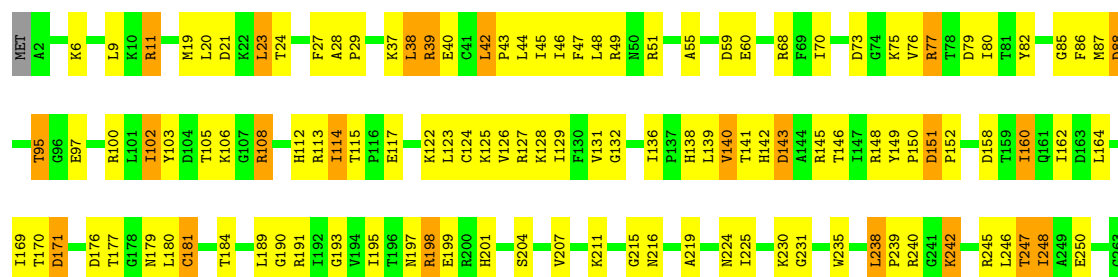
• Molecule 6: RIBOSOMAL PROTEIN US3

Chain D: 63% 27% 7%



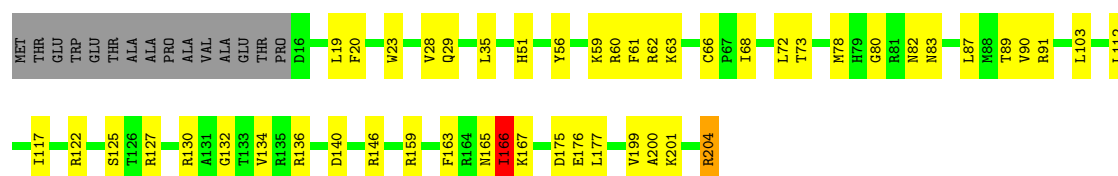
• Molecule 7: RIBOSOMAL PROTEIN ES4

Chain E: 54% 37% 8%



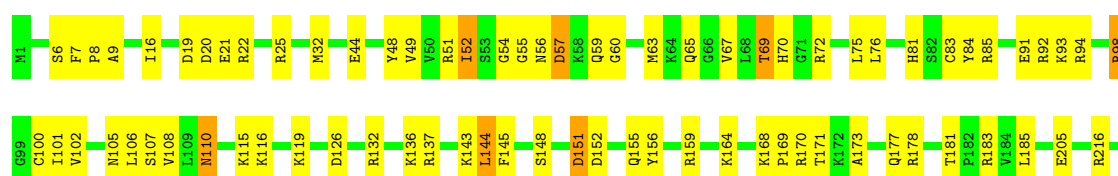
• Molecule 8: RIBOSOMAL PROTEIN US7

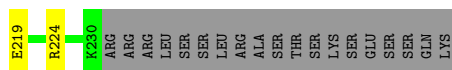
Chain F: 69% 23% 7%



• Molecule 9: RIBOSOMAL PROTEIN ES6

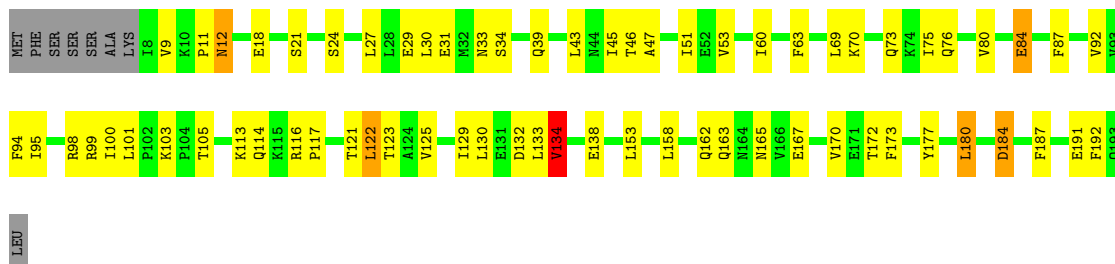
Chain G: 61% 29% 8%





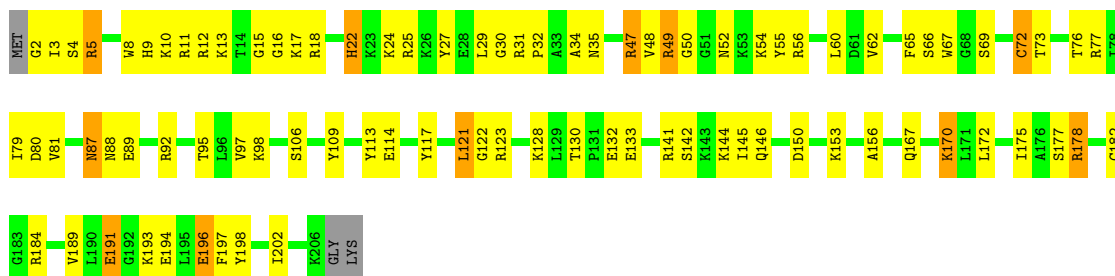
- Molecule 10: RIBOSOMAL PROTEIN ES7

Chain H:  61% 31% . . .



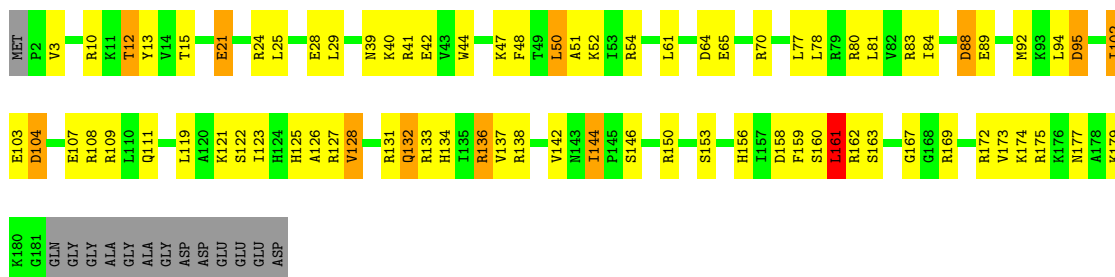
- Molecule 11: RIBOSOMAL PROTEIN ES8

Chain I:  56% 37% 5%



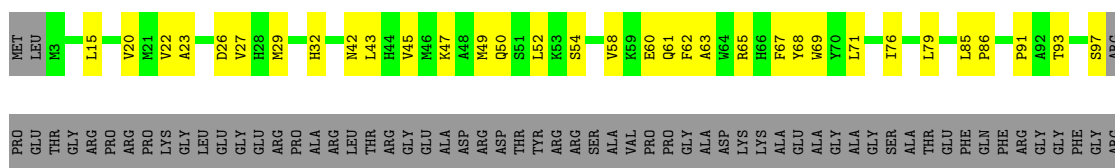
- Molecule 12: RIBOSOMAL PROTEIN US4

Chain J:  53% 34% 6% • 7%



- Molecule 13: RIBOSOMAL PROTEIN ES10

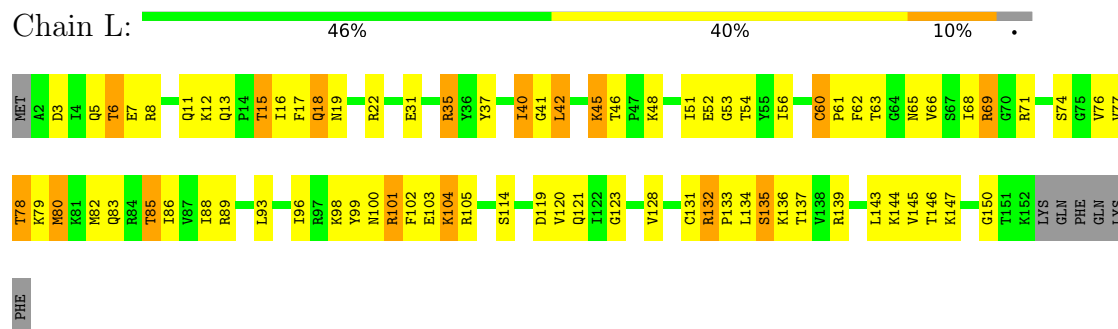
Chain K:  38% 20% 42%



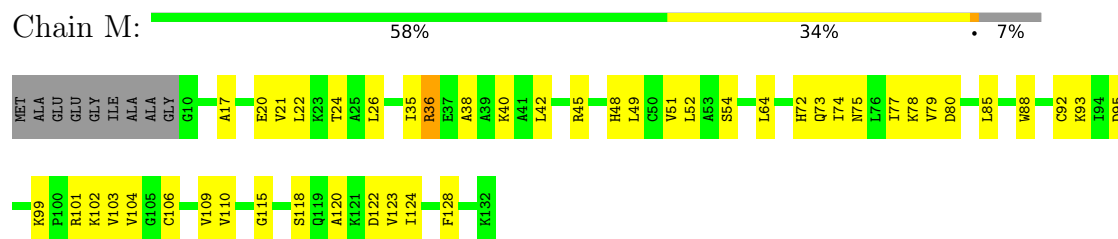


GLY  
ARG  
GLY  
GLN  
PRO  
PRO  
GLN

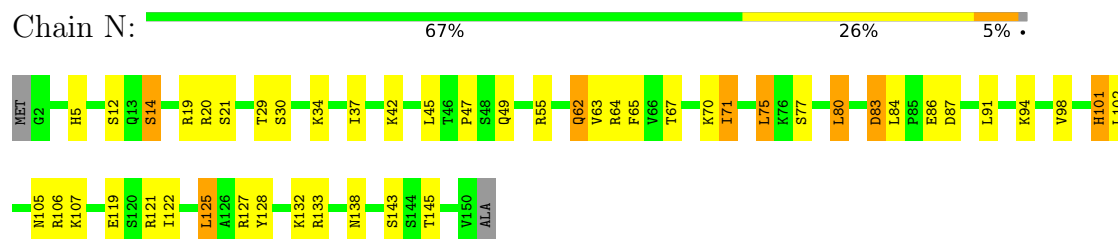
• Molecule 14: RIBOSOMAL PROTEIN US17



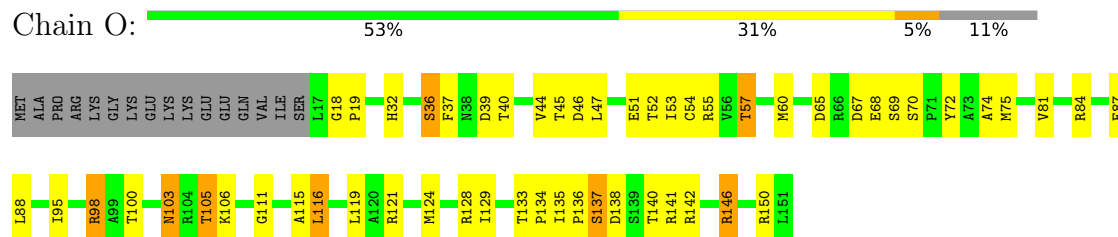
• Molecule 15: RIBOSOMAL PROTEIN ES12



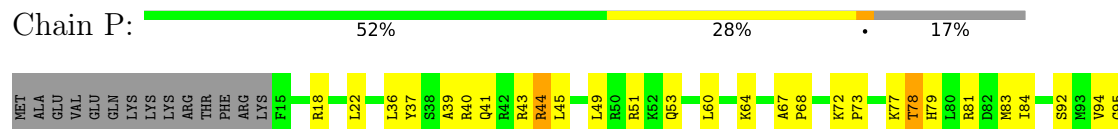
• Molecule 16: RIBOSOMAL PROTEIN US15



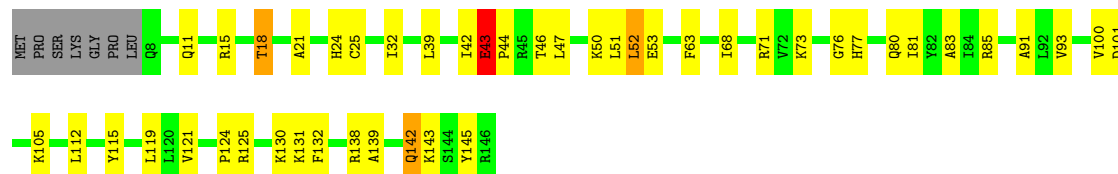
• Molecule 17: RIBOSOMAL PROTEIN US11



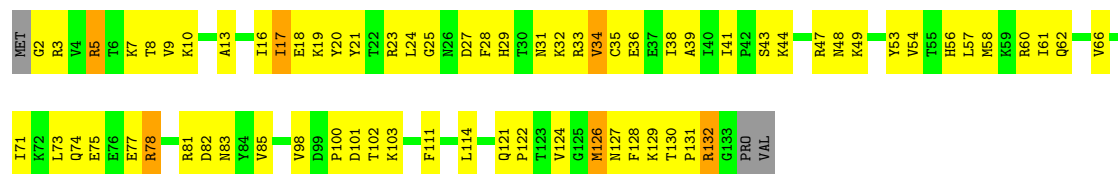
• Molecule 18: RIBOSOMAL PROTEIN US19



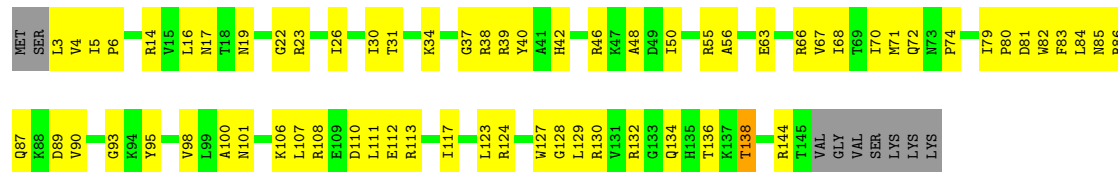
● Molecule 19: RIBOSOMAL PROTEIN US9



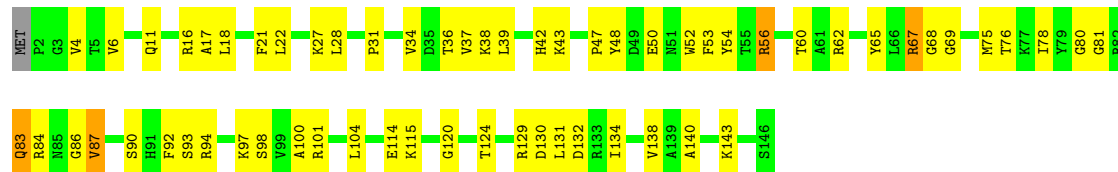
• Molecule 20: RIBOSOMAL PROTEIN ES17



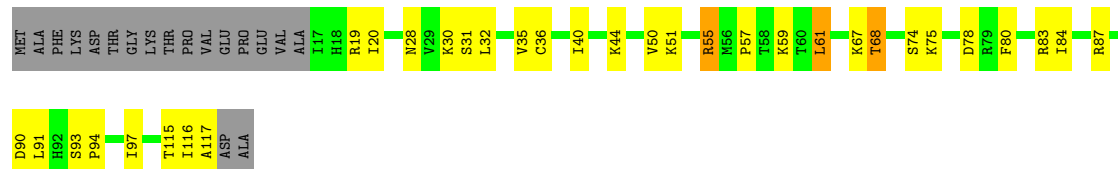
● Molecule 21: RIBOSOMAL PROTEIN US13



• Molecule 22: RIBOSOMAL PROTEIN ES19



• Molecule 23: RIBOSOMAL PROTEIN US10



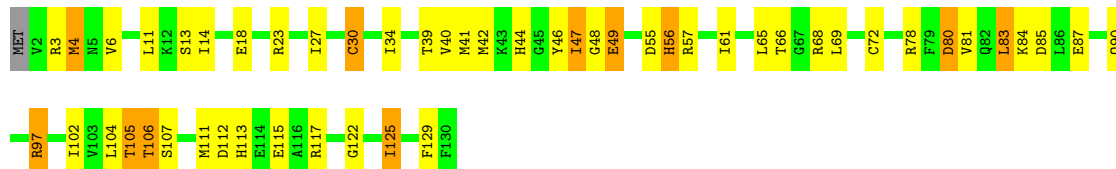
- Molecule 24: RIBOSOMAL PROTEIN ES21

Chain V: 



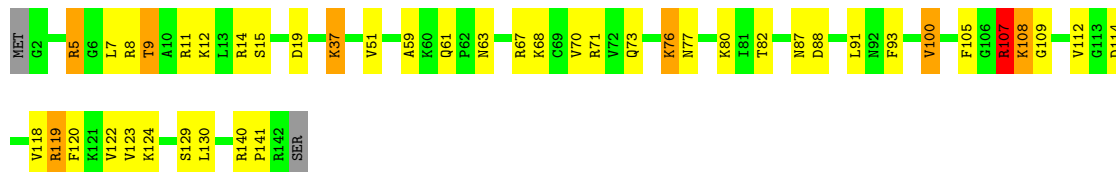
- Molecule 25: RIBOSOMAL PROTEIN US8

Chain W: 



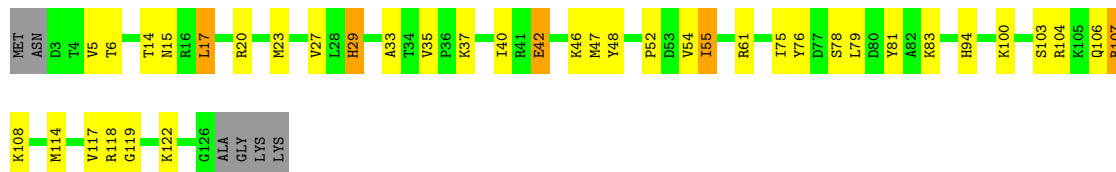
- Molecule 26: RIBOSOMAL PROTEIN US12

Chain X: 



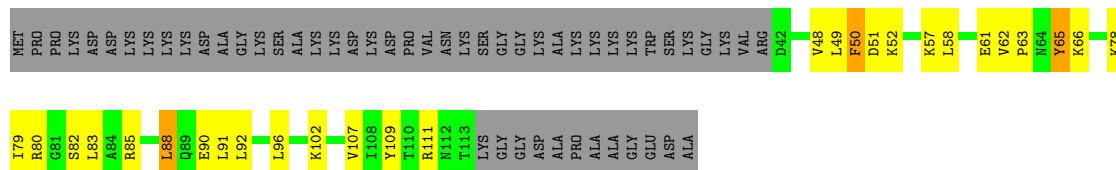
- Molecule 27: RIBOSOMAL PROTEIN ES24

Chain Y: 



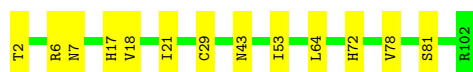
- Molecule 28: RIBOSOMAL PROTEIN ES25

Chain Z: 



- Molecule 29: RIBOSOMAL PROTEIN ES26

Chain a: 



- Molecule 30: RIBOSOMAL PROTEIN ES27

Chain b: 87% 13%



- Molecule 31: RIBOSOMAL PROTEIN ES28

Chain c: 95% 5%



- Molecule 32: RIBOSOMAL PROTEIN US14

Chain d: 95% 5%



- Molecule 33: RIBOSOMAL PROTEIN ES30

Chain e: 84% 16%



- Molecule 34: RIBOSOMAL PROTEIN ES31

Chain f: 96% 4%



- Molecule 35: RIBOSOMAL PROTEIN RACK1

Chain g: 94% 6%



- Molecule 36: RIBOSOMAL PROTEIN EL41

Chain h: 88% 13%



- Molecule 37: RIBOSOMAL PROTEIN EL19

Chain r:  92% 8%



• Molecule 38: RIBOSOMAL PROTEIN EL24

Chain w:  97% .



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	404357	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL FRAMES	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20.00	Depositor
Minimum defocus (nm)	1500.00	Depositor
Maximum defocus (nm)	3400.00	Depositor
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	2	0.74	11/39755 (0.0%)	1.24	222/61954 (0.4%)
10	H	0.44	0/1524	0.61	0/2042
11	I	0.51	0/1711	0.66	1/2282 (0.0%)
12	J	0.57	0/1524	0.67	0/2035
13	K	0.32	0/824	0.46	0/1112
14	L	0.62	0/1250	0.72	0/1673
15	M	0.32	0/963	0.50	0/1291
16	N	0.51	0/1226	0.66	0/1649
17	O	0.52	0/1023	0.75	0/1372
18	P	0.34	0/1003	0.52	0/1341
19	Q	0.35	0/1126	0.55	1/1506 (0.1%)
2	3	0.40	0/6127	1.02	8/9547 (0.1%)
20	R	0.39	0/1080	0.58	0/1449
21	S	0.33	0/1202	0.50	0/1610
22	T	0.35	0/1148	0.50	0/1538
23	U	0.34	0/813	0.52	0/1092
24	V	0.51	0/631	0.63	0/844
25	W	0.65	0/1051	0.73	0/1406
26	X	0.62	0/1116	0.71	0/1490
27	Y	0.51	0/1031	0.64	0/1370
28	Z	0.28	0/580	0.48	0/780
29	a	0.56	0/830	0.64	0/1112
3	A	0.48	0/1742	0.63	0/2367
30	b	0.51	0/653	0.69	0/876
31	c	0.38	0/481	0.59	0/643
32	d	0.36	0/469	0.59	0/623
33	e	0.46	0/447	0.59	0/587
34	f	0.30	0/595	0.50	0/785
35	g	0.31	0/2497	0.52	0/3399
36	h	0.57	0/232	0.65	0/295
37	r	0.29	0/117	0.44	0/149
38	w	0.37	0/368	0.43	0/485

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
4	B	0.52	0/1756	0.68	0/2350
5	C	0.61	0/1726	0.77	4/2332 (0.2%)
6	D	0.35	0/1780	0.53	0/2397
7	E	0.57	0/2118	0.69	0/2849
8	F	0.34	0/1516	0.55	0/2037
9	G	0.42	0/1887	0.60	0/2513
All	All	0.60	11/85922 (0.0%)	1.00	236/125182 (0.2%)

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
10	H	0	1
26	X	0	2
27	Y	0	1
35	g	0	1
6	D	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1353	A	N9-C4	-6.78	1.33	1.37
1	2	1085	C	N1-C6	-6.62	1.33	1.37
1	2	599	A	N9-C4	-6.35	1.34	1.37
1	2	1000	C	N1-C6	-6.09	1.33	1.37
1	2	808	A	N9-C4	-5.94	1.34	1.37

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	N1-C2-O2	10.93	125.45	118.90
1	2	501	C	C2-N1-C1'	10.11	129.93	118.80
1	2	1842	C	C6-N1-C2	-9.59	116.46	120.30
1	2	501	C	C6-N1-C1'	-9.28	109.67	120.80
1	2	1139	C	C6-N1-C2	-9.27	116.59	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
6	D	193	ASP	Peptide
10	H	134	VAL	Peptide
26	X	107	ARG	Peptide
26	X	112	VAL	Peptide
27	Y	118	ARG	Peptide

## 5.2 Too-close contacts

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	2	35552	0	17948	699	0
2	3	5485	0	2776	79	0
3	A	1705	0	1706	54	0
4	B	1729	0	1803	57	0
5	C	1690	0	1777	55	0
6	D	1752	0	1848	57	0
7	E	2076	0	2177	81	0
8	F	1495	0	1549	32	0
9	G	1864	0	2018	61	0
10	H	1501	0	1593	41	0
11	I	1682	0	1769	58	0
12	J	1499	0	1618	59	0
13	K	800	0	818	23	0
14	L	1229	0	1302	51	0
15	M	953	0	990	27	0
16	N	1202	0	1289	34	0
17	O	1010	0	1034	43	0
18	P	984	0	1028	34	0
19	Q	1109	0	1174	35	0
20	R	1066	0	1116	52	0
21	S	1184	0	1244	64	0
22	T	1128	0	1158	56	0
23	U	803	0	873	26	0
24	V	625	0	628	17	0
25	W	1034	0	1080	29	0
26	X	1098	0	1167	36	0
27	Y	1014	0	1082	23	0
28	Z	574	0	627	24	0
29	a	816	0	867	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	640	0	665	0	0
31	c	479	0	507	0	0
32	d	458	0	448	0	0
33	e	442	0	487	0	0
34	f	585	0	615	0	0
35	g	2440	0	2396	0	0
36	h	231	0	277	0	0
37	r	118	0	132	0	0
38	w	452	0	493	0	0
39	2	98	0	0	0	0
40	a	1	0	0	0	0
40	d	1	0	0	0	0
40	f	1	0	0	0	0
41	2	141	0	0	14	0
41	C	2	0	0	0	0
41	e	1	0	0	0	0
All	All	80749	0	62079	1639	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 13.

The worst 5 of 1639 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)
15:M:20:GLU:HB3	15:M:120:ALA:HB2	1.50	0.94
1:2:1622:U:H3	18:P:122:THR:HG1	1.11	0.90
22:T:69:GLY:HA2	22:T:120:GLY:HA3	1.55	0.89
1:2:1256:G:H21	1:2:1659:U:H5'	1.37	0.89
1:2:560:A:H5'	12:J:174:LYS:HG3	1.56	0.88

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	
3	A	214/295 (72%)	202 (94%)	11 (5%)	1 (0%)	31	71
4	B	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
5	C	216/293 (74%)	213 (99%)	3 (1%)	0	100	100
6	D	223/243 (92%)	214 (96%)	8 (4%)	1 (0%)	36	74
7	E	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
8	F	187/204 (92%)	169 (90%)	16 (9%)	2 (1%)	16	56
9	G	228/249 (92%)	217 (95%)	11 (5%)	0	100	100
10	H	184/194 (95%)	172 (94%)	11 (6%)	1 (0%)	31	71
11	I	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
12	J	178/194 (92%)	172 (97%)	5 (3%)	1 (1%)	27	67
13	K	93/165 (56%)	89 (96%)	4 (4%)	0	100	100
14	L	149/158 (94%)	145 (97%)	4 (3%)	0	100	100
15	M	121/132 (92%)	112 (93%)	9 (7%)	0	100	100
16	N	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
17	O	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
18	P	118/145 (81%)	116 (98%)	2 (2%)	0	100	100
19	Q	137/146 (94%)	131 (96%)	6 (4%)	0	100	100
20	R	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
21	S	141/152 (93%)	136 (96%)	5 (4%)	0	100	100
22	T	143/146 (98%)	138 (96%)	4 (3%)	1 (1%)	24	64
23	U	99/119 (83%)	94 (95%)	5 (5%)	0	100	100
24	V	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
25	W	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
26	X	139/143 (97%)	130 (94%)	8 (6%)	1 (1%)	24	64
27	Y	122/130 (94%)	118 (97%)	4 (3%)	0	100	100
28	Z	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
29	a	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
30	b	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
31	c	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
32	d	53/55 (96%)	51 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	e	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
34	f	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
35	g	312/315 (99%)	295 (95%)	15 (5%)	2 (1%)	27	67
36	h	22/24 (92%)	22 (100%)	0	0	100	100
37	r	11/13 (85%)	11 (100%)	0	0	100	100
38	w	47/62 (76%)	47 (100%)	0	0	100	100
All	All	4860/5459 (89%)	4641 (96%)	209 (4%)	10 (0%)	53	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	189	ILE
10	H	170	VAL
12	J	161	LEU
35	g	145	GLU
26	X	108	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	180/243 (74%)	159 (88%)	21 (12%)	6	30
4	B	194/231 (84%)	175 (90%)	19 (10%)	9	36
5	C	184/225 (82%)	140 (76%)	44 (24%)	1	6
6	D	189/202 (94%)	177 (94%)	12 (6%)	20	54
7	E	224/225 (100%)	189 (84%)	35 (16%)	3	20
8	F	159/170 (94%)	149 (94%)	10 (6%)	20	54
9	G	200/218 (92%)	180 (90%)	20 (10%)	8	35
10	H	167/174 (96%)	152 (91%)	15 (9%)	10	41
11	I	178/180 (99%)	153 (86%)	25 (14%)	4	25
12	J	160/168 (95%)	135 (84%)	25 (16%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	K	86/136 (63%)	85 (99%)	1 (1%)	74	87
14	L	135/142 (95%)	104 (77%)	31 (23%)	1	7
15	M	104/108 (96%)	99 (95%)	5 (5%)	28	61
16	N	130/131 (99%)	112 (86%)	18 (14%)	4	25
17	O	105/119 (88%)	87 (83%)	18 (17%)	2	16
18	P	107/130 (82%)	102 (95%)	5 (5%)	29	62
19	Q	115/121 (95%)	104 (90%)	11 (10%)	9	37
20	R	118/122 (97%)	104 (88%)	14 (12%)	6	29
21	S	124/132 (94%)	118 (95%)	6 (5%)	28	61
22	T	115/116 (99%)	108 (94%)	7 (6%)	20	55
23	U	93/107 (87%)	87 (94%)	6 (6%)	19	53
24	V	66/67 (98%)	50 (76%)	16 (24%)	1	6
25	W	112/113 (99%)	91 (81%)	21 (19%)	1	13
26	X	113/115 (98%)	103 (91%)	10 (9%)	11	42
27	Y	108/112 (96%)	95 (88%)	13 (12%)	5	29
28	Z	64/103 (62%)	60 (94%)	4 (6%)	20	54
29	a	89/89 (100%)	76 (85%)	13 (15%)	3	22
30	b	74/74 (100%)	63 (85%)	11 (15%)	3	22
31	c	54/54 (100%)	51 (94%)	3 (6%)	23	58
32	d	48/48 (100%)	45 (94%)	3 (6%)	20	54
33	e	45/45 (100%)	36 (80%)	9 (20%)	1	11
34	f	65/65 (100%)	62 (95%)	3 (5%)	29	62
35	g	272/273 (100%)	257 (94%)	15 (6%)	24	58
36	h	23/23 (100%)	20 (87%)	3 (13%)	4	26
37	r	12/12 (100%)	11 (92%)	1 (8%)	12	45
38	w	35/35 (100%)	33 (94%)	2 (6%)	23	57
All	All	4247/4628 (92%)	3772 (89%)	475 (11%)	10	32

5 of 475 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	104	ASP
16	N	29	THR

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Mol	Chain	Res	Type
32	d	8	TRP
12	J	144	ILE
14	L	69	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
11	I	168	GLN
16	N	58	HIS
35	g	20	GLN
13	K	61	GLN
17	O	32	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1656/1868 (88%)	595 (35%)	83 (5%)
2	3	254/257 (98%)	148 (58%)	25 (9%)
All	All	1910/2125 (89%)	743 (38%)	108 (5%)

5 of 743 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	4	C
1	2	5	U
1	2	8	U
1	2	9	U

5 of 108 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1181	A
1	2	1425	G
2	3	252	A
1	2	1250	A
1	2	1316	C

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 101 ligands modelled in this entry, 101 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	177:C	O3'	222:G	P	17.37
1	3	334:C	O3'	339:A	P	15.84