



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:46 PM BST

PDB ID : 3J0P  
EMDB ID: : EMD-5328  
Title : Core of mammalian 80S pre-ribosome in complex with tRNAs fitted to a 10.6A cryo-em map: rotated PRE state 1  
Authors : Budkevich, T.; Giesebrecht, J.; Altman, R.; Munro, J.; Mielke, T.; Nierhaus, K.; Blanchard, S.; Spahn, C.M.  
Deposited on : 2011-10-06  
Resolution : 10.60 Å(reported)  
Based on PDB ID : 2XZM, 3O58

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 : unknown  
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) : trunk27241

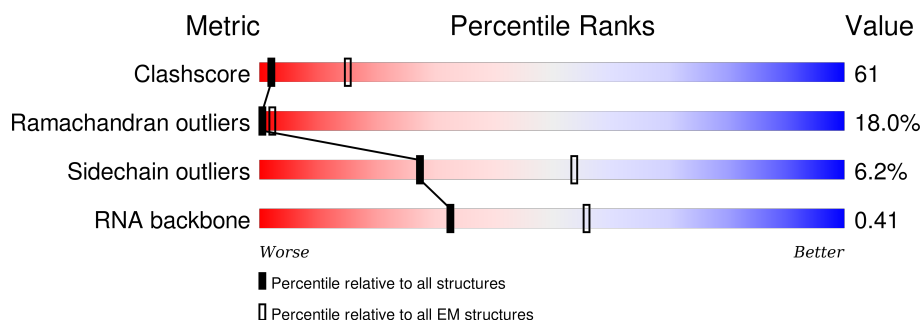
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.60 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.









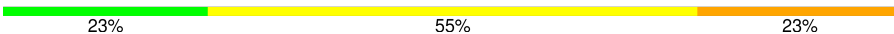
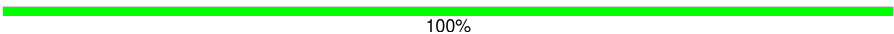


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	a	48	65% 25% 6% .
2	c	17	71% 29%
3	d	7	71% 14% 14%
4	g	31	71% 23% 6%
5	G	13	31% 54% 15%
6	f	21	76% 24%
7	h	111	88% 11% .
8	S	125	32% 62% 5% .

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Mol	Chain	Length	Quality of chain
9	L	141	
10	X	68	
11	2	112	
12	3	12	
13	7	50	
14	B	213	
15	Y	75	
16	y	3	
17	W	77	
18	w	2	

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 16039 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 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	48	Total	C	N	O	P	0	0
			1029	459	190	332	48		

- Molecule 2 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	17	Total	C	N	O	P	0	0
			362	162	66	117	17		

- Molecule 3 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	7	Total	C	N	O	P	0	0
			155	69	33	46	7		

- Molecule 4 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	31	Total	C	N	O	P	0	0
			660	295	118	216	31		

- Molecule 5 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	13	Total	C	N	O	P	0	0
			276	123	49	91	13		

- Molecule 6 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	21	Total	C	N	O	P	0	0
			452	200	79	152	21		

- Molecule 7 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	111	Total	C	N	O	P	0	0
			2368	1060	431	766	111		

- Molecule 8 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	125	Total	C	N	O	S	0	0
			985	632	173	176	4		

- Molecule 9 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	141	Total	C	N	O	S	0	0
			1097	691	221	180	5		

- Molecule 10 is a protein called Ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	68	Total	C	N	O	S	0	0
			554	350	113	90	1		

- Molecule 11 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	112	Total	C	N	O	P	0	0
			2392	1070	435	775	112		

- Molecule 12 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	12	Total	C	N	O	P	0	0
			259	116	50	81	12		

- Molecule 13 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	50	Total	C	N	O	P	0	0
			1054	471	173	360	50		

- Molecule 14 is a protein called Ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	B	213	Total	C	N	O	0	0
			1055	629	213	213		

- Molecule 15 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	75	Total	C	N	O	P	0	0
			1597	713	285	525	74		

- Molecule 16 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	y	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 17 is a RNA chain called tRNA.

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

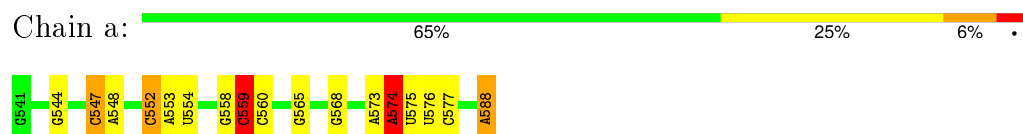
- Molecule 18 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	2	Total	C	N	O	P	0	0
			44	20	10	12	2		

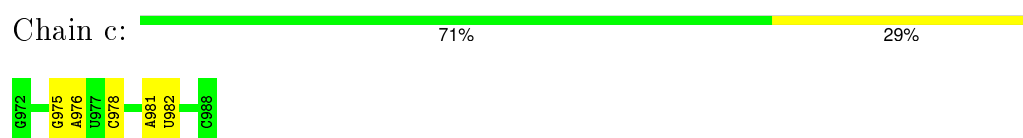
### 3 Residue-property plots

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

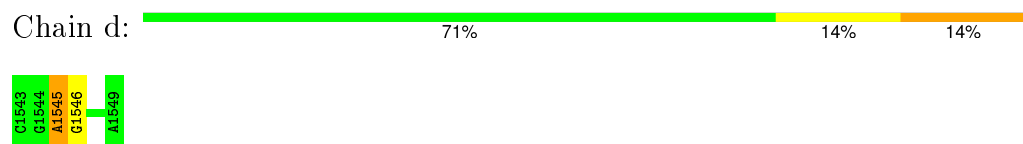
- Molecule 1: 40S ribosomal RNA fragment



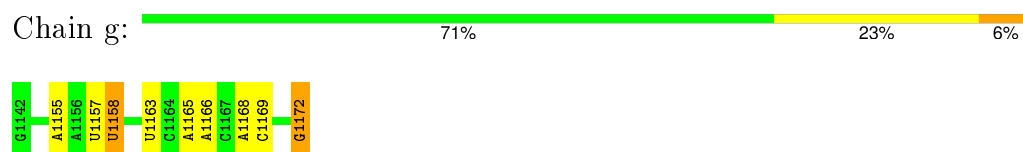
- Molecule 2: 40S ribosomal RNA fragment



- Molecule 3: 40S ribosomal RNA fragment



- Molecule 4: 40S ribosomal RNA fragment

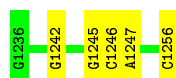


- Molecule 5: 40S ribosomal RNA fragment



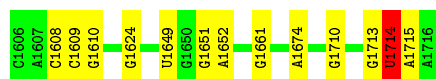
- Molecule 6: 40S ribosomal RNA fragment





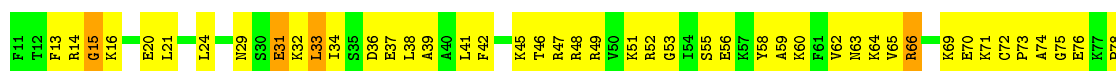
- Molecule 7: 40S ribosomal RNA fragment

Chain h: 88% 11%



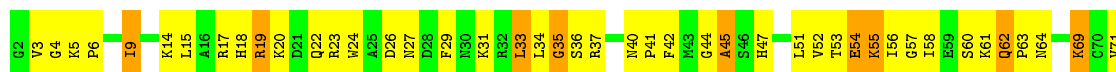
- Molecule 8: Ribosomal protein S15

Chain S: 32% 62% 5%



- Molecule 9: Ribosomal protein S23

Chain L: 33% 51% 16%



- Molecule 10: Ribosomal protein S30

Chain X: 41% 51% 7%



- Molecule 11: 60S ribosomal RNA fragment

Chain 2: 36% 49% 13%



- Molecule 12: 60S ribosomal RNA fragment



Chain 3: 

G2477  
C2478  
C2479  
A2480  
G2481  
U2482  
G2483  
A2484  
A2485  
U2486  
U2487  
A2488

- Molecule 13: 60S ribosomal RNA fragment

Chain 7: 

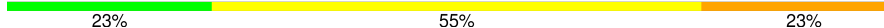
C2824  
C2825  
U2826  
U2827  
G2828  
G2829  
G2830  
C2831  
C2832  
A2833  
R2834  
U2835  
C2836  
A2837  
A2838  
G2839  
G2840  
C2841  
U2842  
U2843  
C2844  
A2845  
U2846  
A2847  
C2848  
C2849  
C2850  
A2851  
C2852  
A2853  
U2854  
U2855  
G2856  
C2857  
U2858  
U2859  
U2860  
U2861  
U2862  
G2863  
A2864  
U2865  
U2866  
C2867  
U2868  
C2869  
C2870  
G2871  
A2872  
U2873

- Molecule 14: Ribosomal protein L10a

Chain B: 

L4  
L5  
H12  
E22  
E23  
K24  
K25  
R26  
N107  
N108  
N109  
V32  
V36  
V115  
L116  
L117  
K118  
Q119  
V120  
P121  
R122  
L123  
L124  
K125  
P126  
F49  
L53  
K54  
L55  
P56  
P57  
C58  
P59  
R60  
P61  
L65  
G66  
L67  
P68  
G69  
D73  
A77  
R85  
S86  
D89  
L90  
R91  
R92  
L93  
R94  
R95  
R96  
R97  
K98  
L99  
K100  
K101  
K102  
L103  
S104  
K105  
K106  
F189  
F190  
V191  
S192  
L193  
L194  
K195  
N196  
N197  
V201  
G202  
S203  
L204  
V205  
V206  
K207  
S208  
S209  
N210  
G211  
P212  
A213  
L216  
V178  
M181  
Q182  
S186  
V187  
N188  
F189  
F190  
V191  
S192  
L193  
L194  
K195  
N196  
N197  
V201  
G202  
S203  
L204  
V205  
V206  
K207  
S208  
S209  
N210  
G211  
P212  
A213  
L216

- Molecule 15: tRNA

Chain Y: 

G1  
C2  
C3  
G4  
G5  
G6  
A7  
A8  
A9  
C10  
C11  
U12  
G15  
U16  
C17  
G18  
G19  
U20  
A21  
G22  
A23  
G24  
C25  
A26  
G27  
G28  
G29  
U33  
G34  
A35  
A36  
A37  
A38  
U39  
C40  
C41  
C42  
C43  
G44  
U45  
G46  
U47  
C48  
U51  
G52  
G53  
U54  
U55  
C56  
G57  
A58  
U59  
U60  
G63  
A64  
G65  
U66  
C67  
C68  
G69  
G70  
G71  
C72  
A73  
C74  
C75

- Molecule 16: mRNA fragment

Chain y: 

There are no outlier residues recorded for this chain.

- Molecule 17: tRNA

Chain W: 

C1  
G2  
C3  
G4  
G5  
G6  
C7  
U8  
G9  
G10  
A11  
G12  
C13  
A14  
G15  
C16  
U17A  
G18  
G19  
U20  
A21  
G22  
C23  
U24  
C25  
G26  
U27  
C28  
G29  
G30  
G31  
C32  
C33  
U34  
A35  
U36  
A37  
A38  
C39  
C40  
C41  
G42  
A43  
A44  
G45  
G46  
U47  
C48  
G49  
U50  
C51  
G52  
G53  
U54  
U55  
C56  
A57  
A58  
A59  
U60  
C61  
C62  
G63  
G64  
C65  
C66  
C67  
C68  
C69  
G70  
G71  
A72  
A73  
C74  
C75  
A76

- Molecule 18: mRNA fragment

Chain w:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	22212	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF CORRECTION OF EACH DEFOCUS GROUP VOLUME PRIOR TO BACK PROJECTION	Depositor
Microscope	FEI POLARA	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	a	0.69	2/1151 (0.2%)	0.99	8/1793 (0.4%)
10	X	0.35	0/566	0.71	0/753
11	2	1.10	4/2677 (0.1%)	1.68	69/4170 (1.7%)
12	3	0.18	0/290	0.43	0/450
13	7	1.07	2/1174 (0.2%)	2.34	33/1825 (1.8%)
14	B	0.34	0/1054	0.63	9/1468 (0.6%)
15	Y	0.47	0/1784	0.74	0/2780
16	y	0.39	0/65	0.69	0/98
17	W	2.74	133/1832 (7.3%)	2.53	181/2855 (6.3%)
18	w	0.40	0/49	0.79	0/74
2	c	0.64	0/404	0.91	1/627 (0.2%)
3	d	0.49	0/174	0.84	0/270
4	g	0.60	0/737	0.87	2/1146 (0.2%)
5	G	0.52	0/307	0.82	0/476
6	f	0.58	0/504	0.87	0/785
7	h	0.45	0/2650	0.74	1/4127 (0.0%)
8	S	0.39	0/1003	0.66	1/1342 (0.1%)
9	L	0.43	0/1114	0.74	0/1485
All	All	1.10	141/17535 (0.8%)	1.38	305/26524 (1.1%)

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
1	a	0	3
17	W	0	5
3	d	0	1
4	g	0	2
7	h	0	2
All	All	0	13

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	W	59	A	N9-C4	-13.33	1.29	1.37
17	W	2	G	C8-N7	-13.19	1.23	1.30
17	W	40	C	N1-C6	-12.02	1.29	1.37
13	7	2845	A	C6-N1	-10.99	1.27	1.35
17	W	22	G	N7-C5	-10.51	1.32	1.39

The worst 5 of 305 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	2845	A	N1-C6-N6	39.32	142.19	118.60
13	7	2845	A	C6-N1-C2	38.58	141.75	118.60
13	7	2845	A	C5-C6-N1	-33.94	100.73	117.70
13	7	2845	A	N1-C2-N3	-22.70	117.95	129.30
17	W	54	U	C5-C6-N1	13.53	129.47	122.70

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	547	C	Sidechain
1	a	559	C	Sidechain
1	a	574	A	Sidechain
3	d	1545	A	Sidechain
4	g	1157	U	Sidechain

## 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	a	1029	0	521	0	0
2	c	362	0	185	0	0
3	d	155	0	78	0	0
4	g	660	0	335	0	0
5	G	276	0	142	11	0
6	f	452	0	226	0	0
7	h	2368	0	1194	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S	985	0	1026	98	0
9	L	1097	0	1169	102	0
10	X	554	0	604	42	0
11	2	2392	0	1207	403	0
12	3	259	0	121	226	0
13	7	1054	0	532	145	0
14	B	1055	0	447	168	0
15	Y	1597	0	811	76	0
16	y	60	0	30	0	0
17	W	1640	0	824	217	0
18	w	44	0	23	0	0
All	All	16039	0	9475	1234	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 61.

The worst 5 of 1234 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)
12:3:2484:A:C6	17:W:60:U:N3	1.69	1.60
12:3:2485:A:C2	17:W:18:G:H2'	1.27	1.59
14:B:121:PRO:CB	17:W:57:A:H5'	1.27	1.58
12:3:2477:G:C8	14:B:99:LEU:CA	1.83	1.47
12:3:2484:A:C4	17:W:60:U:C4	2.04	1.45

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
8	S	123/125 (98%)	90 (73%)	25 (20%)	8 (6%)	<b>1</b> <b>25</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	L	139/141 (99%)	106 (76%)	18 (13%)	15 (11%)	0	11
10	X	66/68 (97%)	48 (73%)	12 (18%)	6 (9%)	1	17
14	B	211/213 (99%)	76 (36%)	67 (32%)	68 (32%)	0	0
All	All	539/547 (98%)	320 (59%)	122 (23%)	97 (18%)	0	4

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	S	15	GLY
9	L	45	ALA
9	L	62	GLN
9	L	87	PRO
9	L	88	MET

### 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	
8	S	105/105 (100%)	101 (96%)	4 (4%)	40	73
9	L	113/113 (100%)	102 (90%)	11 (10%)	10	40
10	X	57/57 (100%)	55 (96%)	2 (4%)	43	74
All	All	275/275 (100%)	258 (94%)	17 (6%)	27	60

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	L	55	LYS
9	L	69	LYS
9	L	106	LEU
9	L	33	LEU
9	L	132	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
8	S	133	HIS
10	X	42	ASN
9	L	78	ASN
8	S	84	HIS
9	L	98	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	47/48 (97%)	15 (31%)	0
11	2	111/112 (99%)	54 (48%)	9 (8%)
12	3	11/12 (91%)	6 (54%)	1 (9%)
13	7	49/50 (98%)	29 (59%)	5 (10%)
15	Y	74/75 (98%)	20 (27%)	1 (1%)
16	y	2/3 (66%)	0	0
17	W	76/77 (98%)	17 (22%)	0
18	w	1/2 (50%)	0	0
2	c	16/17 (94%)	4 (25%)	0
3	d	6/7 (85%)	2 (33%)	0
4	g	30/31 (96%)	8 (26%)	0
5	G	12/13 (92%)	2 (16%)	1 (8%)
6	f	20/21 (95%)	5 (25%)	0
7	h	110/111 (99%)	12 (10%)	0
All	All	565/579 (97%)	174 (30%)	17 (3%)

5 of 174 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	544	G
1	a	547	C
1	a	548	A
1	a	552	C
1	a	553	A

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	2	2281	A
11	2	2290	C
13	7	2851	A
11	2	2280	A
13	7	2859	U



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.