

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 14, 2020 – 05:02 pm BST

PDB ID	:	3LWQ
Title	:	Structure of H/ACA RNP bound to a substrate RNA containing $3MU$
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Deposited on		
Resolution	:	2.68  Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

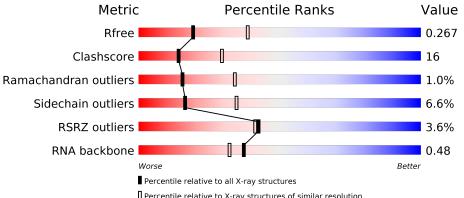
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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.



L	Percentile	relative to	X-ray	structures	of similar	resolution

Metric	Whole archive	Similar resolution
Metric	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R <sub>free</sub>	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)
RNA backbone	3102	1007 (2.98-2.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of cha	in		
1	А	340	% 63%	28%	b	• 7%
2	В	60	62%	18%	5%	15%
3	С	123	45%	50%		
4	D	58	7%	28%	17%	5%

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Mol	Chain	Length		Quality of chai	n	
			31%			
5	Ε	13	31%	31%	31%	8%

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
5	UR3	Ε	10	-	-	Х	-



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5357 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Pseudouridine synthase Cbf5.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	А	316	Total 2510	C 1623	N 428	O 449	S 10	0	0	0

• Molecule 2 is a protein called Ribosome biogenesis protein Nop10.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
2	В	51	Total	C	N 84	0	S 4	0	0	0
			4Z0	268	04	69	4			

• Molecule 3 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	119	Total 907	C 579	N 149	0 176	${ m S} { m 3}$	0	0	0

• Molecule 4 is a RNA chain called H/ACA RNA.

Mol	Chain	Residues		$\mathbf{A}^{1}$	toms			ZeroOcc	AltConf	Trace
4	D	58	Total 1236	${ m C} 552$	N 227	O 400	Р 57	0	0	0

• Molecule 5 is a RNA chain called 5'-R(\*GP\*AP\*GP\*CP\*GP\*(UR3)P\*GP\*CP\*GP\*GP\*U P\*UP\*U)-3.

Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
5	Е	13	Total 278	C 125	N 49	O 92	Р 12	0	0	0

• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

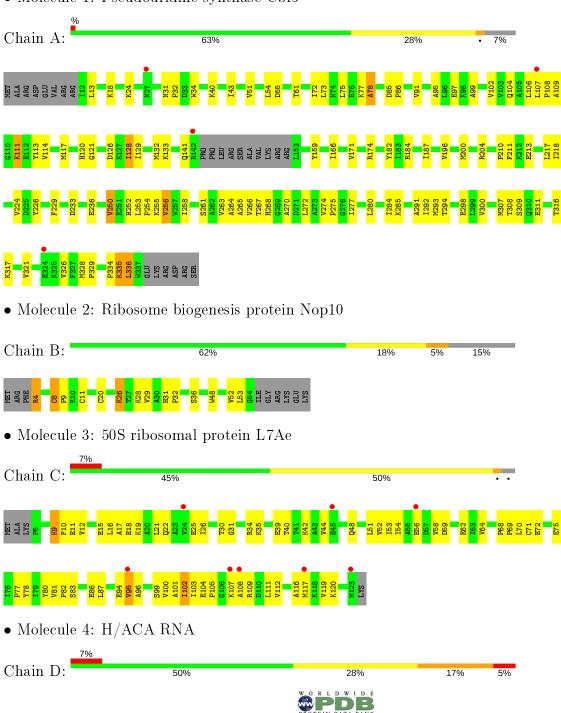


$\mathbb{N}$	ſol	Chain	Residues	Ator	ns	ZeroOcc	AltConf
	6	В	1	Total 1	Zn 1	0	0



# 3 Residue-property plots (i)

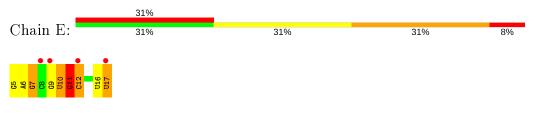
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Pseudouridine synthase Cbf5

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• Molecule 5: 5'-R(\*GP\*AP\*GP\*CP\*GP\*(UR3)P\*GP\*CP\*GP\*GP\*UP\*UP\*U)-3





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	189.15Å $64.33$ Å $84.05$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	32.97 - 2.68	Depositor
Resolution (A)	49.32 - 2.68	EDS
% Data completeness	45.2(32.97-2.68)	Depositor
(in resolution range)	85.0(49.32 - 2.68)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.09	Depositor
$< I/\sigma(I) > 1$	$3.45 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
D D.	0.211 , $0.271$	Depositor
$R, R_{free}$	0.206 , $0.267$	DCC
$R_{free}$ test set	1286 reflections $(5.09\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	65.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 57.1	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5357	wwPDB-VP
Average B, all atoms $(Å^2)$	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, UR3

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	
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.45	0/2567	0.61	0/3474
2	В	0.54	0/437	0.70	2/586~(0.3%)
3	С	0.31	0/919	0.50	0/1241
4	D	0.58	0/1381	1.29	13/2152~(0.6%)
5	Е	0.69	0/287	1.31	3/447~(0.7%)
All	All	0.49	0/5591	0.89	18/7900~(0.2%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
4	D	41	С	N1-C1'-C2'	-9.52	101.52	112.00
4	D	24	G	P-O3'-C3'	8.96	130.45	119.70
4	D	40	U	P-O3'-C3'	8.59	130.00	119.70
4	D	40	U	N1-C1'-C2'	6.58	122.56	114.00
5	Е	11	G	C1'-O4'-C4'	-6.55	104.66	109.90

There are no chirality outliers.

There are no planarity outliers.

### 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	А	2510	0	2575	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	425	0	430	12	0
3	С	907	0	952	37	0
4	D	1236	0	633	23	0
5	Е	278	0	143	20	0
6	В	1	0	0	0	0
All	All	5357	0	4733	157	0

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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 16.

The worst 5 of 157 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)
2:B:4:ARG:HG2	2:B:4:ARG:HH11	1.06	1.08
2:B:4:ARG:HG2	2:B:4:ARG:NH1	1.85	0.87
1:A:129:ILE:HG23	1:A:133:LYS:HE3	1.58	0.85
1:A:113:TYR:OH	5:E:10:UR3:H3U1	1.78	0.83
5:E:10:UR3:O2'	5:E:11:G:H5'	1.82	0.80

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 X-ray entries followed by that with respect to entries of similar resolution.

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	А	312/340~(92%)	296~(95%)	12~(4%)	4 (1%)	12 27
2	В	49/60~(82%)	46~(94%)	3~(6%)	0	100 100
3	С	117/123~(95%)	103~(88%)	13 (11%)	1 (1%)	17 37
All	All	478/523~(91%)	445~(93%)	28 (6%)	5 (1%)	15 34

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	78	ALA
1	А	91	VAL
3	С	95	VAL
1	А	336	LEU
1	А	128	ILE

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	А	267/289~(92%)	255~(96%)	12 (4%)	27 52
2	В	46/54~(85%)	41 (89%)	5 (11%)	6 13
3	С	96/99~(97%)	86~(90%)	10 (10%)	7 14
All	All	409/442~(92%)	382~(93%)	27 (7%)	16 35

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
2	В	4	ARG
2	В	28	LYS
3	С	94	GLU
2	В	11	CYS
1	А	126	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	53	ASN
1	А	63	HIS
1	А	141	GLN
1	А	268	HIS
3	С	48	GLN

5.3.3 RNA (i)



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	57/58~(98%)	14 (24%)	4(7%)
5	Е	12/13~(92%)	6~(50%)	1 (8%)
All	All	69/71~(97%)	20 (28%)	5 (7%)

 $5~{\rm of}~20~{\rm RNA}$  backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	10	A
4	D	25	А
4	D	26	U
4	D	27	С
4	D	28	А

All (5) RNA pucker outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
4	D	24	G
4	D	32	А
4	D	40	U
4	D	56	С
5	Е	11	G

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

1 non-standard protein/DNA/RNA residue is 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		
IVIOI	rybe	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
5	UR3	Е	10	5	14,22,23	0.83	0	$15,\!32,\!35$	0.94	1(6%)

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
5	UR3	Е	10	5	-	2/5/25/26	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Е	10	UR3	O4'-C1'-C2'	-2.10	103.85	106.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Ε	10	UR3	C2'-C1'-N1-C6
5	Ε	10	UR3	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Ε	10	UR3	7	0

#### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

#### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	316/340~(92%)	0.24	4 (1%) 77 78	36,62,98,154	0
2	В	51/60~(85%)	0.19	0 100 100	47, 66, 92, 102	0
3	С	119/123~(96%)	0.52	8 (6%) 17 15	57, 101, 146, 160	0
4	D	58/58~(100%)	0.22	4 (6%) 16 14	64, 86, 178, 202	0
5	Ε	12/13~(92%)	1.78	4 (33%) 0 0	128, 154, 187, 202	0
All	All	556/594~(93%)	0.33	20 (3%) 42 41	36, 72, 136, 202	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
5	Ε	17	U	5.5
1	А	142	ARG	5.0
5	Е	12	С	5.0
3	С	117	MET	4.9
3	С	107	LYS	4.6

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

$\mathbf{M}$	ol	Type	Chain	Res	Atoms	RSCC	$\mathbf{RSR}$	$\mathbf{B} ext{-factors}(\mathbf{\mathring{A}}^2)$	$\mathbf{Q}{<}0.9$
Сл		UR3	Ε	10	21/22	0.81	0.26	$139,\!152,\!178,\!190$	0

### 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.



#### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	ZN	В	61	1/1	0.96	0.33	$580,\!580,\!580,\!580$	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

