

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 06:55 pm BST

PDB ID : 1U63

Title : THE STRUCTURE OF A RIBOSOMAL PROTEIN L1-mRNA COMPLEX Authors : Nevskaya, N.; Tishchenko, S.; Gabdoulkhakov, A.; Nikonova, E.; Nikonov, O.;

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Deposited on : 2004-07-29

Resolution : 3.40 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 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

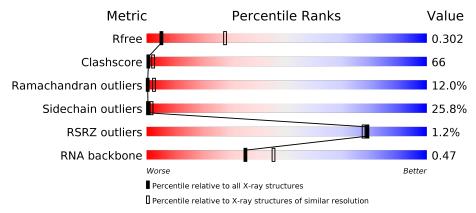
Validation Pipeline (wwPDB-VP) : 2.11

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 3.40 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 chain						
1	В	49	12%	45%	33%	10%			
1	D	49	20%	41%	29%	10%			
2	A	219	17%	56%	21%	. .			
2	С	219	15%	57%	24%	• •			



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5510 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 RNA chain called 49 NT FRAGMENT OF MRNA FOR L1.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	D	49	Total	С	N	О	Р	0	0	0
1	Б	49	1055	470	199	337	49	0		U
1	D	40	Total C N O	О	Р	0	0	0		
1	D	49	1055	470	199	337	49	0	U	U

• Molecule 2 is a protein called 50S ribosomal protein L1P.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	A	214	Total 1700	C 1088		O 302			0	0	0
2	С	214	Total 1700	C 1088	N 303	O 302	S 1	Se 6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

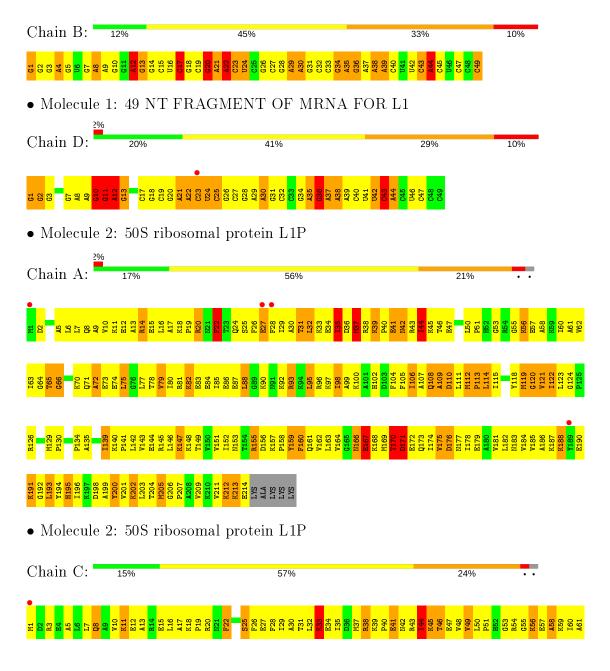
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	112	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	119	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	129	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	169	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	205	MSE	MET	MODIFIED RESIDUE	UNP P54050
С	37	MSE	MET	MODIFIED RESIDUE	UNP P54050
С	112	MSE	MET	MODIFIED RESIDUE	UNP P54050
С	119	MSE	MET	MODIFIED RESIDUE	UNP P54050
С	129	MSE	MET	MODIFIED RESIDUE	UNP P54050
С	169	MSE	MET	MODIFIED RESIDUE	UNP P54050
С	205	MSE	MET	MODIFIED RESIDUE	UNP P54050



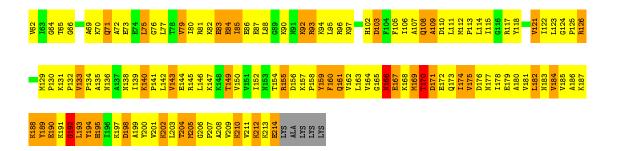
3 Residue-property plots (i)

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: 49 NT FRAGMENT OF MRNA FOR L1









4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	212.29Å 68.90Å 115.87Å	Depositor
a, b, c, α , β , γ	90.00° 122.99° 90.00°	Depositor
Resolution (Å)	8.00 - 3.40	Depositor
Resolution (A)	28.97 - 3.40	EDS
% Data completeness	92.7 (8.00-3.40)	Depositor
(in resolution range)	92.5 (28.97-3.40)	EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$2.06 \; ({\rm at} \; 3.39 {\rm \AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
D D.	0.276 , 0.302	Depositor
R, R_{free}	0.278 , 0.302	DCC
R_{free} test set	941 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.24 , 54.4	EDS
L-test for twinning ²	$< L >=0.44, < L^2>=0.26$	Xtriage
Estimated twinning fraction	0.399 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5510	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	В	0.63	$2/1181 \ (0.2\%)$	1.31	$16/1839 \ (0.9\%)$	
1	D	0.70	$2/1181 \ (0.2\%)$	1.47	23/1839 (1.3%)	
2	A	0.70	1/1718 (0.1%)	0.97	$2/2294 \ (0.1\%)$	
2	С	0.66	1/1718 (0.1%)	0.97	3/2294 (0.1%)	
All	All	0.68	$6/5798 \; (0.1\%)$	1.18	$44/8266 \ (0.5\%)$	

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	В	3	2
1	D	9	3
All	All	12	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	1	G	OP3-P	-6.92	1.52	1.61
1	D	1	G	OP3-P	-6.75	1.53	1.61
2	A	169	MSE	CG-SE	-5.76	1.75	1.95
2	С	169	MSE	CG-SE	-5.73	1.75	1.95
1	D	43	С	C4'-C3'	-5.57	1.47	1.52

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	В	20	G	N9-C1'-C2'	22.85	143.71	114.00
1	D	43	С	N1-C1'-C2'	21.21	141.57	114.00
1	D	11	G	N9-C1'-C2'	19.49	139.34	114.00
1	В	8	A	O5'-P-OP2	-17.98	89.12	110.70
1	D	43	С	O4'-C1'-N1	-16.60	94.92	108.20



5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	В	20	G	C4',C3',C1'
1	D	11	G	C4',C3',C1'
1	D	12	A	C4',C3',C1'
1	D	43	С	C4',C3',C1'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	20	G	Sidechain
1	В	44	A	Sidechain
1	D	11	G	Sidechain
1	D	12	A	Sidechain
1	D	43	С	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	В	1055	0	534	94	0
1	D	1055	0	534	75	0
2	A	1700	0	1824	256	0
2	С	1700	0	1824	287	0
All	All	5510	0	4716	678	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 66.

The worst 5 of 678 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)
1:D:23:C:H3'	1:D:24:U:H5"	1.28	1.13
1:D:43:C:H4'	1:D:44:A:OP2	1.41	1.10
1:B:34:G:H2'	1:B:35:A:H5"	1.31	1.09
2:A:62:VAL:HG12	2:A:106:ILE:HG13	1.26	1.09
2:C:44:ILE:HD12	2:C:44:ILE:H	1.15	1.05



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
2	A	212/219 (97%)	156 (74%)	29 (14%)	27 (13%)	0 2
2	С	212/219 (97%)	139 (66%)	49 (23%)	24 (11%)	0 3
All	All	424/438 (97%)	295 (70%)	78 (18%)	51 (12%)	0 3

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	${f Res}$	Type
2	A	35	ILE
2	A	82	LYS
2	A	121	VAL
2	A	122	ILE
2	A	135	ALA

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	Pe	rce	ntil	les
2	A	182/180 (101%)	134 (74%)	48 (26%)		0	1	
2	С	182/180 (101%)	136 (75%)	46 (25%)		0	2	
All	All	364/360 (101%)	270 (74%)	94 (26%)		0	2	

5 of 94 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	A	198	ASP
2	С	22	PHE
2	С	190	GLU
2	A	200	TYR
2	A	214	GLU

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

Mol	Chain	Res	Type
2	A	173	GLN
2	A	183	ASN
2	С	91	ASN
2	A	166	ASN
2	С	21	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	В	48/49 (97%)	20 (41%)	3 (6%)
1	D	48/49 (97%)	17 (35%)	5 (10%)
All	All	96/98 (97%)	37 (38%)	8 (8%)

5 of 37 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	В	2	G
1	В	4	A
1	В	8	A
1	В	12	A
1	В	13	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	11	G
1	D	43	С
1	D	36	G
1	В	44	A
1	D	12	A



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)

There are no ligands in this entry.

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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	В	49/49 (100%)	-0.56	0 100 100	56, 79, 117, 150	0
1	D	49/49 (100%)	-0.37	1 (2%) 65 64	53, 82, 139, 153	0
2	A	208/219 (94%)	-0.37	4 (1%) 66 65	9, 77, 134, 153	0
2	С	$208/219 \ (94\%)$	-0.41	1 (0%) 91 90	21, 79, 132, 146	0
All	All	514/536~(95%)	-0.40	6 (1%) 79 77	9, 79, 134, 153	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1	MET	4.7
2	С	1	MET	2.9
2	A	189	TYR	2.6
2	A	28	PHE	2.2
2	A	27	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

