



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 11:31 AM EDT

PDB ID : 1U63
Title : THE STRUCTURE OF A RIBOSOMAL PROTEIN L1-mRNA COMPLEX
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Deposited on : 2004-07-29
Resolution : 3.40 Å(reported)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

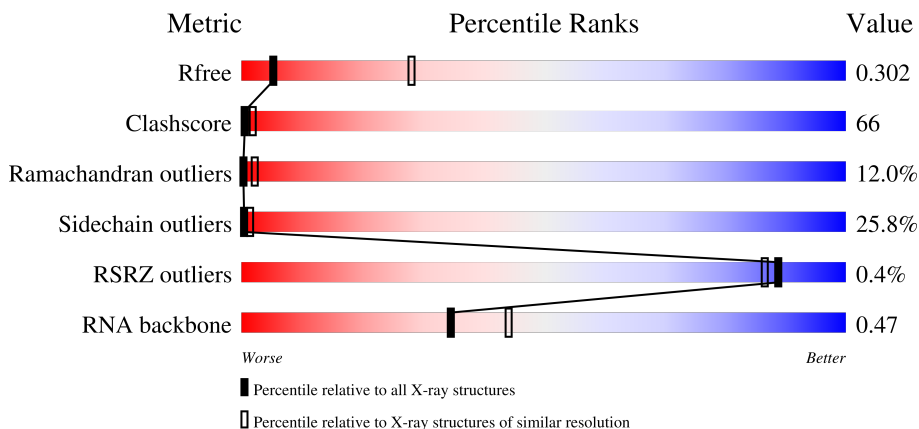
1 Overall quality at a glance

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)
RNA backbone	3690	1033 (3.80-3.00)

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 of 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 $\leq 5\%$. 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	B	49	<div> <div>2%</div> <div>12% 45% 33% 10%</div> </div>
1	D	49	<div> <div>2%</div> <div>20% 41% 29% 10%</div> </div>
2	A	219	<div> <div>17% 56% 21% . .</div> </div>
2	C	219	<div> <div>15% 57% 24% . .</div> </div>

2 Entry composition

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	Atoms					ZeroOcc	AltConf	Trace
1	B	49	Total	C	N	O	P	0	0	0
			1055	470	199	337	49			
1	D	49	Total	C	N	O	P	0	0	0
			1055	470	199	337	49			

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

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

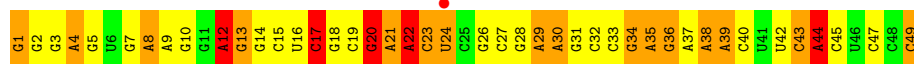
There are 12 discrepancies between the modelled and reference sequences:

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
C	37	MSE	MET	modified residue	UNP P54050
C	112	MSE	MET	modified residue	UNP P54050
C	119	MSE	MET	modified residue	UNP P54050
C	129	MSE	MET	modified residue	UNP P54050
C	169	MSE	MET	modified residue	UNP P54050
C	205	MSE	MET	modified residue	UNP P54050

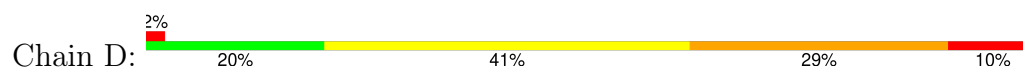
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

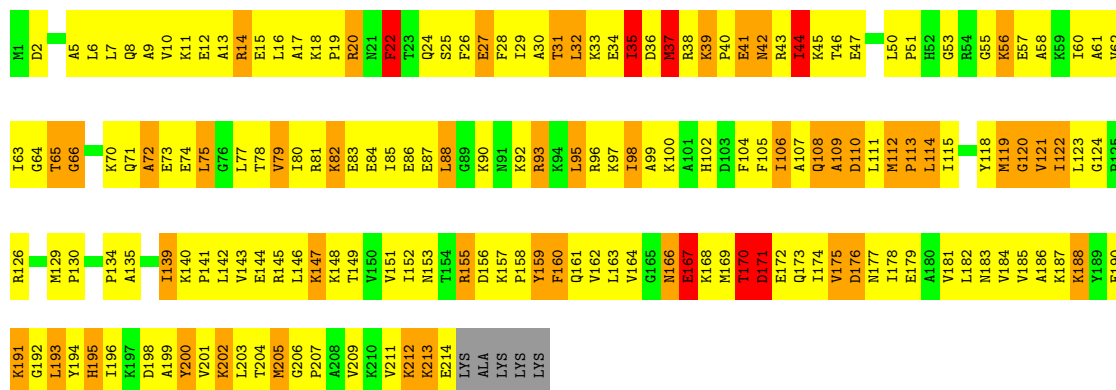
• Molecule 1: 49 NT FRAGMENT OF MRNA FOR L1



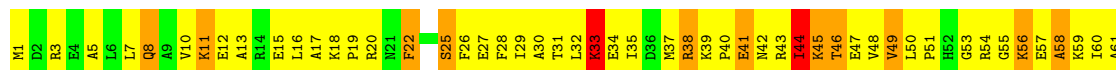
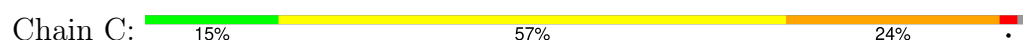
• Molecule 1: 49 NT FRAGMENT OF MRNA FOR L1



• Molecule 2: 50S ribosomal protein L1P



• Molecule 2: 50S ribosomal protein L1P



K188	M129	V62
I189	P130	I63
E190	K131	G64
G191	P132	T65
G192	V133	G66
L193	P134	
Y194	A135	A69
H195	N136	K70
I196	A137	Q71
K197	N138	A72
D198	I139	E73
A199	K140	E74
Y200	P141	L75
V201	L142	G76
K202	V143	L77
L203	E144	T78
T204	R145	V79
M205	L146	I80
G206	K147	R81
P207	K148	K82
A208	T149	E83
V209	V150	E84
K210	V151	I85
V211	I152	E86
K212	M153	E87
K213	T154	L88
E214	R155	G89
LYS	D156	K90
ALA	K157	N91
LYS	P158	K92
LYS	Y159	R93
LYS	F160	K94
	Q161	L95
	V162	R96
	L163	K97
	V164	
	G165	H102
	M166	D103
	E167	F104
	K168	F105
	M169	I106
	T170	A107
	D171	Q108
	E172	A109
	Q173	D110
	I174	L111
	V175	M112
	D176	P113
	N177	L114
	I178	I115
	E179	G116
	A180	R117
	V181	Y118
	L182	
	N183	V121
	V184	I122
	V185	L123
	A186	G124
	K187	P125
		R126

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.29Å 68.90Å 115.87Å 90.00° 122.99° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40 8.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	92.7 (8.00-3.40) 93.1 (8.00-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.302 0.278 , 0.302	Depositor DCC
R_{free} test set	2388 reflections (6.54%)	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 , 107.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.399 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	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	C	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	B	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	Observed(Å)	Ideal(Å)
1	B	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	C	169	MSE	CG-SE	-5.73	1.75	1.95
1	D	43	C	C4'-C3'	-5.57	1.47	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	G	N9-C1'-C2'	22.85	143.71	114.00
1	D	43	C	N1-C1'-C2'	21.21	141.57	114.00
1	D	11	G	N9-C1'-C2'	19.49	139.34	114.00
1	B	8	A	O5'-P-OP2	-17.98	89.12	110.70
1	D	43	C	O4'-C1'-N1	-16.60	94.92	108.20

5 of 12 chirality outliers are listed below:

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

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	G	Sidechain
1	B	44	A	Sidechain
1	D	11	G	Sidechain
1	D	12	A	Sidechain
1	D	43	C	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	B	1055	0	534	94	0
1	D	1055	0	534	75	0
2	A	1700	0	1824	256	0
2	C	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	Interatomic distance (Å)	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:32:LEU:HD12	2:C:158:PRO:HA	1.30	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	1
2	C	212/219 (97%)	139 (66%)	49 (23%)	24 (11%)	0	2
All	All	424/438 (97%)	295 (70%)	78 (18%)	51 (12%)	0	2

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	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	Percentiles	
2	A	182/180 (101%)	134 (74%)	48 (26%)	0	1
2	C	182/180 (101%)	136 (75%)	46 (25%)	0	1
All	All	364/360 (101%)	270 (74%)	94 (26%)	0	1

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

Mol	Chain	Res	Type
2	C	38	ARG
2	C	126	ARG
2	C	42	ASN
2	C	75	LEU
2	C	159	TYR

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

Mol	Chain	Res	Type
2	C	91	ASN
2	C	161	GLN
2	C	195	HIS
2	A	166	ASN
2	A	173	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	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	B	2	G
1	B	4	A
1	B	8	A
1	B	12	A
1	B	13	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	43	C
1	D	38	A
1	D	12	A
1	D	11	G
1	D	36	G

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 oligosaccharides 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, 95th 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	OWAB(Å ²)	Q<0.9
1	B	49/49 (100%)	-0.88	1 (2%) 64 55	56, 79, 117, 150	0
1	D	49/49 (100%)	-0.76	1 (2%) 64 55	53, 82, 139, 153	0
2	A	208/219 (94%)	-0.92	0 100 100	9, 77, 134, 153	0
2	C	208/219 (94%)	-0.93	0 100 100	21, 79, 132, 146	0
All	All	514/536 (95%)	-0.91	2 (0%) 89 86	9, 79, 134, 153	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	C	3.4
1	B	24	U	2.7

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 monosaccharides 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.