



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID : 1P6V
Title : Crystal structure of the tRNA domain of transfer-messenger RNA in complex with SmpB
Authors : Gutmann, S.; Haebel, P.W.; Metzinger, L.; Sutter, M.; Felden, B.; Ban, N.
Deposited on : 2003-04-30
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : trunk26865

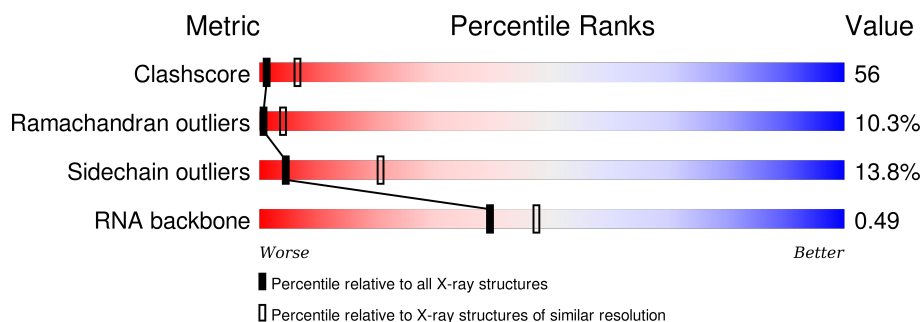
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RNA backbone	2183	1079 (3.70-2.70)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	68	
1	D	68	
2	A	156	
2	C	156	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3519 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 45-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	45	Total	C	N	O	P	0	0	0
			955	426	167	318	44			
1	D	24	Total	C	N	O	P	0	0	0
			510	228	91	168	23			

- Molecule 2 is a protein called SsrA-binding protein.

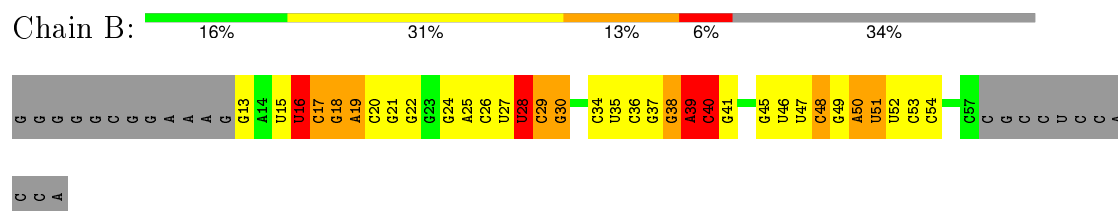
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	125	Total	C	N	O	S	0	0	0
			1027	671	179	176	1			
2	C	125	Total	C	N	O	S	0	0	0
			1027	671	179	176	1			

3 Residue-property plots

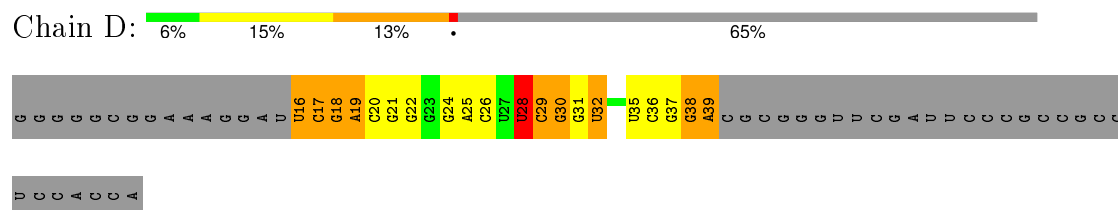
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

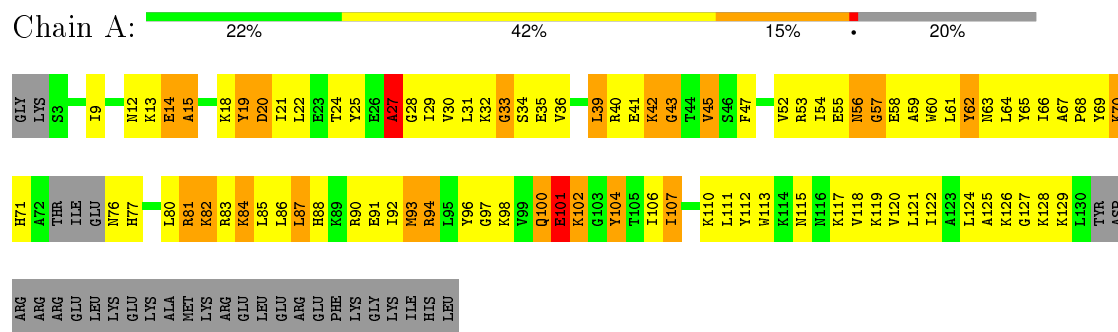
• Molecule 1: 45-MER



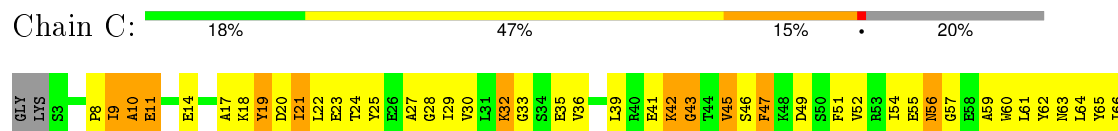
• Molecule 1: 45-MER



• Molecule 2: SsrA-binding protein



• Molecule 2: SsrA-binding protein



L130	A67
TRR	P68
ASP	Y69
ARG	K70
ARG	H71
ARG	A72
LEU	THR
GLU	I1E
LVS	GLU
LVS	N76
GLU	H77
LVS	D78
ALA	P79
MET	R81
LVS	L80
ARG	K82
GLU	R83
LEU	K84
GLU	L85
ARG	L86
GLU	L87
PHE	H88
LVS	K89
LYS	R90
LYS	E91
I1E	I92
HS	M93
LEU	R94
	L95
	Y96
	G97
	K98
	V99
	Q100
	E101
	K102
	G103
	Y104
	T105
	I106
	I107
	P108
	L109
	K110
	L111
	Y112
	W113
	V118
	K119
	V120
	L121
	L122
	A123
	L124
	A125
	K126
	G127
	K128
	K129

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.68 Å 99.68 Å 207.05 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.20	Depositor
% Data completeness (in resolution range)	94.4 (19.94-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.302 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3519	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

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 > 5$	RMSZ	# $ Z > 5$
1	B	0.53	0/1065	0.88	5/1659 (0.3%)
1	D	0.63	0/569	0.85	0/886
2	A	0.44	0/1046	0.81	4/1400 (0.3%)
2	C	0.36	0/1046	0.65	0/1400
All	All	0.48	0/3726	0.80	9/5345 (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
1	B	0	3
1	D	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	C	N1-C1'-C2'	6.63	122.62	114.00
1	B	16	U	N1-C1'-C2'	6.52	122.48	114.00
2	A	62	TYR	N-CA-C	6.31	128.04	111.00
1	B	18	G	C2'-C3'-O3'	6.12	123.49	113.70
2	A	19	TYR	N-CA-C	5.86	126.83	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	16	U	Sidechain
1	B	28	U	Sidechain

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Mol	Chain	Res	Type	Group
1	B	40	C	Sidechain
1	D	28	U	Sidechain
1	D	32	U	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	B	955	0	487	56	0
1	D	510	0	261	57	0
2	A	1027	0	1098	124	0
2	C	1027	0	1098	159	0
All	All	3519	0	2944	365	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 56.

The worst 5 of 365 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:A:84:LYS:H	2:A:84:LYS:HD3	1.16	1.08
2:C:84:LYS:H	2:C:84:LYS:HE2	0.95	1.07
2:C:107:ILE:H	2:C:107:ILE:HD13	1.23	1.00
2:A:27:ALA:HB2	2:A:120:VAL:N	1.78	0.99
2:A:27:ALA:CB	2:A:120:VAL:H	1.76	0.98

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	121/156 (78%)	87 (72%)	20 (16%)	14 (12%)	0	3
2	C	121/156 (78%)	88 (73%)	22 (18%)	11 (9%)	1	5
All	All	242/312 (78%)	175 (72%)	42 (17%)	25 (10%)	1	4

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	27	ALA
2	A	42	LYS
2	A	43	GLY
2	A	70	LYS
2	A	81	ARG

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 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	109/137 (80%)	97 (89%)	12 (11%)	8	33
2	C	109/137 (80%)	91 (84%)	18 (16%)	3	13
All	All	218/274 (80%)	188 (86%)	30 (14%)	4	21

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	32	LYS
2	C	56	ASN
2	C	107	ILE
2	C	49	ASP
2	C	63	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	115	ASN
2	C	12	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	44/68 (64%)	13 (29%)	7 (15%)
1	D	24/68 (35%)	6 (25%)	4 (16%)
All	All	68/136 (50%)	19 (27%)	11 (16%)

5 of 19 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	15	U
1	B	16	U
1	B	17	C
1	B	19	A
1	B	29	C

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	39	A
1	B	40	C
1	D	18	G
1	B	38	G
1	D	16	U

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.