wwPDB X-ray Structure Validation Summary Report (i)

Nov 4, 2023 – 07:25 AM EDT

PDB ID	:	4TZP
Title	:	As Grown, Untreated Co-crystals of the Ternary Complex Containing a T-box Stem I RNA, its cognate tRNAGly, and B. subtilis YbxF protein
Authors	:	Zhang, J.; Ferre-D'Amare, A.R.
Deposited on	:	2014-07-10
Resolution	:	8.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

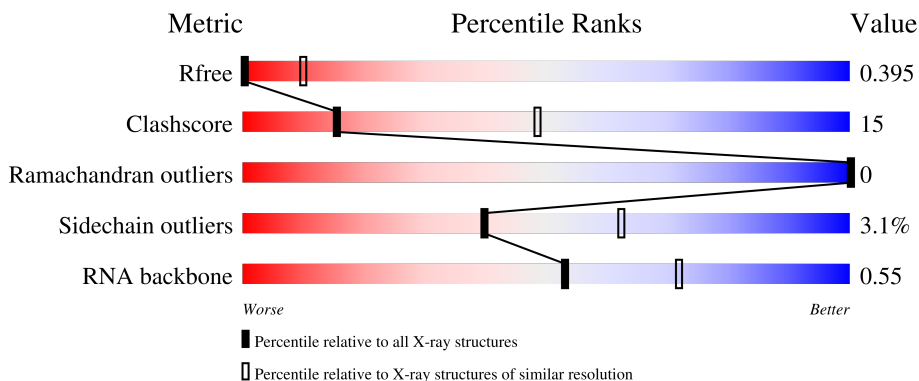|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 8.50 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	Percentile Ranks	Value
Rfree		0.395
Clashscore		15
Ramachandran outliers		0
Sidechain outliers		3.1%
RNA backbone		0.55

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RNA backbone	3102	1079 (11.50-3.00)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	82	65% / 33% / ••
1	D	82	62% / 34% / ••
2	B	75	52% / 32% / 9% / 7%
2	E	75	61% / 32% / 7%
3	C	102	46% / 42% / 10% / •
3	F	102	48% / 36% / 13% / •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8508 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 Ribosome-associated protein L7Ae-like.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	Se	0	0	0
			524	328	88	105	1	2			
1	D	81	Total	C	N	O	S	Se	0	0	0
			524	328	88	105	1	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P46350
D	1	GLY	-	expression tag	UNP P46350

- Molecule 2 is a RNA chain called engineered tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O	P	0	0	0
			1480	658	264	488	70			
2	E	75	Total	C	N	O	P	0	0	0
			1592	708	289	520	75			

- Molecule 3 is a RNA chain called glyQ T-box Stem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	102	Total	C	N	O	P	0	0	0
			2194	982	411	700	101			
3	F	102	Total	C	N	O	P	0	0	0
			2194	982	411	700	101			

3 Residue-property plots ⓘ

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. 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.
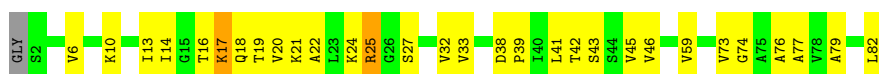
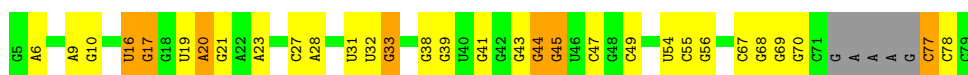- Molecule 1: Ribosome-associated protein L7Ae-like

Chain A:
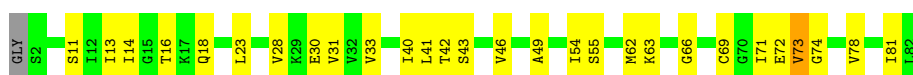
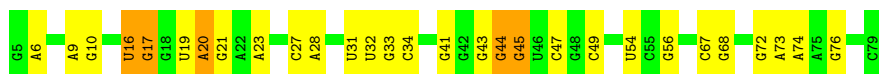- Molecule 1: Ribosome-associated protein L7Ae-like

Chain D:

- Molecule 2: engineered tRNA

Chain B:
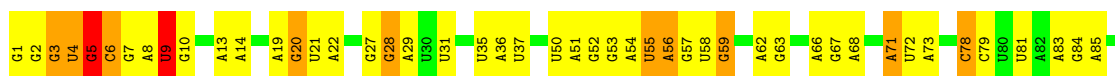

- Molecule 2: engineered tRNA

Chain E:

- Molecule 3: glyQ T-box Stem I

Chain C:

- Molecule 3: glyQ T-box Stem I

Chain F:

48%   36%   13%   •

G1 G2 G3 U4 G5 C6 G7 A8 U9 G10 A11 G12 A13 A14 A19 G20 U21 A22 G27 G28 A29 U30 U31 U48 C49 U50 A51 G52 G53 A54 U55 A56 G57 U58 G59 A62 G63 A66 G67 A68 A71 U72 A73 C78 C79 U80 U81 A82 A83 G84 A85 G88

C91 U92 U93 C94 G95 A96 G97 C98 C102
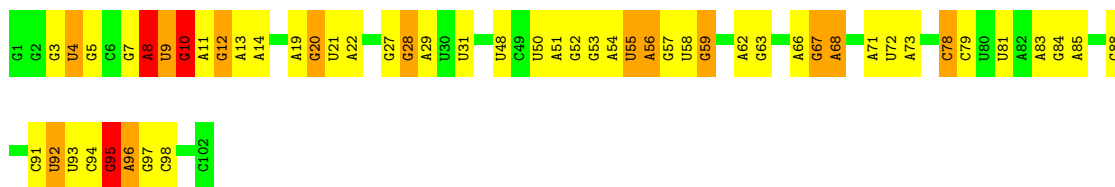
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	108.73Å 108.75Å 291.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 8.50 48.64 – 8.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.63-8.50) 94.8 (48.64-8.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 8.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.267 , 0.373 0.308 , 0.395	Depositor DCC
R_{free} test set	160 reflections (9.69%)	wwPDB-VP
Wilson B-factor (Å^2)	525.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.10 , -71.3	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.180 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8508	wwPDB-VP
Average B, all atoms (Å^2)	480.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

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	A	0.35	0/523	0.59	0/709
1	D	0.55	0/523	0.86	2/709 (0.3%)
2	B	0.21	0/1652	0.77	2/2572 (0.1%)
2	E	0.14	0/1780	0.70	1/2775 (0.0%)
3	C	0.28	0/2461	0.86	9/3838 (0.2%)
3	F	0.50	3/2461 (0.1%)	1.15	28/3838 (0.7%)
All	All	0.35	3/9400 (0.0%)	0.90	42/14441 (0.3%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	95	G	N9-C4	10.30	1.46	1.38
3	F	10	G	N1-C2	-5.66	1.33	1.37
3	F	8	A	N9-C8	5.20	1.42	1.37

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	95	G	C4-N9-C1'	13.78	144.42	126.50
3	F	95	G	N3-C4-C5	-13.71	121.74	128.60
3	F	95	G	N3-C4-N9	12.45	133.47	126.00
3	F	10	G	N3-C2-N2	12.25	128.47	119.90
3	F	95	G	C8-N9-C1'	-11.88	111.56	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	VAL	Peptide

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	524	0	505	31	0
1	D	524	0	505	65	0
2	B	1480	0	750	17	0
2	E	1592	0	804	11	0
3	C	2194	0	1101	38	0
3	F	2194	0	1101	77	0
All	All	8508	0	4766	187	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 15.

The worst 5 of 187 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:21:LYS:O	1:D:25:ARG:NH1	1.81	1.13
1:D:25:ARG:NH1	3:F:96:A:N7	2.00	1.07
2:B:70:G:H1	2:B:77:C:H42	1.05	1.01
3:F:94:C:N4	3:F:95:G:O6	2.01	0.94
1:D:16:THR:O	1:D:19:THR:OG1	1.90	0.89

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	A	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
1	D	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
All	All	158/164 (96%)	148 (94%)	10 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	48/63 (76%)	48 (100%)	0	100	100
1	D	48/63 (76%)	45 (94%)	3 (6%)	18	43
All	All	96/126 (76%)	93 (97%)	3 (3%)	40	62

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	25	ARG
1	D	45	VAL
1	D	59	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	68/75 (90%)	15 (22%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	74/75 (98%)	17 (22%)	1 (1%)
3	C	101/102 (99%)	27 (26%)	0
3	F	101/102 (99%)	26 (25%)	0
All	All	344/354 (97%)	85 (24%)	2 (0%)

5 of 85 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	A
2	B	17	G
2	B	19	U
2	B	20	A
2	B	21	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	16	U
2	E	16	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 monosaccharides 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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.