



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:29 AM GMT

PDB ID : 1TN1
Title : CRYSTALLOGRAPHIC AND BIOCHEMICAL INVESTIGATION OF THE
LEAD(II)-CATALYZED HYDROLYSIS OF YEAST PHENYLALANINE
TRNA
Authors : Dewan, J.C.; Brown, R.S.; Hingerty, B.E.; Klug, A.
Deposited on : 1986-12-04
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

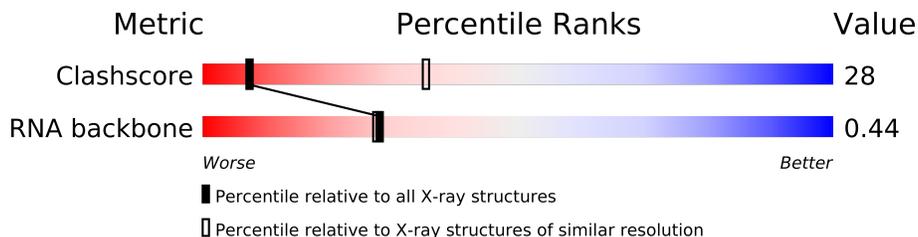
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	79885	1594 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	76	

2 Entry composition (i)

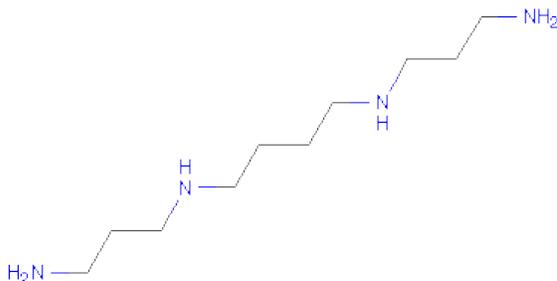
There are 5 unique types of molecules in this entry. The entry contains 1781 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TRNAPHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	76	1652	746	294	536	76	0	0	0

- Molecule 2 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	14	10	4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	5	5	5	0	0

- Molecule 4 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Pb 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total 107	O 107	0	0

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: TRNAPHE

Chain A:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.70Å 33.20Å 63.00Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.227 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1781	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

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: 5MU, OMC, MG, OMG, H2U, YG, PB, 2MG, 5MC, 1MA, M2G, 7MG, SPM, PSU

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	4.46	249/1487 (16.7%)	5.81	472/2315 (20.4%)

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	9

The worst 5 of 249 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	G	C8-N7	24.19	1.45	1.30
1	A	53	G	C8-N7	23.51	1.45	1.30
1	A	19	G	C8-N7	23.30	1.45	1.30
1	A	4	G	C8-N7	23.17	1.44	1.30
1	A	3	G	C8-N7	22.44	1.44	1.30

The worst 5 of 472 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	G	N3-C4-C5	-30.49	113.36	128.60
1	A	45	G	N3-C4-C5	-29.98	113.61	128.60
1	A	51	G	N3-C4-C5	-29.19	114.00	128.60
1	A	20	G	N3-C4-C5	-28.66	114.27	128.60
1	A	22	G	N3-C4-C5	-28.41	114.39	128.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	G	Sidechain
1	A	21	A	Sidechain
1	A	24	G	Sidechain
1	A	27	C	Sidechain
1	A	38	A	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1652	0	858	64	12
2	A	14	0	25	13	0
3	A	5	0	0	0	0
4	A	3	0	0	1	0
5	A	107	0	0	40	8
All	All	1781	0	883	71	13

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 71 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:65:G:H1'	5:A:115:HOH:O	1.19	1.26
4:A:84:PB:PB	5:A:182:HOH:O	0.82	1.24
1:A:3:G:OP2	5:A:152:HOH:O	1.53	1.22
2:A:77:SPM:C8	5:A:182:HOH:O	1.91	1.16
1:A:3:G:P	5:A:152:HOH:O	2.03	1.16

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:124:HOH:O	5:A:126:HOH:O[2_656]	0.90	1.30
1:A:13:C:O2'	5:A:94:HOH:O[1_545]	1.28	0.92
1:A:13:C:C2'	5:A:94:HOH:O[1_545]	1.37	0.83
1:A:13:C:C3'	5:A:94:HOH:O[1_545]	1.39	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:C:N4	5:A:154:HOH:O[2_646]	1.60	0.60

5.3 Torsion angles

5.3.1 Protein backbone [i](#)

There are no protein chains in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein chains in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	75/76 (98%)	17 (22%)	2 (2%)

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	A
1	A	13	C
1	A	16	H2U
1	A	17	H2U
1	A	18	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	18	G
1	A	46	7MG

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

14 non-standard protein/DNA/RNA residues are 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		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	10	1	24,26,27	1.64	5 (20%)	32,38,41	6.18	9 (28%)
1	H2U	A	16	1	19,21,22	1.35	3 (15%)	27,30,33	1.62	7 (25%)
1	H2U	A	17	1	19,21,22	1.49	1 (5%)	27,30,33	1.75	5 (18%)
1	M2G	A	26	1	25,27,28	1.84	5 (20%)	34,40,43	4.50	13 (38%)
1	OMC	A	32	1,4	20,22,23	1.27	2 (10%)	25,31,34	1.97	8 (32%)
1	OMG	A	34	1	24,26,27	1.38	4 (16%)	32,38,41	5.50	8 (25%)
1	YG	A	37	1,4	40,42,43	2.09	12 (30%)	50,62,65	18.87	18 (36%)
1	PSU	A	39	1	19,21,22	1.50	4 (21%)	23,30,33	1.47	3 (13%)
1	5MC	A	40	1	20,22,23	1.25	1 (5%)	26,32,35	1.74	3 (11%)
1	7MG	A	46	1	24,26,27	2.37	5 (20%)	34,39,42	1.80	9 (26%)
1	5MC	A	49	1	20,22,23	1.80	6 (30%)	26,32,35	1.67	5 (19%)
1	5MU	A	54	1	20,22,23	1.43	3 (15%)	25,32,35	2.03	3 (12%)
1	PSU	A	55	1	19,21,22	1.54	4 (21%)	23,30,33	1.29	2 (8%)
1	1MA	A	58	1	23,25,26	1.90	3 (13%)	32,37,40	2.56	7 (21%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	10	1	-	1/10/27/28	0/1/3/3
1	H2U	A	16	1	-	0/8/38/39	0/2/2/2
1	H2U	A	17	1	-	1/8/38/39	0/2/2/2
1	M2G	A	26	1	-	0/12/29/30	0/1/3/3
1	OMC	A	32	1,4	-	0/8/27/28	0/2/2/2
1	OMG	A	34	1	-	0/10/27/28	0/1/3/3
1	YG	A	37	1,4	-	0/25/42/43	0/1/4/4
1	PSU	A	39	1	-	0/8/25/26	0/2/2/2
1	5MC	A	40	1	-	0/6/25/26	0/2/2/2
1	7MG	A	46	1	-	0/8/37/38	0/1/3/3
1	5MC	A	49	1	-	0/6/25/26	0/2/2/2
1	5MU	A	54	1	-	0/6/25/26	0/2/2/2
1	PSU	A	55	1	-	0/8/25/26	0/2/2/2
1	1MA	A	58	1	-	0/8/25/26	0/1/3/3

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	7MG	C8-N9	-8.76	1.39	1.46
1	A	58	1MA	C6-N1	-6.42	1.28	1.38
1	A	37	YG	O23-C21	-6.16	1.25	1.34
1	A	17	H2U	P-OP1	5.35	1.52	1.46
1	A	37	YG	P-OP1	4.85	1.52	1.46

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	YG	C6-C5-N7	-132.67	127.18	134.24
1	A	10	2MG	C6-C5-N7	-31.87	129.85	134.14
1	A	34	OMG	C6-C5-N7	-28.52	130.30	134.14
1	A	26	M2G	C6-C5-N7	-21.54	131.24	134.14
1	A	10	2MG	C5-C4-N3	-8.16	114.11	125.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	17	H2U	OP2-P-O5'-C5'
1	A	10	2MG	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SPM	A	77	4	13,13,13	0.62	0	12,12,12	1.02	1 (8%)

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
2	SPM	A	77	4	-	0/11/11/11	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	77	SPM	C11-N10-C9	-2.04	105.90	113.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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