



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:36 PM GMT

PDB ID : 2NQP
Title : Crystal structure of pseudouridine synthase TruA in complex with leucyl tRNA
Authors : Hur, S.; Stroud, R.M.
Deposited on : 2006-10-31
Resolution : 3.50 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>

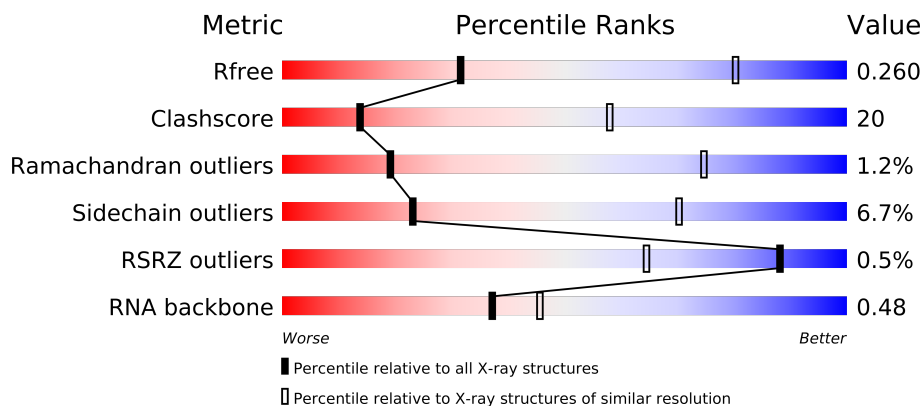
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 3.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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.

Mol	Chain	Length	Quality of chain
1	F	87	
2	A	270	
2	B	270	
2	C	270	
2	D	270	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9765 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 transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	71	Total	C	N	O	P	21	0	0
			1441	636	256	480	69			

- Molecule 2 is a protein called tRNA pseudouridine synthase A.

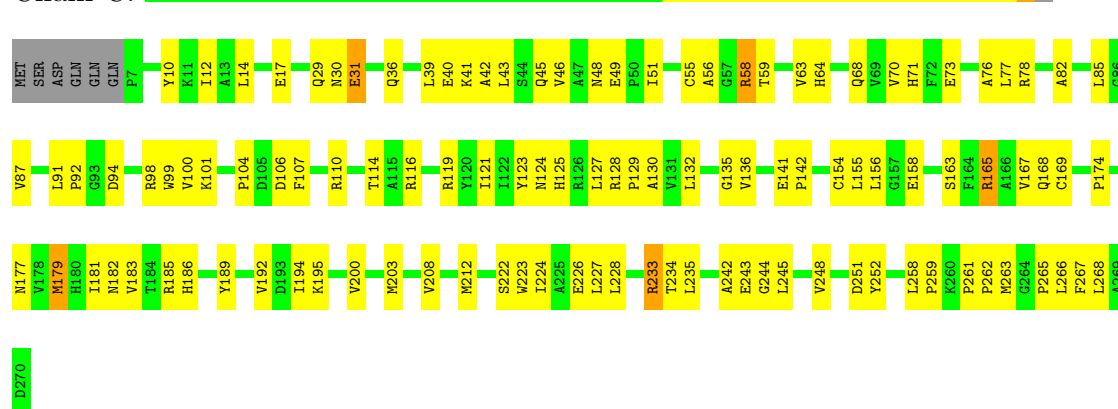
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	264	Total	C	N	O	S	0	0	0
			2088	1327	379	374	8			
2	B	264	Total	C	N	O	S	0	0	0
			2083	1325	377	373	8			
2	C	264	Total	C	N	O	S	0	0	0
			2057	1306	373	370	8			
2	D	263	Total	C	N	O	S	18	0	0
			2090	1328	381	373	8			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	K	0	0
			1	1		
3	F	5	Total	K	0	0
			5	5		

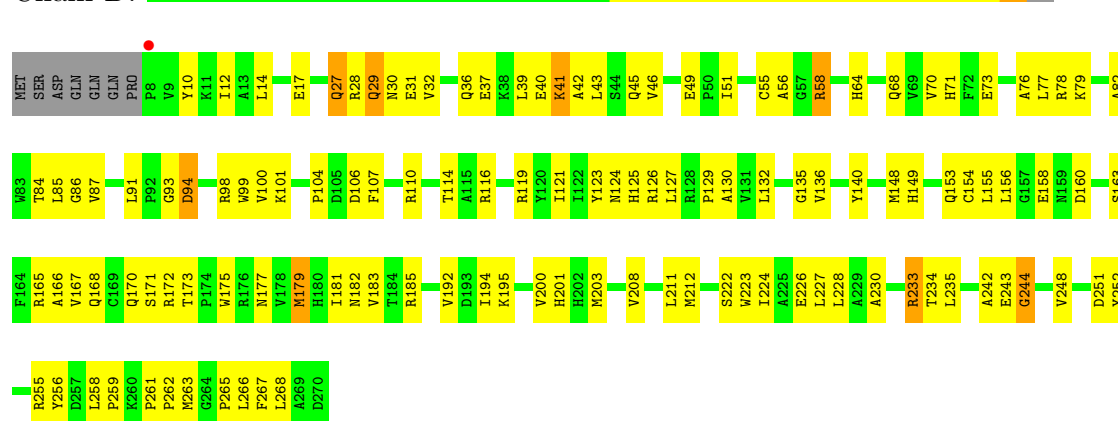
- Molecule 2: tRNA pseudouridine synthase A

Chain C:



- Molecule 2: tRNA pseudouridine synthase A

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.28Å 128.59Å 159.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 77.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-3.50) 92.4 (77.07-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.279 0.240 , 0.260	Depositor DCC
R_{free} test set	2812 reflections (11.15%)	DCC
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 12.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 30274 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9765	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	F	0.63	2/1604 (0.1%)	0.88	5/2498 (0.2%)
2	A	0.52	0/2142	0.65	0/2915
2	B	0.51	0/2139	0.65	0/2912
2	C	0.47	0/2112	0.64	0/2881
2	D	0.49	0/2145	0.62	0/2917
All	All	0.52	2/10142 (0.0%)	0.69	5/14123 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	46(L)	U	C2-N3	-5.32	1.34	1.37
1	F	18	G	O3'-P	-5.20	1.54	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	19	G	O4'-C1'-N9	-8.26	101.59	108.20
1	F	46(L)	U	OP1-P-OP2	-6.44	109.94	119.60
1	F	19	G	OP1-P-OP2	-6.44	109.94	119.60
1	F	46(K)	C	P-O3'-C3'	-5.32	113.32	119.70
1	F	46(L)	U	C6-N1-C2	5.11	124.07	121.00

There are no chirality outliers.

There are no planarity outliers.

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	F	1441	0	11	15	0
2	A	2088	0	2039	93	0
2	B	2083	0	2039	85	0
2	C	2057	0	1982	86	0
2	D	2090	0	2059	97	0
3	C	1	0	0	0	0
3	F	5	0	0	0	0
All	All	9765	0	8130	354	0

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 20.

The worst 5 of 354 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:130:ALA:HB3	2:B:17:GLU:HG2	1.46	0.95
2:A:17:GLU:HG2	2:B:130:ALA:HB3	1.51	0.92
2:C:130:ALA:HB1	2:D:94:ASP:O	1.70	0.88
2:A:41:LYS:CA	2:A:42:ALA:N	2.41	0.83
2:D:165:ARG:HG2	2:D:166:ALA:H	1.43	0.82

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	
2	A	260/270 (96%)	230 (88%)	28 (11%)	2 (1%)	27	82
2	B	262/270 (97%)	228 (87%)	31 (12%)	3 (1%)	21	77
2	C	262/270 (97%)	229 (87%)	29 (11%)	4 (2%)	15	69
2	D	261/270 (97%)	226 (87%)	31 (12%)	4 (2%)	15	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1045/1080 (97%)	913 (87%)	119 (11%)	13 (1%)	19 75

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	243	GLU
2	B	243	GLU
2	C	243	GLU
2	D	243	GLU
2	C	168	GLN

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	214/223 (96%)	200 (94%)	14 (6%)	24 71
2	B	214/223 (96%)	198 (92%)	16 (8%)	19 65
2	C	207/223 (93%)	198 (96%)	9 (4%)	40 84
2	D	216/223 (97%)	198 (92%)	18 (8%)	16 59
All	All	851/892 (95%)	794 (93%)	57 (7%)	23 70

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	172	ARG
2	C	77	LEU
2	D	171	SER
2	B	173	THR
2	B	233	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	170	GLN
2	C	45	GLN

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Mol	Chain	Res	Type
2	D	153	GLN
2	B	218	ASN
2	C	64	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	F	65/87 (74%)	14 (21%)	3 (4%)

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	F	7	A
1	F	9	G
1	F	10	G
1	F	14	A
1	F	17	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	F	18	G
1	F	58	A
1	F	60	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	F	71/87 (81%)	0.53	5 (7%)	16	7	27, 80, 197, 241	5 (7%)
2	A	264/270 (97%)	-0.09	0	100	100	8, 18, 43, 60	0
2	B	264/270 (97%)	-0.10	0	100	100	8, 21, 42, 64	0
2	C	264/270 (97%)	0.17	0	100	100	8, 34, 67, 81	0
2	D	263/270 (97%)	0.14	1 (0%)	90	71	10, 30, 53, 76	5 (1%)
All	All	1126/1167 (96%)	0.06	6 (0%)	88	64	8, 27, 67, 241	10 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	70	G	7.0
1	F	67	C	2.8
1	F	3	C	2.4
2	D	8	PRO	2.4
1	F	45(D)	G	2.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	K	F	79	1/1	0.21	-	74,74,74,74	0
3	K	F	78	1/1	0.12	-	28,28,28,28	0
3	K	F	81	1/1	0.32	-	67,67,67,67	0
3	K	C	271	1/1	0.15	-	26,26,26,26	0
3	K	F	80	1/1	0.11	-	72,72,72,72	0
3	K	F	77	1/1	0.73	-	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.