



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:46 PM GMT

PDB ID : 1NGS
Title : COMPLEX OF TRANSKETOLASE WITH THIAMIN DIPHOSPHATE,
CA2+ AND ACCEPTOR SUBSTRATE ERYTHROSE-4-PHOSPHATE
Authors : Nilsson, U.; Lindqvist, Y.; Schneider, G.
Deposited on : 1996-09-25
Resolution : 2.40 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>

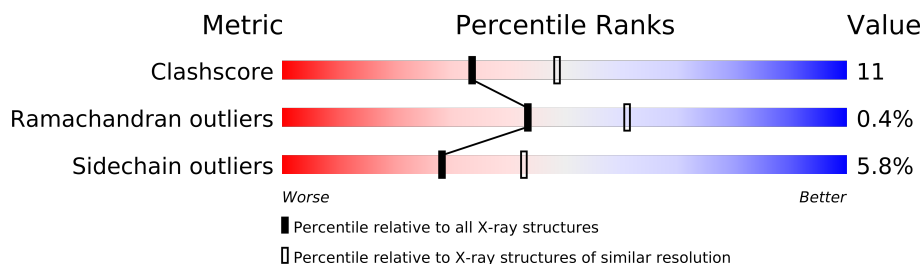
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **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 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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	680	
1	B	680	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10928 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.

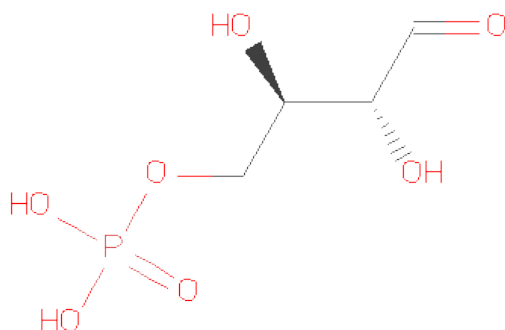
- Molecule 1 is a protein called TRANSKETOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	678	Total	C	N	O	S	0	0	0
			5198	3312	884	990	12			
1	B	678	Total	C	N	O	S	0	0	0
			5198	3312	884	990	12			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

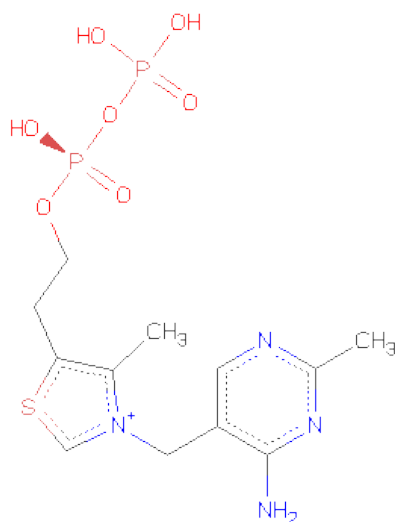
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ERYTHROSE-4-PHOSPHATE (three-letter code: E4P) (formula: C₄H₉O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			12	4	7	1		
3	B	1	Total	C	O	P	0	0
			12	4	7	1		

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	237	Total	O	0	0
			237	237		
5	B	217	Total	O	0	0
			217	217		

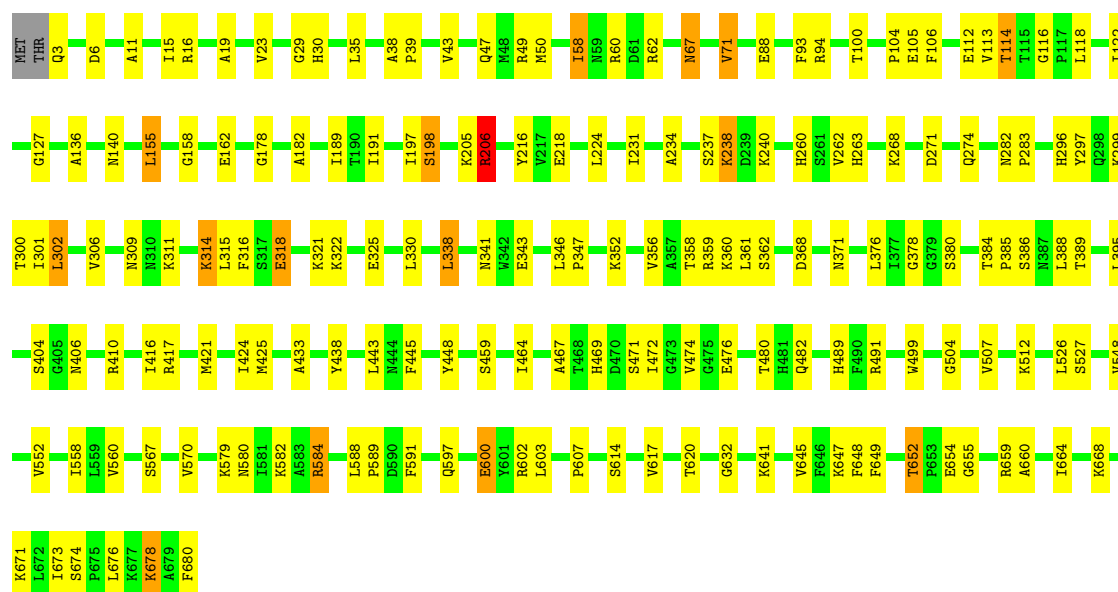
3 Residue-property plots

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.

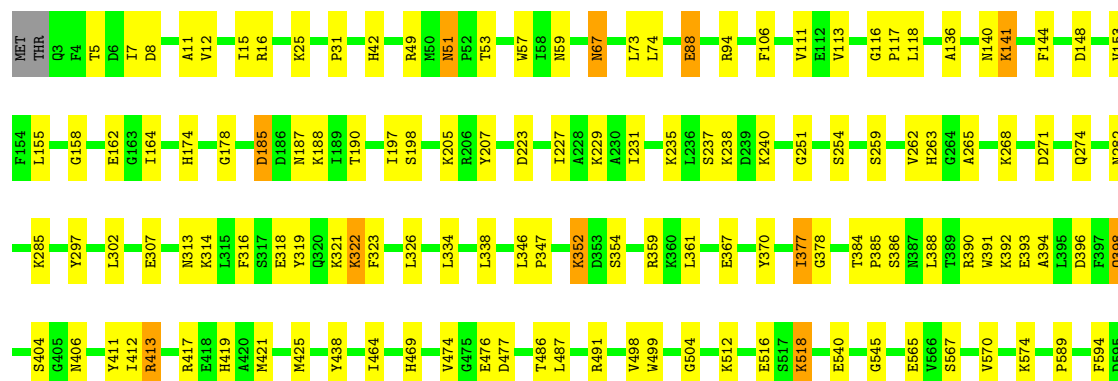
• Molecule 1: TRANSKETOLASE

Chain A: 



• Molecule 1: TRANSKETOLASE

Chain B: 



K596	E600	Y601	R602	M613	S614	V615	E616	V617	K625	Q629	R635	F636	F646	K647	F648	F649	E658	R659	K662	K671	S674	K677	F680
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.50Å 113.30Å 160.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10928	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, E4P, TPP

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	0.50	1/5324 (0.0%)	0.82	6/7230 (0.1%)
1	B	0.59	4/5324 (0.1%)	0.81	7/7230 (0.1%)
All	All	0.55	5/10648 (0.0%)	0.81	13/14460 (0.1%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	GLU	CG-CD	14.33	1.73	1.51
1	B	88	GLU	CB-CG	13.39	1.77	1.52
1	B	88	GLU	CD-OE1	-10.22	1.14	1.25
1	A	600	GLU	CD-OE1	-6.28	1.18	1.25
1	B	600	GLU	CD-OE1	-5.45	1.19	1.25

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	GLU	OE1-CD-OE2	-9.87	111.45	123.30
1	A	206	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	58	ILE	CA-CB-CG1	-9.17	93.58	111.00
1	A	206	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	88	GLU	CG-CD-OE2	6.40	131.11	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	TYR	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	5198	0	5139	133	1
1	B	5198	0	5139	104	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	7	1	0
3	B	12	0	7	1	0
4	A	26	0	16	3	0
4	B	26	0	16	4	0
5	A	237	0	0	13	2
5	B	217	0	0	13	0
All	All	10928	0	10324	229	2

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 11.

The worst 5 of 229 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:88:GLU:CB	1:B:88:GLU:CG	1.77	1.61
1:A:58:ILE:CG1	1:A:58:ILE:CD1	1.84	1.51
1:A:58:ILE:HG12	5:A:981:HOH:O	1.47	1.09
1:B:307:GLU:HG3	5:B:1094:HOH:O	1.58	0.99
1:A:652:THR:HG22	1:A:655:GLY:H	1.35	0.91

All (2) 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)
1:B:313:ASN:OD1	5:A:1009:HOH:O[3_555]	2.12	0.08
1:A:579:LYS:NZ	5:A:954:HOH:O[3_555]	2.17	0.03

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	676/680 (99%)	645 (95%)	28 (4%)	3 (0%)	43 61
1	B	676/680 (99%)	644 (95%)	29 (4%)	3 (0%)	43 61
All	All	1352/1360 (99%)	1289 (95%)	57 (4%)	6 (0%)	43 61

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	B	617	VAL
1	A	617	VAL
1	B	198	SER
1	A	198	SER

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	552/554 (100%)	519 (94%)	33 (6%)	27 41
1	B	552/554 (100%)	521 (94%)	31 (6%)	30 45
All	All	1104/1108 (100%)	1040 (94%)	64 (6%)	28 43

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	LEU
1	B	73	LEU
1	B	625	LYS
1	A	600	GLU
1	A	678	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	ASN
1	B	51	ASN
1	B	120	GLN
1	A	580	ASN
1	B	149	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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, 2 are monoatomic - leaving 4 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
4	TPP	A	682	2	27,27,27	2.20	4 (14%)	40,40,40	1.77	11 (27%)
3	E4P	A	900	-	11,11,11	1.58	2 (18%)	15,15,15	1.51	3 (20%)
4	TPP	B	682	2	27,27,27	2.14	5 (18%)	40,40,40	2.23	14 (35%)
3	E4P	B	900	-	11,11,11	1.46	2 (18%)	15,15,15	1.58	2 (13%)

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
4	TPP	A	682	2	-	0/17/17/17	0/2/2/2
3	E4P	A	900	-	-	0/11/12/12	0/0/0/0
4	TPP	B	682	2	-	0/17/17/17	0/2/2/2
3	E4P	B	900	-	-	0/11/12/12	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	682	TPP	C4-N3	-7.94	1.30	1.39
4	B	682	TPP	C4-N3	-6.76	1.32	1.39
4	B	682	TPP	C5-S1	-5.98	1.69	1.73
4	A	682	TPP	C5-S1	-5.51	1.69	1.73
3	A	900	E4P	P-O4	-3.50	1.48	1.60

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	682	TPP	PA-O3A-PB	5.24	147.05	131.68
4	B	682	TPP	C6-C5-C4	-4.90	123.88	127.44
3	B	900	E4P	C3-C2-C1	-4.85	106.67	111.28
4	B	682	TPP	O2A-PA-O7	-4.85	84.04	108.51
4	A	682	TPP	PA-O3A-PB	4.58	145.12	131.68

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.