



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:30 PM GMT

PDB ID : 2XA2  
Title : CRYSTAL STRUCTURE OF TREHALOSE SYNTHASE TRET MUTANT  
E326A FROM P.HORIKOSHII IN COMPLEX WITH UDPG  
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Deposited on : 2010-03-26  
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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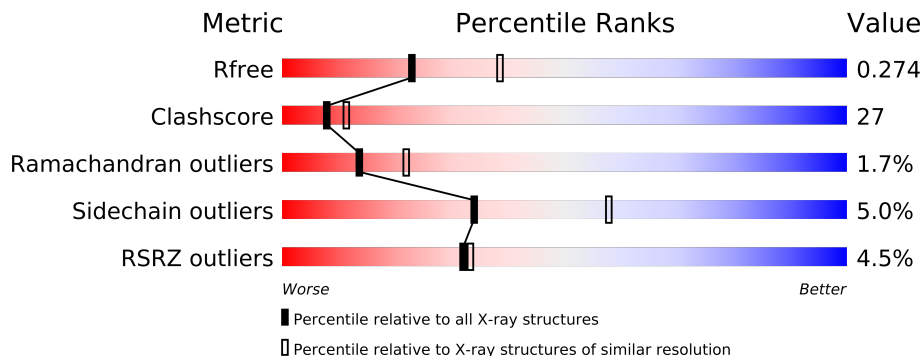
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 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	A	416	
1	B	416	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	UPG	A	1415	-	X
2	UPG	B	1415	-	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6940 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.

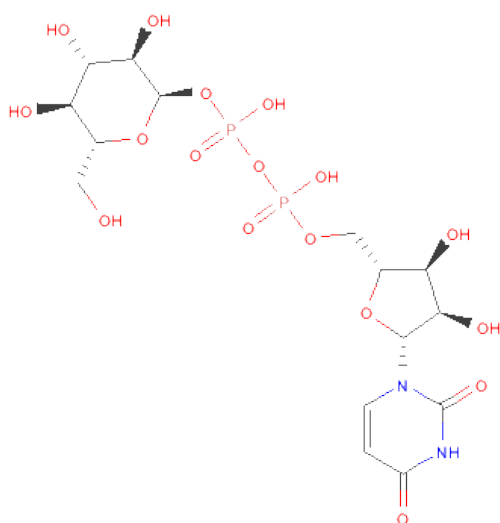
- Molecule 1 is a protein called TREHALOSE-SYNTHASE TRET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	1
			3374	2181	572	612	9			
1	B	413	Total	C	N	O	S	0	0	1
			3374	2181	572	612	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	ALA	GLU	ENGINEERED MUTATION	UNP O58762
A	372	VAL	LYS	CONFLICT	UNP O58762
B	326	ALA	GLU	ENGINEERED MUTATION	UNP O58762
B	372	VAL	LYS	CONFLICT	UNP O58762

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula:  $C_{15}H_{24}N_2O_{17}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is water.

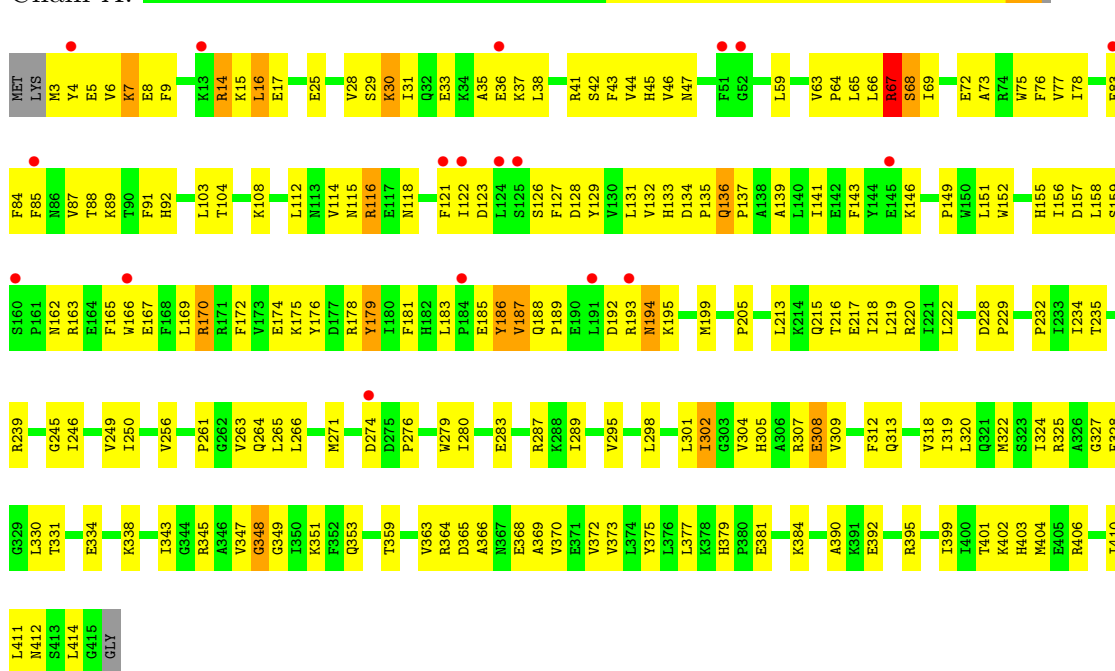
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	52	Total	O	0	0
			52	52		

### 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.

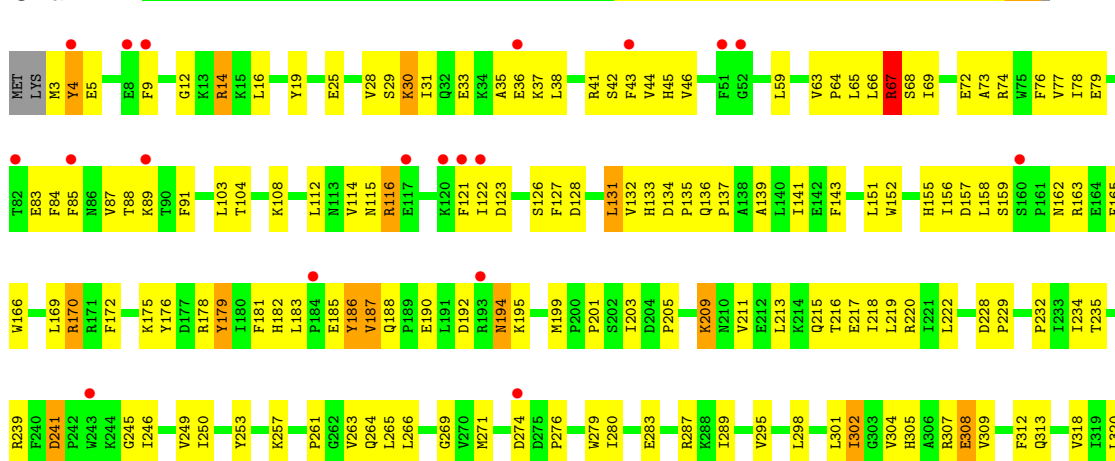
#### • Molecule 1: TREHALOSE-SYNTHASE TRET

Chain A:



#### • Molecule 1: TREHALOSE-SYNTHASE TRET

Chain B:



T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.84Å 63.14Å 91.52Å 90.00° 98.83° 90.00°	Depositor
Resolution (Å)	29.36 – 2.50 29.36 – 2.47	Depositor EDS
% Data completeness (in resolution range)	81.6 (29.36-2.50) 80.0 (29.36-2.47)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.225 , 0.275 0.221 , 0.274	Depositor DCC
$R_{free}$ test set	1256 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 28.9	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 26465 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: UPG

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	0.39	0/3451	0.79	9/4658 (0.2%)
1	B	0.39	0/3451	0.78	9/4658 (0.2%)
All	All	0.39	0/6902	0.79	18/9316 (0.2%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH1	-14.09	113.25	120.30
1	A	67	ARG	NE-CZ-NH2	13.64	127.12	120.30
1	A	170	ARG	NE-CZ-NH1	-13.34	113.63	120.30
1	B	67	ARG	NE-CZ-NH1	13.16	126.88	120.30
1	B	67	ARG	NE-CZ-NH2	-13.08	113.76	120.30

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	A	3374	0	3412	190	0
1	B	3374	0	3412	180	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	22	2	0
2	B	36	0	22	6	0
3	A	68	0	0	2	0
3	B	52	0	0	1	0
All	All	6940	0	6868	370	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 27.

The worst 5 of 370 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:343:ILE:HD13	1:B:372:VAL:HG23	1.49	0.95
1:A:343:ILE:HD13	1:A:372:VAL:HG23	1.49	0.94
1:B:228:ASP:H	1:B:264:GLN:HE22	1.16	0.94
1:A:42:SER:HB2	1:A:128:ASP:H	1.30	0.93
1:B:42:SER:HB2	1:B:128:ASP:H	1.30	0.92

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	411/416 (99%)	352 (86%)	51 (12%)	8 (2%)	12	19
1	B	411/416 (99%)	354 (86%)	51 (12%)	6 (2%)	15	25
All	All	822/832 (99%)	706 (86%)	102 (12%)	14 (2%)	14	22

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	176	TYR
1	B	68	SER
1	A	16	LEU

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Mol	Chain	Res	Type
1	B	12	GLY

### 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	370/372 (100%)	353 (95%)	17 (5%)	37	62
1	B	370/372 (100%)	350 (95%)	20 (5%)	31	53
All	All	740/744 (100%)	703 (95%)	37 (5%)	34	58

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	GLU
1	B	131	LEU
1	B	365	ASP
1	B	4	TYR
1	B	14	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	HIS
1	B	32	GLN
1	B	133	HIS
1	A	215	GLN
1	A	264	GLN

### 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 ⓘ

2 ligands 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	$\# Z  > 2$
2	UPG	A	1415	-	38,38,38	1.27	3 (7%)	54,58,58	2.17	11 (20%)
2	UPG	B	1415	-	38,38,38	1.26	3 (7%)	54,58,58	2.16	11 (20%)

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	UPG	A	1415	-	-	0/21/59/59	0/3/3/3
2	UPG	B	1415	-	-	0/21/59/59	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1415	UPG	O4C-C1C	3.83	1.47	1.41
2	B	1415	UPG	O4C-C1C	3.68	1.47	1.41
2	A	1415	UPG	C6-N1	3.03	1.40	1.35
2	B	1415	UPG	C6-N1	2.94	1.40	1.35
2	B	1415	UPG	O5'-C1'	2.05	1.47	1.41

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1415	UPG	PB-O3A-PA	-7.10	110.88	131.68
2	A	1415	UPG	PB-O3A-PA	-7.03	111.07	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1415	UPG	O5C-PA-O1A	-6.04	85.73	109.37
2	A	1415	UPG	C2-N1-C1C	6.03	121.99	118.21
2	A	1415	UPG	O5C-PA-O1A	-6.02	85.79	109.37

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	413/416 (99%)	0.29	18 (4%) 33 34	4, 39, 76, 91	0
1	B	413/416 (99%)	0.26	19 (4%) 31 32	4, 39, 73, 83	0
All	All	826/832 (99%)	0.27	37 (4%) 32 33	4, 39, 74, 91	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	TYR	4.4
1	B	52	GLY	4.2
1	A	121	PHE	4.0
1	A	52	GLY	4.0
1	A	125	SER	3.7

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	UPG	A	1415	36/36	0.37	5.62	92,110,115,116	0
2	UPG	B	1415	36/36	0.36	4.82	86,108,113,114	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.