



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:37 AM GMT

PDB ID : 2OWC  
Title : Structure of a covalent intermediate in Thermus thermophilus amylomaltase  
Authors : Barends, T.R.M.; Bultema, J.B.; Kaper, T.; van der Maarel, M.J.E.C.; Dijkhuizen, L.; Dijkstra, B.W.  
Deposited on : 2007-02-16  
Resolution : 2.05 Å(reported)

This is a full wwPDB validation 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>

---

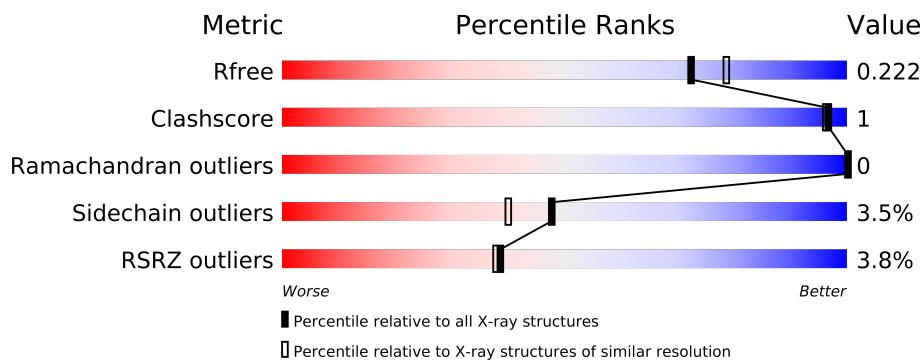
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.05 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	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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	502	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4539 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.

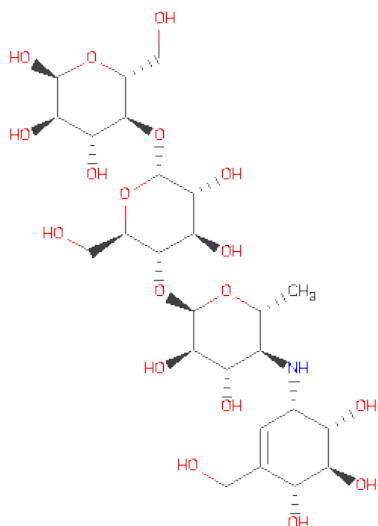
- Molecule 1 is a protein called 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	499	4083	2653	711	708	11	0	2	0

There are 5 discrepancies between the modelled and reference sequences:

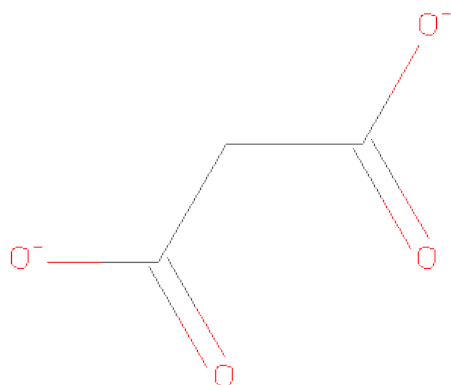
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q72J82
A	-1	SER	-	CLONING ARTIFACT	UNP Q72J82
A	0	HIS	-	CLONING ARTIFACT	UNP Q72J82
A	?	SUI	ASP	MODIFIED RESIDUE	UNP Q72J82
A	370	SUI	GLY	MODIFIED RESIDUE	UNP Q72J82

- Molecule 2 is malonate ion (three-letter code: ACR) (formula:  $C_{25}H_{43}NO_{18}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	32	19	1	12	0	0

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	409	Total 411	O 411	0	2

i

- Molecule 1: 4-alpha-glucanotransferase

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.41Å 92.41Å 154.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.62 – 2.05 29.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.62-2.05) 100.0 (29.59-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.186 , 0.216 0.194 , 0.222	Depositor DCC
$R_{free}$ test set	3061 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 38.4	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60598 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: GOL, MLI, SUI, ACR

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	0.41	0/4212	0.57	0/5726

There are no bond length outliers.

There are no bond angle outliers.

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	4083	0	3941	8	0
2	A	32	0	31	0	0
3	A	7	0	2	0	0
4	A	6	0	8	0	0
5	A	411	0	0	4	0
All	All	4539	0	3982	8	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 1.

All (8) close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:291[B]:ARG:NH1	5:A:3000[B]:HOH:O	1.61	0.96
1:A:291[B]:ARG:NH2	5:A:3000[B]:HOH:O	2.06	0.87
1:A:416:ARG:HD3	1:A:416:ARG:O	1.89	0.73
1:A:291[B]:ARG:CZ	5:A:3000[B]:HOH:O	2.11	0.71
1:A:433:TRP:HA	1:A:436:MET:HE3	1.88	0.54
1:A:156:TRP:HA	1:A:159:TRP:CD2	2.49	0.48
1:A:416:ARG:C	1:A:416:ARG:HD3	2.37	0.45
1:A:291[A]:ARG:NH2	5:A:3000[A]:HOH:O	1.76	0.43

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	498/502 (99%)	493 (99%)	5 (1%)	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	402/402 (100%)	388 (96%)	14 (4%)	48	40

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	34	ARG
1	A	37	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	171	LEU
1	A	173	GLU
1	A	239	ARG
1	A	249	ASP
1	A	280	LEU
1	A	289	LEU
1	A	296	ARG
1	A	331	VAL
1	A	373	GLU
1	A	465	TYR
1	A	500	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	SUI	A	370	1	11,11,12	9.11	3 (27%)	12,15,17	2.28	5 (41%)

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
1	SUI	A	370	1	-	0/2/19/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	SUI	C2A-N2	-21.67	1.30	1.47
1	A	370	SUI	O-C	20.61	1.25	1.11
1	A	370	SUI	C1-N2	-3.00	1.34	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	SUI	CB-CG-N2	3.90	110.59	108.12
1	A	370	SUI	OD-CG-CB	-3.59	122.31	127.31
1	A	370	SUI	O1-C1-N2	2.94	128.20	124.14
1	A	370	SUI	OD-CG-N2	2.72	127.09	123.89
1	A	370	SUI	C2A-N2-CG	2.16	124.94	123.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates i

There are no carbohydrates in this entry.

## 5.6 Ligand geometry i

3 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	$\# Z  > 2$
4	GOL	A	5001	-	5,5,5	0.39	0	5,5,5	0.36	0
2	ACR	A	600	1	33,34,47	0.65	0	46,50,70	1.26	4 (8%)
3	MLI	A	6001	-	2,6,6	2.01	1 (50%)	0,7,7	0.00	-

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	GOL	A	5001	-	-	0/4/4/4	0/0/0/0
2	ACR	A	600	1	1/1/14/22	0/12/69/98	0/3/3/4
3	MLI	A	6001	-	-	0/0/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	6001	MLI	C1-C2	2.12	1.51	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	ACR	C1A-N4B-C4B	4.73	124.64	116.56
2	A	600	ACR	O5C-C5C-C4C	-3.40	106.20	110.48
2	A	600	ACR	C6A-C5A-C4A	2.55	118.17	114.53
2	A	600	ACR	C2B-C3B-C4B	-2.12	107.43	110.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	600	ACR	C1C

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	499/502 (99%)	-0.10	19 (3%) 38 38	16, 24, 43, 60	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	TYR	6.2
1	A	251	PHE	5.2
1	A	254	THR	5.2
1	A	467	GLY	5.0
1	A	469	PRO	4.8
1	A	2	GLU	4.1
1	A	253	GLU	4.1
1	A	384	HIS	3.6
1	A	470	SER	3.3
1	A	500	LEU	2.9
1	A	1	MET	2.7
1	A	252	SER	2.6
1	A	84	ARG	2.5
1	A	122	GLU	2.4
1	A	249	ASP	2.4
1	A	307	SER	2.4
1	A	86	GLU	2.2
1	A	313	GLU	2.2
1	A	121	PRO	2.1

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

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
1	SUI	A	370	11/12	0.07	-0.74	22,24,25,26	0

### 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
3	MLI	A	6001	7/7	0.13	2.00	38,38,39,39	0
4	GOL	A	5001	6/6	0.17	0.27	34,38,39,40	0
2	ACR	A	600	32/44	0.10	-0.55	18,22,30,32	0

### 6.5 Other polymers

There are no such residues in this entry.