



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:27 am BST

PDB ID : 5WQS  
Title : Crystal structure of Apo Beta-Amylase from Sweet potato  
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Deposited on : 2016-11-28  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

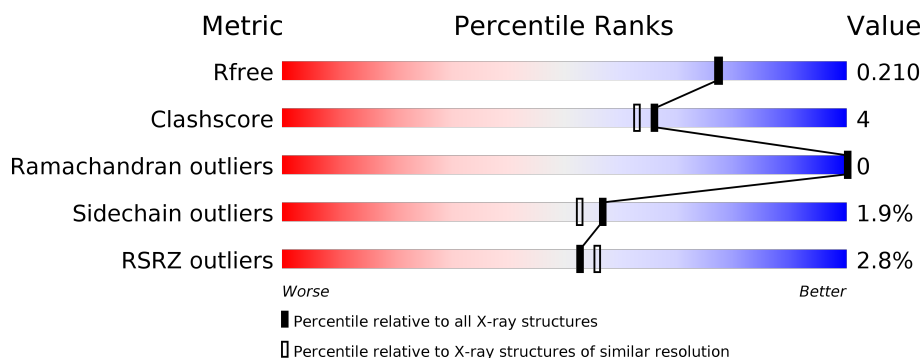
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	498	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

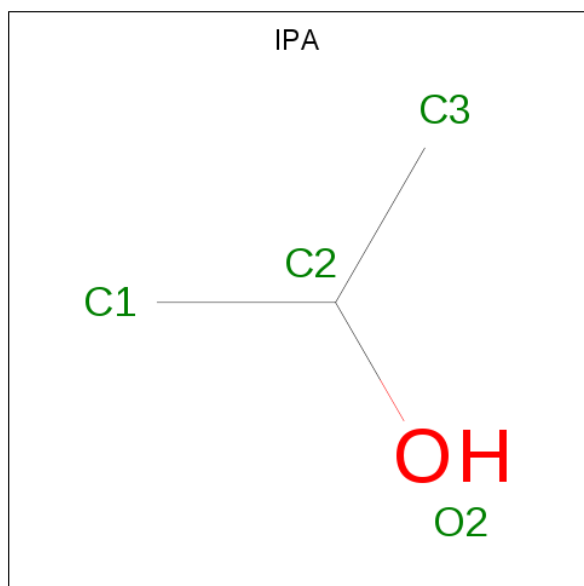
- Molecule 1 is a protein called Beta-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	496	3934	2516	662	733	23	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	LEU	ASN	conflict	UNP P10537

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

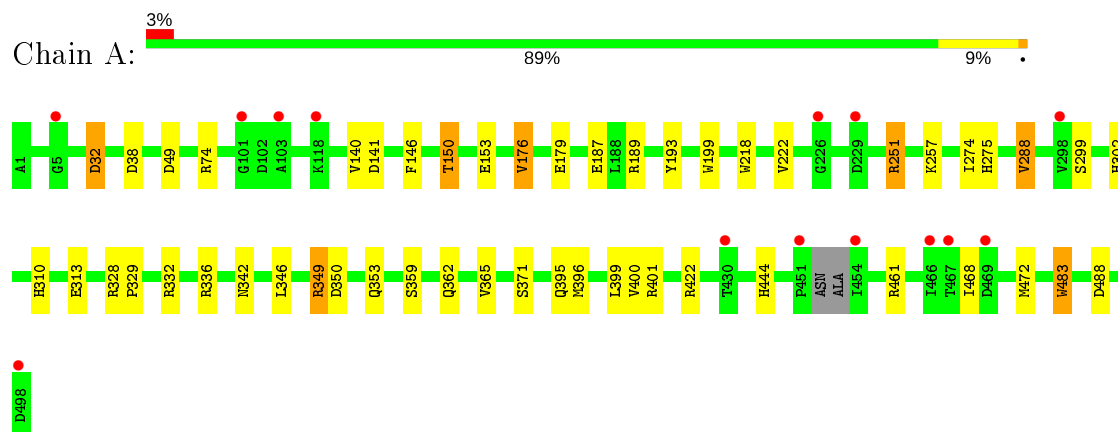
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	267	Total 267	O 267	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Beta-amylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.35Å 128.35Å 66.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.76 – 1.90 29.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (90.76-1.90) 99.2 (29.59-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.166 , 0.202 0.176 , 0.210	Depositor DCC
$R_{free}$ test set	2213 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.93	3/4041 (0.1%)	1.14	22/5483 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	SER	CB-OG	8.89	1.53	1.42
1	A	401	ARG	CD-NE	-5.92	1.36	1.46
1	A	488	ASP	CB-CG	-5.29	1.40	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	ARG	NE-CZ-NH2	-23.69	108.45	120.30
1	A	401	ARG	NE-CZ-NH1	22.49	131.55	120.30
1	A	336	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	A	251	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	251	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	A	74	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	336	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	349	ARG	NE-CZ-NH2	9.67	125.13	120.30
1	A	288	VAL	CB-CA-C	-9.16	94.00	111.40
1	A	74	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	288	VAL	CG1-CB-CG2	7.91	123.55	110.90
1	A	461	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	A	401	ARG	CD-NE-CZ	7.08	133.51	123.60
1	A	488	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	349	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	176	VAL	CG1-CB-CG2	6.21	120.84	110.90
1	A	461	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	472	MET	CG-SD-CE	5.41	108.85	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	336	ARG	CG-CD-NE	-5.20	100.88	111.80
1	A	332	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	176	VAL	N-CA-CB	-5.03	100.43	111.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3934	0	3816	31	0
2	A	4	0	8	0	0
3	A	267	0	0	3	1
All	All	4205	0	3824	31	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:HG21	3:A:833:HOH:O	1.67	0.94
1:A:350:ASP:H	1:A:362:GLN:HE21	1.26	0.81
1:A:399:LEU:HD23	1:A:483:TRP:HE1	1.47	0.79
1:A:399:LEU:HD21	3:A:811:HOH:O	1.87	0.74
1:A:141:ASP:OD2	1:A:275:HIS:HD2	1.70	0.73
1:A:140:VAL:HG11	1:A:146:PHE:HZ	1.56	0.69
1:A:346:LEU:O	1:A:399:LEU:HD12	1.93	0.69
1:A:187:GLU:OE1	1:A:299:SER:HB3	1.94	0.68
1:A:140:VAL:HG11	1:A:146:PHE:CZ	2.29	0.67
1:A:444:HIS:HD2	3:A:705:HOH:O	1.87	0.57
1:A:140:VAL:O	1:A:140:VAL:HG12	2.07	0.53
1:A:349:ARG:HH21	1:A:395:GLN:NE2	2.10	0.49
1:A:218:TRP:CZ2	1:A:222:VAL:HG11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:OE1	1:A:342[B]:ASN:ND2	2.47	0.47
1:A:179:GLU:OE1	1:A:342[A]:ASN:ND2	2.40	0.47
1:A:302:HIS:HD2	1:A:359:SER:OG	1.98	0.47
1:A:49:ASP:OD2	1:A:444:HIS:HE1	1.98	0.46
1:A:310:HIS:HD2	1:A:313:GLU:OE1	1.99	0.46
1:A:140:VAL:CG1	1:A:146:PHE:CE2	2.99	0.46
1:A:274:ILE:HD11	1:A:468:ILE:HD11	1.97	0.46
1:A:353:GLN:HG3	1:A:359:SER:OG	2.16	0.46
1:A:150:THR:HG22	1:A:153:GLU:CG	2.47	0.45
1:A:189:ARG:HD3	1:A:299:SER:OG	2.16	0.44
1:A:399:LEU:CD2	1:A:483:TRP:HE1	2.24	0.44
1:A:365:VAL:HG11	1:A:399:LEU:HD22	1.99	0.44
1:A:193:TYR:HB2	1:A:199:TRP:CD2	2.54	0.43
1:A:396:MET:O	1:A:400:VAL:HG13	2.20	0.42
1:A:32:ASP:OD1	1:A:32:ASP:N	2.54	0.41
1:A:328:ARG:N	1:A:329:PRO:CD	2.83	0.40
1:A:187:GLU:OE1	1:A:299:SER:CB	2.66	0.40
1:A:140:VAL:O	1:A:140:VAL:CG1	2.68	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
3:A:796:HOH:O	3:A:796:HOH:O[8_556]	1.30	0.90

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	493/498 (99%)	485 (98%)	8 (2%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	416/416 (100%)	408 (98%)	8 (2%)	57	53

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	38	ASP
1	A	150	THR
1	A	176	VAL
1	A	251	ARG
1	A	257	LYS
1	A	288	VAL
1	A	483	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	99	ASN
1	A	275	HIS
1	A	278	GLN
1	A	302	HIS
1	A	310	HIS
1	A	362	GLN
1	A	395	GLN
1	A	429	GLN
1	A	432	ASN
1	A	444	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z  > 2$
2	IPA	A	501	-	3,3,3	0.87	0	3,3,3	0.46	0

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	496/498 (99%)	-0.01	14 (2%) 53 56	20, 30, 52, 88	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ALA	4.3
1	A	454	ILE	4.3
1	A	101	GLY	3.6
1	A	466	ILE	3.6
1	A	467	THR	2.8
1	A	229	ASP	2.7
1	A	498	ASP	2.2
1	A	298	VAL	2.2
1	A	226	GLY	2.2
1	A	118	LYS	2.2
1	A	430	THR	2.1
1	A	469	ASP	2.1
1	A	5	GLY	2.1
1	A	451	PRO	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IPA	A	501	4/4	0.82	0.14	39,42,44,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.