



# wwPDB X-ray Structure Validation Summary Report

Sep 11, 2014 – 09:21 PM EDT

PDB ID : 2AAA  
Title : CALCIUM BINDING IN ALPHA-AMYLASES: AN X-RAY DIFFRACTION STUDY AT 2.1 ANGSTROMS RESOLUTION OF TWO ENZYMES FROM ASPERGILLUS  
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Deposited on : 1991-02-27  
Resolution : 2.12 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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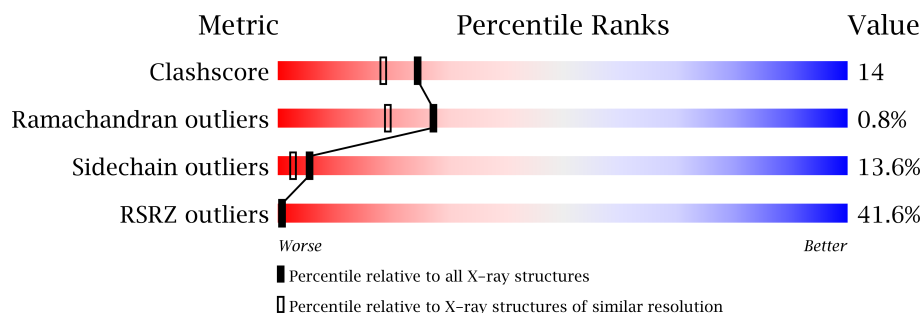
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
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) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.12 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	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (2.14-2.10)

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	484	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4021 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 ALPHA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3669	2321	580	751	17			

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

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

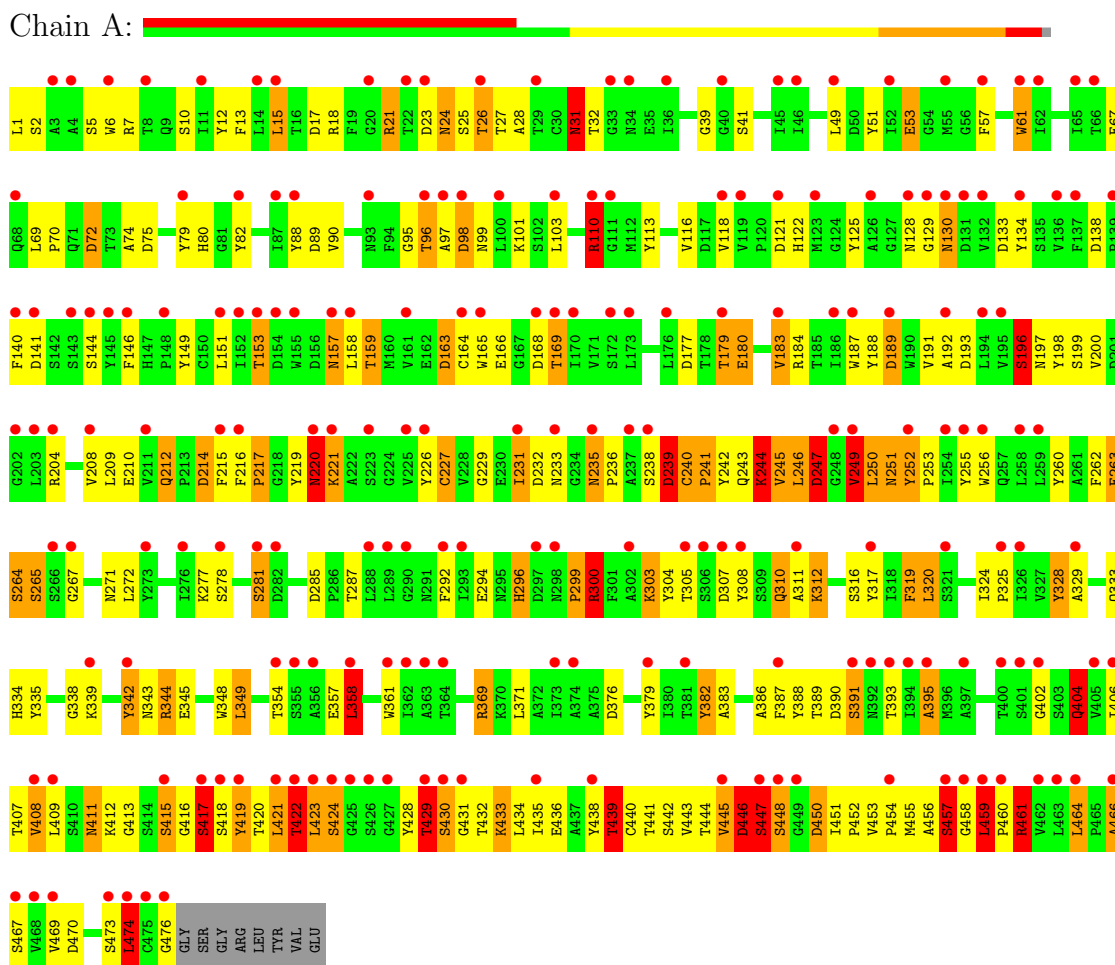
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	350	Total	O	0	0
			350	350		

### 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: ALPHA-AMYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.10Å 98.30Å 138.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.12 24.57 – 2.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.12) 97.7 (24.57-2.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	19.71 (at 2.11Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.169 , (Not available) 0.368 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 91.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31209 reflections	Xtriage
$F_o, F_c$ correlation	0.68	EDS
Total number of atoms	4021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: CA

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	1.28	6/3764 (0.2%)	2.71	307/5149 (6.0%)

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	A	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	ASP	N-CA	8.42	1.63	1.46
1	A	2	SER	CB-OG	6.81	1.51	1.42
1	A	476	GLY	C-O	6.75	1.34	1.23
1	A	238	SER	CB-OG	5.87	1.49	1.42
1	A	180	GLU	CD-OE1	-5.50	1.19	1.25

The worst 5 of 307 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASN	CA-CB-CG	23.12	164.27	113.40
1	A	110	ARG	NE-CZ-NH1	20.86	130.73	120.30
1	A	247	ASP	N-CA-CB	20.38	147.28	110.60
1	A	239	ASP	CB-CA-C	19.24	148.88	110.40
1	A	304	TYR	CB-CG-CD2	-18.73	109.76	121.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	21	ARG	Sidechain
1	A	300	ARG	Sidechain
1	A	344	ARG	Sidechain
1	A	461	ARG	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	3669	0	3423	99	246
2	A	2	0	0	0	0
3	A	350	0	0	15	41
All	All	4021	0	3423	99	249

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 14.

The worst 5 of 99 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:422:THR:HG22	1:A:450:ASP:HB3	1.34	1.06
1:A:436:GLU:OE1	1:A:439:THR:HB	1.59	1.03
1:A:95:GLY:HA2	3:A:581:HOH:O	1.65	0.96
1:A:402:GLY:H	1:A:404:GLN:HE22	1.19	0.91
1:A:296:HIS:H	1:A:296:HIS:HD2	1.22	0.88

The worst 5 of 249 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:A:442:SER:N	1:A:461:ARG:NH1[3.554]	0.51	1.69
1:A:420:THR:C	1:A:451:ILE:O[3.554]	0.58	1.62
1:A:436:GLU:OE1	1:A:441:THR:OG1[3.554]	0.64	1.56
1:A:419:TYR:CD2	1:A:450:ASP:O[3.554]	0.66	1.54
1:A:416:GLY:O	1:A:431:GLY:C[3.554]	0.67	1.53

## 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	474/484 (98%)	452 (95%)	18 (4%)	4 (1%)	27	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	ASP
1	A	417	SER
1	A	446	ASP
1	A	457	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	403/409 (98%)	348 (86%)	55 (14%)	5	3

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	296	HIS
1	A	447	SER
1	A	264	SER
1	A	277	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	A	235	ASN
1	A	251	ASN
1	A	333	GLN
1	A	233	ASN
1	A	392	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 2 ligands modelled in this entry, 2 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, 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	476/484 (98%)	1.97	198 (41%) 1 1	8, 16, 31, 50	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	ILE	7.6
1	A	356	ALA	6.1
1	A	430	SER	5.7
1	A	363	ALA	5.7
1	A	148	PRO	5.5

### 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(Å <sup>2</sup> )	Q<0.9
2	CA	A	486	1/1	0.15	-1.74	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	485	1/1	0.08	-4.51	17,17,17,17	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.