

# wwPDB X-ray Structure Validation Summary Report (i)

#### Mar 4, 2024 – 01:03 PM EST

PDB ID : 1JI2

Title : Improved X-ray Structure of Thermoactinomyces vulgaris R-47 alpha-Amylase

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Deposited on : 2001-06-28

Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Xtriage (Phenix) : 1.13 EDS : 2.36

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)

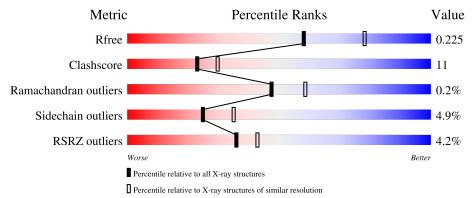
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	585	78%	20%	•
1	В	585	79%	18%	•



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10450 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 ALPHA-AMYLASE II.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	585	Total	С	N	О	S	0	0	0
1	Λ	969	4776	3056	831	874	15	0		0
1	B	585	Total	С	N	О	S	0	0	0
1	ъ	300	4776	3056	831	874	15		U	

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

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

• Molecule 3 is water.

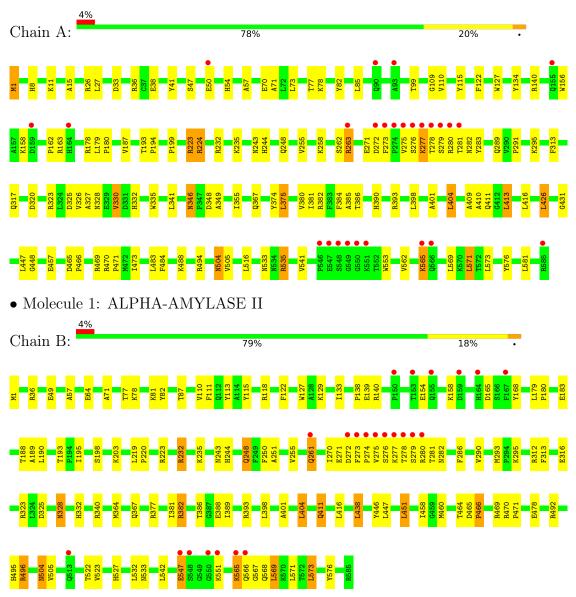
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	454	Total O 454 454	0	0
3	В	442	Total O 442 442	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ALPHA-AMYLASE II





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	112.46Å 117.68Å 112.67Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	37.05 - 2.30	Depositor
Resolution (A)	37.05 - 2.30	EDS
% Data completeness	99.7 (37.05-2.30)	Depositor
(in resolution range)	99.8 (37.05-2.30)	EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.82  (at  2.29Å)	Xtriage
Refinement program	CNS	Depositor
$R, R_{free}$	0.179 , $0.224$	Depositor
it, it free	0.180 , $0.225$	DCC
$R_{free}$ test set	6776 reflections $(10.13%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36 , 51.2	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.32$	Xtriage
	0.016  for  -h,l,k	
	0.012  for -k,-h,-l	
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
	0.003 for $l,h,k$	
	0.003 for k,l,h	
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10450	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

#### 5.1 Standard geometry (i)

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.34	0/4906	0.58	0/6641
1	В	0.34	0/4906	0.58	1/6641 (0.0%)
All	All	0.34	0/9812	0.58	$1/13282 \ (0.0\%)$

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	В	113	TYR	N-CA-C	-5.21	96.93	111.00

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	4776	0	4607	109	0
1	В	4776	0	4607	106	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	454	0	0	8	0
3	В	442	0	0	11	0
All	All	10450	0	9214	213	0



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 11.

The worst 5 of 213 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:275:VAL:HA	1:A:282:ASN:HD21	1.29	0.97
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.47	0.94
1:A:224:ARG:HE	1:A:224:ARG:HA	1.30	0.93
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.62	0.82
1:B:280:ARG:HE	1:B:281:THR:H	1.26	0.82

There are no symmetry-related clashes.

#### 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	Perce	ntiles
1	A	583/585 (100%)	558 (96%)	24 (4%)	1 (0%)	47	58
1	В	583/585 (100%)	565 (97%)	17 (3%)	1 (0%)	47	58
All	All	1166/1170 (100%)	1123 (96%)	41 (4%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	547	GLU
1	A	277	LYS

#### 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	493/493 (100%)	469 (95%)	24 (5%)	25 35	
1	В	493/493 (100%)	469 (95%)	24 (5%)	25 35	
All	All	986/986 (100%)	938 (95%)	48 (5%)	25 35	

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	223	ARG
1	В	364	MET
1	В	232	ARG
1	В	323	ARG
1	В	398	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	135	GLN
1	В	544	GLN
1	В	257	GLN
1	В	568	GLN
1	В	509	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 monosaccharides in this entry.



## 5.6 Ligand geometry (i)

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.

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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	585/585 (100%)	0.03	26 (4%)	34	41	16, 26, 46, 73	0
1	В	585/585 (100%)	0.03	23 (3%)	39	46	13, 26, 46, 75	0
All	All	1170/1170 (100%)	0.03	49 (4%)	36	43	13, 26, 46, 75	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	SER	12.3
1	В	278	THR	11.7
1	В	279	SER	9.0
1	A	278	THR	8.6
1	В	280	ARG	7.9

### 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 monosaccharides 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	CA	A	1001	1/1	0.99	0.06	23,23,23,23	0
2	CA	В	1002	1/1	0.99	0.05	27,27,27,27	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

