



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5TXC  
Title : AtxE2 Isopeptidase - APO  
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Deposited on : 2016-11-16  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

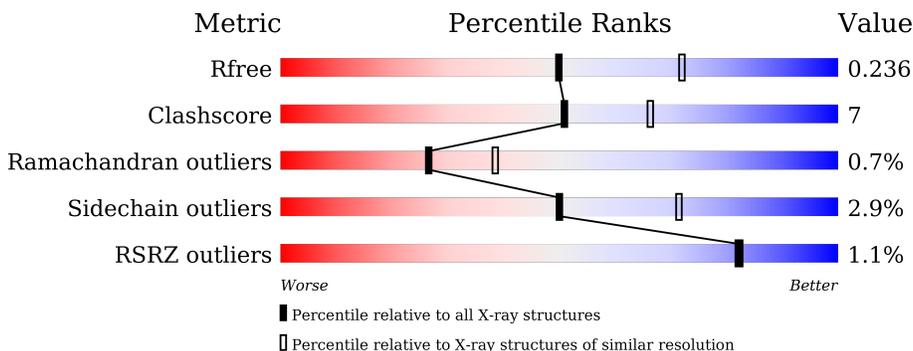
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	705	 77% 14% • 7%
1	B	705	 2% 76% 15% • 7%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 10881 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 AtxE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	653	5158	3245	936	962	15	0	0	0
1	B	653	5158	3245	936	962	15	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	696	GLY	-	expression tag	UNP E8RUP5
A	697	SER	-	expression tag	UNP E8RUP5
A	698	ARG	-	expression tag	UNP E8RUP5
A	699	SER	-	expression tag	UNP E8RUP5
A	700	HIS	-	expression tag	UNP E8RUP5
A	701	HIS	-	expression tag	UNP E8RUP5
A	702	HIS	-	expression tag	UNP E8RUP5
A	703	HIS	-	expression tag	UNP E8RUP5
A	704	HIS	-	expression tag	UNP E8RUP5
A	705	HIS	-	expression tag	UNP E8RUP5
B	696	GLY	-	expression tag	UNP E8RUP5
B	697	SER	-	expression tag	UNP E8RUP5
B	698	ARG	-	expression tag	UNP E8RUP5
B	699	SER	-	expression tag	UNP E8RUP5
B	700	HIS	-	expression tag	UNP E8RUP5
B	701	HIS	-	expression tag	UNP E8RUP5
B	702	HIS	-	expression tag	UNP E8RUP5
B	703	HIS	-	expression tag	UNP E8RUP5
B	704	HIS	-	expression tag	UNP E8RUP5
B	705	HIS	-	expression tag	UNP E8RUP5

- Molecule 2 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	A	372	Total 372	O 372	0	0
2	B	193	Total 193	O 193	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.49Å 201.74Å 109.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.40 49.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.72-2.40) 96.1 (49.72-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.194 , 0.236 0.192 , 0.236	Depositor DCC
$R_{free}$ test set	3166 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.46	1/5285 (0.0%)	0.71	7/7207 (0.1%)
1	B	0.40	0/5285	0.62	2/7207 (0.0%)
All	All	0.43	1/10570 (0.0%)	0.67	9/14414 (0.1%)

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	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	THR	C-N	6.21	1.46	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	LEU	CA-CB-CG	7.10	131.63	115.30
1	A	445	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	398	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	B	235	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	78	ASP	CB-CG-OD1	5.24	123.02	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Peptide
1	A	382	GLY	Peptide
1	A	551	CYS	Peptide
1	B	551	CYS	Peptide

## 5.2 Too-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 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	5158	0	5061	66	0
1	B	5158	0	5061	78	0
2	A	372	0	0	19	1
2	B	193	0	0	19	0
All	All	10881	0	10122	141	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 7.

The worst 5 of 141 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:205:ARG:O	1:B:652:ARG:NH2	2.09	0.85
1:A:205:ARG:NH1	2:A:803:HOH:O	2.10	0.84
1:A:652:ARG:NH1	2:A:805:HOH:O	2.13	0.81
1:A:448:THR:O	2:A:801:HOH:O	2.05	0.74
1:B:131:GLN:N	2:B:801:HOH:O	1.98	0.73

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)
2:A:837:HOH:O	2:A:1076:HOH:O[6_575]	1.92	0.28

## 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	651/705 (92%)	625 (96%)	21 (3%)	5 (1%)	24	35
1	B	651/705 (92%)	626 (96%)	21 (3%)	4 (1%)	30	43
All	All	1302/1410 (92%)	1251 (96%)	42 (3%)	9 (1%)	26	38

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	552	CYS
1	B	83	LEU
1	B	552	CYS
1	A	35	ALA
1	A	164	SER

### 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	547/588 (93%)	529 (97%)	18 (3%)	45	66
1	B	547/588 (93%)	533 (97%)	14 (3%)	54	74
All	All	1094/1176 (93%)	1062 (97%)	32 (3%)	50	71

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	LEU

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Mol	Chain	Res	Type
1	A	628	VAL
1	B	407	LEU
1	A	611	TYR
1	B	115	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	121	ASN

### 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](#)

There are no ligands in this entry.

### 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	653/705 (92%)	-0.40	1 (0%) 95 95	22, 33, 54, 86	0
1	B	653/705 (92%)	-0.05	13 (1%) 68 68	26, 46, 77, 109	0
All	All	1306/1410 (92%)	-0.23	14 (1%) 82 82	22, 39, 71, 109	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	GLY	4.0
1	B	158	VAL	3.9
1	B	273	THR	3.7
1	B	480	THR	3.4
1	B	276	GLN	3.0

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.