



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:37 am BST

PDB ID : 2X3B  
Title : AsaP1 inactive mutant E294A, an extracellular toxic zinc metalloendopeptidase  
Authors : Bogdanovic, X.; Palm, G.J.; Singh, R.K.; Hinrichs, W.  
Deposited on : 2010-01-22  
Resolution : 2.28 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
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

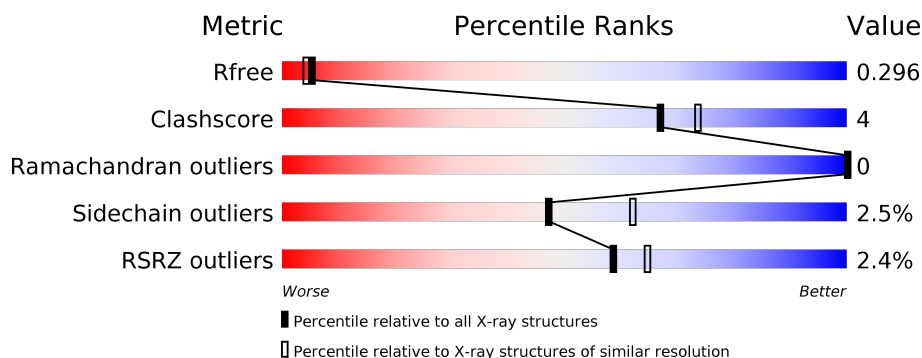
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	343	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>14%</div> </div> </div>
1	B	343	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4805 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 TOXIC EXTRACELLULAR ENDOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	2	0
			2296	1436	398	457	5			
1	B	290	Total	C	N	O	S	0	2	0
			2252	1407	386	454	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	ALA	GLU	engineered mutation	UNP Q8GMV9
B	294	ALA	GLU	engineered mutation	UNP Q8GMV9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

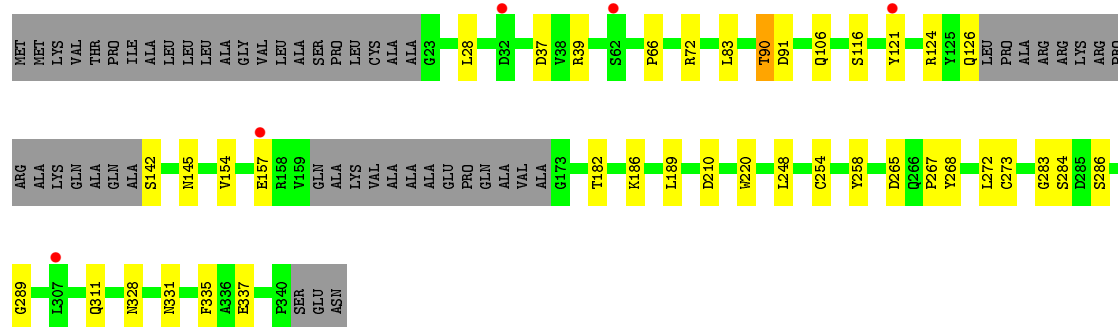
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	116	Total	O	0	0
			116	116		



- Molecule 1: TOXIC EXTRACELLULAR ENDOPEPTIDASE

GLN	ALA	S142	L149	V159	GLF	ALA	ALA	LYS	VAL	ALA	ALA	ALA	ALA	GLU	PRO	GLN	ALA	VAL	ALA	ALA	G173	F177	L189	W220	K238	F250	Y258	C273	V301	N316	T320	N328	N331	F335	P340	GLR	GLU	ASN	ARG	PRO	ARG	ALA	LYS	GLN	ALA				
MET	MET	LYS	VAL	THR	PRO	ILE	ALA	LEU	LEU	LEU	GLY	VAL	LEU	ALA	VAL	SER	PRO	LEU	CYS	ALA	ALA	G23	T29	S34	T35	D36	G48	D49	L54	H57	Q58	S62	L67	L96	L97	K98	Q106	P128	A129	R130	R131	LYS	ARG	PRO	ARG	ALA	LYS	GLN	ALA

Chain B:  %



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.85Å 60.20Å 183.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.81 – 2.28 24.47 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.81-2.28) 99.8 (24.47-2.28)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.244 , 0.293 0.245 , 0.296	Depositor DCC
$R_{free}$ test set	1526 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 3.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.060 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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](#)

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

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	0.38	0/2348	0.52	1/3193 (0.0%)
1	B	0.37	0/2298	0.51	0/3125
All	All	0.38	0/4646	0.52	1/6318 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	149	LEU	CA-CB-CG	5.64	128.27	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	GLU	Peptide

### 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	2296	0	2189	14	0
1	B	2252	0	2145	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	139	0	0	0	0
3	B	116	0	0	0	0
All	All	4805	0	4334	35	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 4.

All (35) 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:189:LEU:HD21	1:A:250:PHE:CD2	2.14	0.83
1:B:124:ARG:HD3	1:B:142:SER:HA	1.60	0.81
1:B:28:LEU:H	1:B:145:ASN:HD21	1.32	0.76
1:A:189:LEU:HD11	1:A:250:PHE:CB	2.24	0.68
1:A:328:ASN:HD22	1:A:331:ASN:HD22	1.42	0.66
1:B:28:LEU:H	1:B:145:ASN:ND2	1.96	0.62
1:B:116:SER:HB2	1:B:154:VAL:HG22	1.82	0.60
1:B:254:CYS:HB3	1:B:272:LEU:O	2.04	0.58
1:B:124:ARG:CD	1:B:142:SER:HA	2.32	0.57
1:B:328:ASN:HD22	1:B:331:ASN:HD22	1.54	0.56
1:A:58:GLN:HA	1:A:67:LEU:HD21	1.90	0.54
1:A:189:LEU:HD11	1:A:250:PHE:HB3	1.90	0.54
1:A:54:LEU:HD22	1:A:128:PRO:HG2	1.89	0.53
1:A:328:ASN:HD22	1:A:331:ASN:ND2	2.07	0.52
1:B:289:GLY:HA3	1:B:337:GLU:OE2	2.13	0.48
1:B:28:LEU:N	1:B:145:ASN:HD21	2.08	0.48
1:A:316:ASN:O	1:A:320:THR:HB	2.14	0.47
1:B:90:THR:HG22	1:B:91:ASP:H	1.79	0.47
1:B:220:TRP:CD1	1:B:335:PHE:HA	2.52	0.45
1:B:328:ASN:HB3	1:B:331:ASN:HD22	1.82	0.45
1:A:238:LYS:HD3	1:A:301:VAL:O	2.17	0.44
1:A:258:TYR:O	1:A:273:CYS:HB2	2.18	0.43
1:A:220:TRP:CD1	1:A:335:PHE:HA	2.54	0.42
1:B:39:ARG:HD3	1:B:106:GLN:NE2	2.34	0.42
1:B:284:SER:OG	1:B:311:GLN:NE2	2.53	0.42
1:B:66:PRO:O	1:B:126:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TYR:O	1:B:273:CYS:HB2	2.20	0.42
1:B:267:PRO:HA	1:B:268:TYR:HA	1.76	0.41
1:A:177:PHE:HE1	1:A:189:LEU:HD13	1.85	0.41
1:B:189:LEU:HD21	1:B:272:LEU:HD11	2.02	0.41
1:B:283:GLY:O	1:B:286:SER:HB3	2.19	0.41
1:B:182:THR:O	1:B:186:LYS:HG3	2.21	0.41
1:A:36:ASP:N	1:A:36:ASP:OD1	2.54	0.41
1:A:130[B]:ARG:HD3	1:A:130[B]:ARG:H	1.86	0.40
1:B:72:ARG:HB2	1:B:121:TYR:CE1	2.56	0.40

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	Percentiles	
1	A	291/343 (85%)	281 (97%)	10 (3%)	0	100	100
1	B	286/343 (83%)	276 (96%)	10 (4%)	0	100	100
All	All	577/686 (84%)	557 (96%)	20 (4%)	0	100	100

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	245/278 (88%)	239 (98%)	6 (2%)	49	63
1	B	242/278 (87%)	236 (98%)	6 (2%)	47	62
All	All	487/556 (88%)	475 (98%)	12 (2%)	47	62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	36	ASP
1	A	96	LEU
1	A	106	GLN
1	A	149	LEU
1	A	320	THR
1	B	37	ASP
1	B	83	LEU
1	B	90	THR
1	B	210	ASP
1	B	248	LEU
1	B	265	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	231	GLN
1	A	311	GLN
1	A	331	ASN
1	B	41	ASN
1	B	106	GLN
1	B	145	ASN
1	B	231	GLN
1	B	245	ASN
1	B	299	ASN
1	B	311	GLN
1	B	331	ASN

### 5.3.3 RNA ⓘ

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](#)

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 ⓘ

### 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	295/343 (86%)	0.14	9 (3%) 49 54	20, 33, 62, 86	0
1	B	290/343 (84%)	0.16	5 (1%) 70 75	20, 32, 45, 48	0
All	All	585/686 (85%)	0.15	14 (2%) 59 65	20, 33, 54, 86	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	SER	8.0
1	A	49	ASP	4.2
1	A	130[A]	ARG	3.5
1	B	121	TYR	3.2
1	A	62	SER	3.1
1	A	57[A]	TRP	3.0
1	A	98	LYS	2.8
1	B	62	SER	2.7
1	B	157	GLU	2.7
1	A	35	THR	2.5
1	A	131	ARG	2.3
1	B	307	LEU	2.3
1	A	48	GLY	2.2
1	B	32	ASP	2.1

### 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 [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	ZN	A	1341	1/1	0.99	0.10	35,35,35,35	0
2	ZN	B	1341	1/1	0.99	0.10	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.