



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:34 am BST

PDB ID : 2X3A  
Title : AsaP1 inactive mutant E294Q, an extracellular toxic zinc metalloendopeptidase  
Authors : Bogdanovic, X.; Palm, G.J.; Singh, R.K.; Hinrichs, W.  
Deposited on : 2010-01-22  
Resolution : 2.00 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

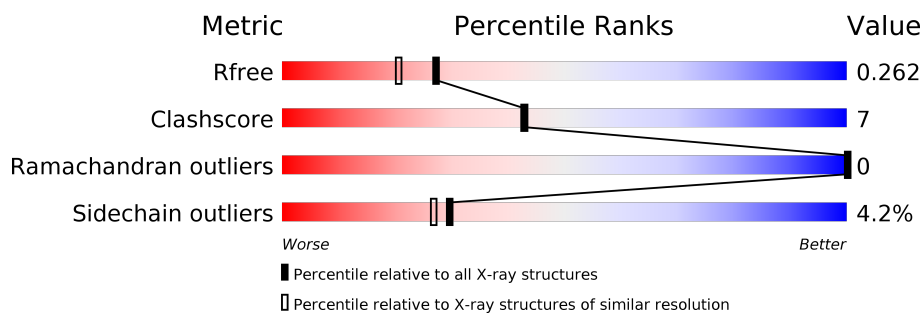
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	343	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2523 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	293	Total	C	N	O	S	0	4	0
			2284	1429	392	458	5			

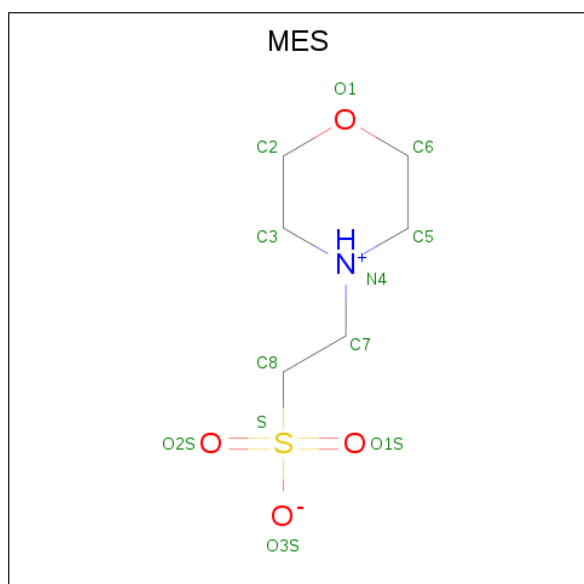
There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

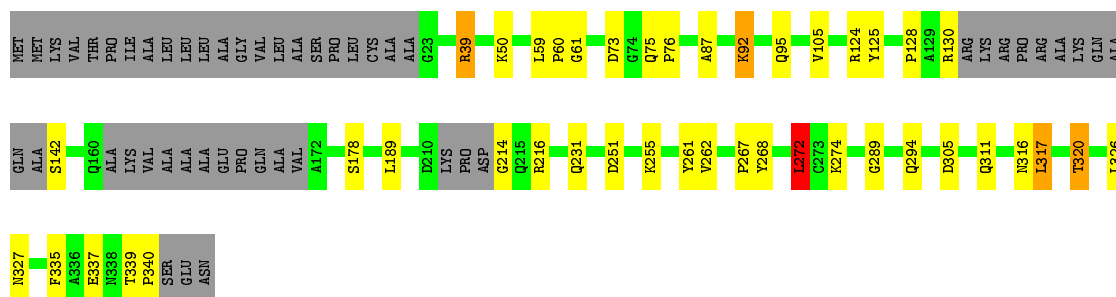
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	199	Total	O	0	0
			199	199		

### 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. 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. 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: TOXIC EXTRACELLULAR ENDOPEPTIDASE

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.25Å 74.47Å 54.70Å 90.00° 112.35° 90.00°	Depositor
Resolution (Å)	57.60 – 2.00 18.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (57.60-2.00) 99.4 (18.33-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.170 , 0.205 0.250 , 0.262	Depositor DCC
$R_{free}$ test set	1258 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% 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: GOL, ZN, SO4, MES

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	1.05	2/2333 (0.1%)	0.93	2/3171 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ARG	CG-CD	5.31	1.65	1.51
1	A	73	ASP	CB-CG	5.03	1.62	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	272	LEU	CA-CB-CG	-6.55	100.23	115.30

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	2284	0	2172	30	0
2	A	1	0	0	0	0
3	A	12	0	13	1	0
4	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	16	2	0
6	A	199	0	0	5	0
All	All	2523	0	2201	31	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 7.

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:305:ASP:OD1	6:A:2172:HOH:O	1.82	0.95
1:A:316:ASN:O	1:A:320:THR:HB	1.76	0.85
1:A:125:TYR:OH	1:A:128:PRO:HD3	1.84	0.78
1:A:124:ARG:HH22	5:A:1346:GOL:H12	1.56	0.71
1:A:231:GLN:HG2	1:A:326:LEU:HD21	1.73	0.69
1:A:261:TYR:CA	1:A:294:GLN:HE22	2.08	0.67
1:A:87:ALA:HB3	6:A:2046:HOH:O	1.97	0.65
1:A:189:LEU:HD21	1:A:272:LEU:HD13	1.80	0.62
1:A:261:TYR:HA	1:A:294:GLN:HE22	1.67	0.60
1:A:214:GLY:N	6:A:2113:HOH:O	2.35	0.59
1:A:261:TYR:C	1:A:294:GLN:HE22	2.09	0.56
1:A:92:LYS:H	1:A:92:LYS:CE	2.20	0.54
1:A:92:LYS:HE2	1:A:92:LYS:H	1.73	0.54
1:A:305:ASP:OD2	1:A:327[B]:ASN:ND2	2.43	0.52
1:A:255:LYS:O	1:A:274:LYS:HE2	2.11	0.51
3:A:1342:MES:O1S	6:A:2196:HOH:O	2.19	0.50
1:A:50:LYS:NZ	6:A:2021:HOH:O	2.39	0.50
1:A:61:GLY:O	5:A:1347:GOL:H12	2.12	0.49
1:A:261:TYR:C	1:A:294:GLN:NE2	2.66	0.48
1:A:262:VAL:HG13	1:A:294:GLN:NE2	2.30	0.46
1:A:125:TYR:CZ	1:A:128:PRO:HD3	2.51	0.46
1:A:216:ARG:HG2	1:A:335:PHE:CE1	2.52	0.44
1:A:261:TYR:CA	1:A:294:GLN:NE2	2.78	0.43
1:A:75:GLN:HA	1:A:76:PRO:HD3	1.94	0.42
1:A:289:GLY:HA3	1:A:337:GLU:OE2	2.19	0.42
1:A:339:THR:HA	1:A:340:PRO:HA	1.82	0.42
1:A:178:SER:O	1:A:251:ASP:HA	2.20	0.41
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.87	0.41
1:A:267:PRO:HA	1:A:268:TYR:HA	1.77	0.41
1:A:60:PRO:HD2	1:A:105:VAL:HG11	2.03	0.40
1:A:231:GLN:HG2	1:A:326:LEU:CD2	2.48	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	289/343 (84%)	279 (96%)	10 (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	244/279 (88%)	234 (96%)	10 (4%)	30	28

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	59	LEU
1	A	92	LYS
1	A	95	GLN
1	A	130	ARG
1	A	142	SER
1	A	272	LEU
1	A	311	GLN
1	A	317	LEU
1	A	320	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	106	GLN
1	A	294	GLN

### 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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	$\# Z  > 2$
3	MES	A	1342	-	12,12,12	1.56	1 (8%)	14,16,16	2.76	4 (28%)
4	SO4	A	1345	-	4,4,4	0.17	0	6,6,6	0.34	0
5	GOL	A	1347	-	5,5,5	0.66	0	5,5,5	1.10	0
4	SO4	A	1344	-	4,4,4	0.71	0	6,6,6	1.00	0
5	GOL	A	1346	-	5,5,5	0.52	0	5,5,5	0.24	0
4	SO4	A	1343	-	4,4,4	0.18	0	6,6,6	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1346	-	-	2/4/4/4	-
3	MES	A	1342	-	-	0/6/14/14	0/1/1/1
5	GOL	A	1347	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1342	MES	C8-S	-4.78	1.70	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1342	MES	O3S-S-C8	5.86	115.24	105.77
3	A	1342	MES	C2-C3-N4	-5.30	102.06	110.10
3	A	1342	MES	O1S-S-C8	-4.55	101.43	106.92
3	A	1342	MES	C7-N4-C3	-3.66	101.87	111.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1347	GOL	O1-C1-C2-O2
5	A	1347	GOL	O1-C1-C2-C3
5	A	1346	GOL	O1-C1-C2-C3
5	A	1347	GOL	C1-C2-C3-O3
5	A	1347	GOL	O2-C2-C3-O3
5	A	1346	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1342	MES	1	0
5	A	1347	GOL	1	0
5	A	1346	GOL	1	0

## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.