



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2019 – 10:57 PM EDT

PDB ID : 5N4B  
Title : Prolyl oligopeptidase B from *Galerina marginata* bound to 25mer macrocyclization substrate - S577A mutant  
Authors : Czekster, C.M.; McMahon, S.A.; Ludewig, H.; Naismith, J.H.  
Deposited on : 2017-02-10  
Resolution : 1.44 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

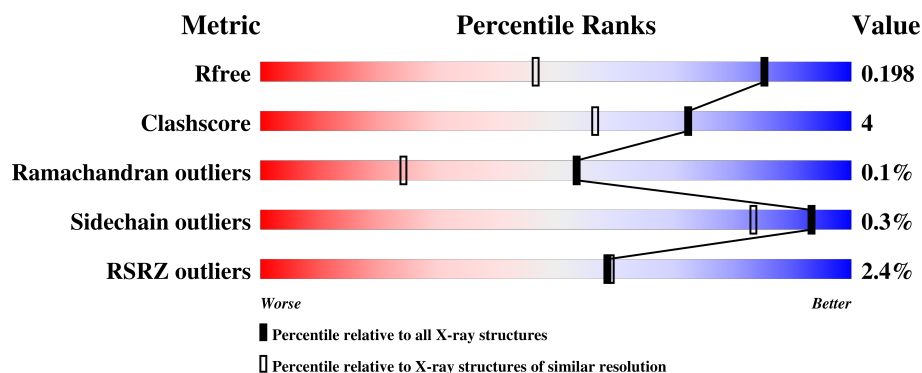
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.44 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))
$R_{free}$	111664	1592 (1.46-1.42)
Clashscore	122126	1643 (1.46-1.42)
Ramachandran outliers	120053	1618 (1.46-1.42)
Sidechain outliers	120020	1618 (1.46-1.42)
RSRZ outliers	108989	1566 (1.46-1.42)

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	731	 91% 7% .
1	B	731	 92% 7% .
2	C	25	 24% 56% 12% 32%
2	D	25	 24% 56% 12% 32%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13794 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 Prolyl oligopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	722	Total	C	N	O	S	0	13	0
			5796	3717	971	1096	12			
1	B	722	Total	C	N	O	S	0	13	0
			5797	3719	971	1096	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP H2E7Q8
A	577	ALA	SER	engineered mutation	UNP H2E7Q8
B	0	GLY	-	expression tag	UNP H2E7Q8
B	577	ALA	SER	engineered mutation	UNP H2E7Q8

- Molecule 2 is a protein called Alpha-amanitin proprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	17	Total	C	N	O	S	0	0	0
			130	78	22	29	1			
2	C	17	Total	C	N	O	S	0	0	0
			130	78	22	29	1			

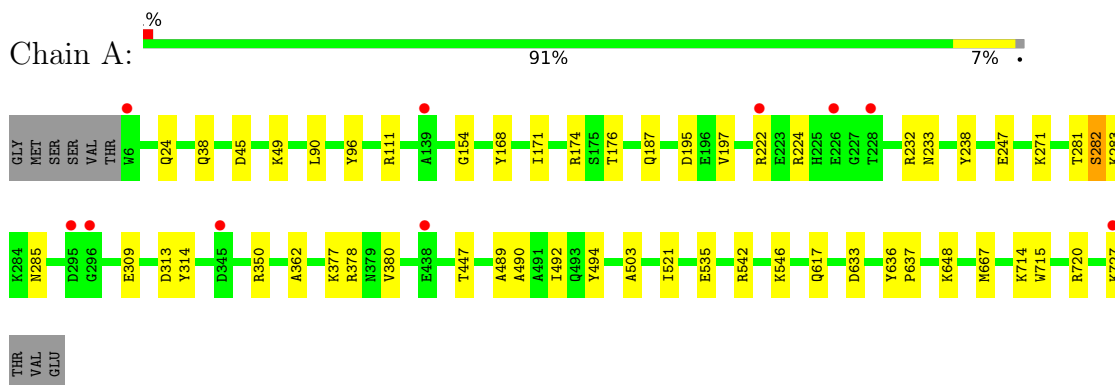
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	954	Total	O	0	0
			954	954		
3	B	939	Total	O	0	0
			939	939		
3	D	24	Total	O	0	0
			24	24		
3	C	24	Total	O	0	0
			24	24		

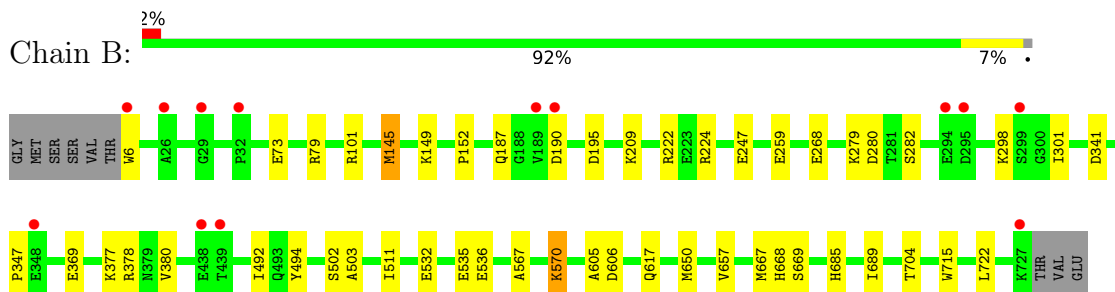
### 3 Residue-property plots [i](#)

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 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: Prolyl oligopeptidase



- Molecule 1: Prolyl oligopeptidase



- Molecule 2: Alpha-amanitin proprotein



- Molecule 2: Alpha-amanitin proprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.08Å 114.72Å 141.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.56 – 1.44 43.56 – 1.44	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.56-1.44) 99.6 (43.56-1.44)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.44Å)	Xtriage
Refinement program	PHENIX (1.11rc2_2522: ???)	Depositor
R, $R_{free}$	0.155 , 0.181 0.177 , 0.198	Depositor DCC
$R_{free}$ test set	14696 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9927e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.70	4/5993 (0.1%)	0.80	6/8139 (0.1%)
1	B	0.73	7/5994 (0.1%)	0.81	8/8141 (0.1%)
2	C	0.68	0/132	0.82	0/179
2	D	0.58	0/132	0.84	0/179
All	All	0.71	11/12251 (0.1%)	0.80	14/16638 (0.1%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	SER	N-CA	-8.17	1.30	1.46
1	B	6	TRP	CB-CG	6.67	1.62	1.50
1	A	535	GLU	CB-CG	6.28	1.64	1.52
1	B	570[A]	LYS	N-CA	5.97	1.58	1.46
1	B	570[B]	LYS	N-CA	5.97	1.58	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	MET	CG-SD-CE	7.03	111.45	100.20
1	B	282	SER	N-CA-C	-6.99	92.14	111.00
1	A	174	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	378	ARG	O-C-N	6.54	133.16	122.70
1	A	350	ARG	NE-CZ-NH2	-6.48	117.06	120.30

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	5796	0	5618	42	0
1	B	5797	0	5621	40	0
2	C	130	0	112	3	0
2	D	130	0	112	4	0
3	A	954	0	0	27	5
3	B	939	0	0	28	5
3	C	24	0	0	1	0
3	D	24	0	0	1	0
All	All	13794	0	11463	86	5

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.

The worst 5 of 86 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:490:ALA:O	3:A:801:HOH:O	1.65	1.14
1:B:145:MET:HG2	3:B:1552:HOH:O	1.64	0.96
1:A:24:GLN:NE2	3:A:802:HOH:O	1.96	0.95
2:C:9:TRP:O	3:C:101:HOH:O	1.91	0.89
1:B:145:MET:CE	3:B:1552:HOH:O	2.24	0.85

All (5) 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)
3:A:840:HOH:O	3:B:1643:HOH:O[3_555]	1.88	0.32
3:A:1668:HOH:O	3:B:1132:HOH:O[4_455]	1.95	0.25
3:A:1523:HOH:O	3:B:1608:HOH:O[3_655]	2.00	0.20
3:A:1622:HOH:O	3:B:1308:HOH:O[3_555]	2.12	0.08
3:A:1609:HOH:O	3:B:1433:HOH:O[3_555]	2.12	0.08

## 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	733/731 (100%)	713 (97%)	19 (3%)	1 (0%)	53	24
1	B	733/731 (100%)	716 (98%)	16 (2%)	1 (0%)	53	24
2	C	15/25 (60%)	14 (93%)	1 (7%)	0	100	100
2	D	15/25 (60%)	14 (93%)	1 (7%)	0	100	100
All	All	1496/1512 (99%)	1457 (97%)	37 (2%)	2 (0%)	53	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	380	VAL
1	A	380	VAL

### 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	616/612 (101%)	614 (100%)	2 (0%)	93	83
1	B	616/612 (101%)	614 (100%)	2 (0%)	93	83
2	C	14/20 (70%)	14 (100%)	0	100	100
2	D	14/20 (70%)	14 (100%)	0	100	100
All	All	1260/1264 (100%)	1256 (100%)	4 (0%)	93	83

All (4) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	195	ASP
1	A	667	MET
1	B	195	ASP
1	B	667	MET

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	285	ASN
1	B	64	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](#)

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	722/731 (98%)	-0.12	10 (1%) 75 75	8, 17, 36, 64	0
1	B	722/731 (98%)	-0.08	13 (1%) 68 68	8, 17, 39, 78	0
2	C	17/25 (68%)	3.31	6 (35%) 0 0	16, 24, 95, 112	0
2	D	17/25 (68%)	3.92	6 (35%) 0 0	14, 22, 119, 140	0
All	All	1478/1512 (97%)	-0.01	35 (2%) 59 59	8, 17, 39, 140	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	9	TRP	14.0
2	D	11	ALA	13.4
2	D	10	THR	12.7
2	C	9	TRP	12.0
2	C	10	THR	10.9

### 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 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.