



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:29 AM GMT

PDB ID : 1E8N  
Title : PROLYL OLIGOPEPTIDASE FROM PORCINE BRAIN, MUTANT, COM-  
PLEXED WITH PEPTIDE  
Authors : Fulop, V.  
Deposited on : 2000-09-27  
Resolution : 1.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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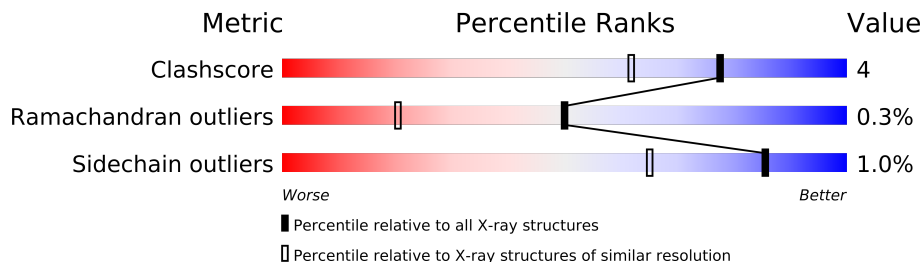
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.50 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))
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	710	
2	I	9	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6700 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ENDOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	710	5700	3659	944	1069	28	0	0	0

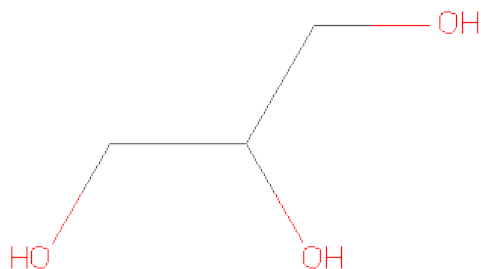
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	ALA	SER	ENGINEERED MUTATION	UNP P23687

- Molecule 2 is a protein called PEPTIDE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	7	50	36	7	7	0	0	0

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

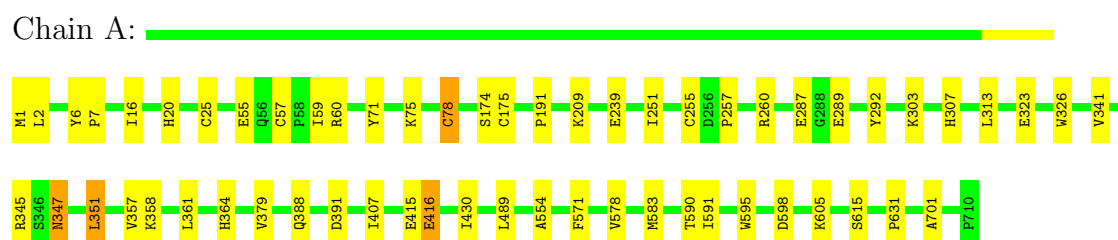
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	917	Total	O	0	0
			917	917		
4	I	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: PROLYL ENDOPEPTIDASE



#### • Molecule 2: PEPTIDE INHIBITOR



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.70Å 99.70Å 110.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.00 – 1.50	Depositor
% Data completeness (in resolution range)	96.1 (19.00-1.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.192 , 0.212	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BE2, GOL

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	0.43	2/5854 (0.0%)	0.68	0/7938
2	I	0.90	0/43	1.09	1/56 (1.8%)
All	All	0.43	2/5897 (0.0%)	0.68	1/7994 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	GLU	CD-OE1	7.56	1.33	1.25
1	A	416	GLU	CD-OE2	-5.47	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	723	GLY	N-CA-C	-5.69	98.88	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5700	0	5516	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	50	0	40	3	0
3	A	30	0	40	4	0
4	A	917	0	0	7	0
4	I	3	0	0	1	0
All	All	6700	0	5596	42	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:345:ARG:HH21	1:A:347:ASN:HD21	1.28	0.77
1:A:591:ILE:HG12	2:I:724:PHE:HB2	1.77	0.67
1:A:174:SER:O	2:I:722:BE2:H3	1.95	0.67
1:A:347:ASN:H	1:A:347:ASN:HD22	1.45	0.65
1:A:59:ILE:HD13	1:A:701:ALA:HB1	1.82	0.61
1:A:287:GLU:HG3	4:A:2559:HOH:O	2.03	0.58
1:A:358:LYS:HD3	1:A:379:VAL:HG13	1.86	0.57
1:A:175:CYS:HB2	4:A:2365:HOH:O	2.05	0.56
1:A:351:LEU:HG	1:A:364:HIS:CD2	2.41	0.56
1:A:358:LYS:CD	1:A:379:VAL:HG13	2.36	0.56
1:A:191:PRO:HG3	1:A:209:LYS:HZ3	1.70	0.55
3:A:794:GOL:H31	4:A:2457:HOH:O	2.06	0.55
1:A:313:LEU:HD21	1:A:341:VAL:HG21	1.90	0.53
1:A:251:ILE:HB	1:A:260:ARG:HB2	1.90	0.53
1:A:430:ILE:HG21	1:A:489:LEU:HD13	1.92	0.52
1:A:292:TYR:O	3:A:794:GOL:O2	2.27	0.51
1:A:1:MET:HG3	1:A:2:LEU:H	1.77	0.49
1:A:78:CYS:HB3	1:A:407:ILE:HG23	1.94	0.49
1:A:416:GLU:OE1	4:A:2676:HOH:O	2.20	0.49
1:A:71:TYR:CZ	1:A:75:LYS:HE2	2.49	0.48
1:A:571:PHE:O	1:A:631:PRO:HB3	2.14	0.48
1:A:595:TRP:CD1	2:I:726:PRO:HD3	2.50	0.47
1:A:59:ILE:HD13	1:A:701:ALA:CB	2.45	0.46
1:A:16:ILE:CD1	1:A:25:CYS:SG	3.04	0.45
1:A:239:GLU:OE1	3:A:794:GOL:H32	2.17	0.45
1:A:388:GLN:HG2	1:A:391:ASP:OD2	2.16	0.45
1:A:416:GLU:OE1	1:A:416:GLU:HA	2.16	0.45
1:A:255:CYS:SG	4:I:2001:HOH:O	2.54	0.44
1:A:191:PRO:HG3	1:A:209:LYS:NZ	2.33	0.44
1:A:554:ALA:HA	1:A:578:VAL:O	2.18	0.43
3:A:790:GOL:H2	4:A:2906:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:GLU:HA	1:A:326:TRP:CE2	2.54	0.42
1:A:303:LYS:HA	1:A:313:LEU:HD23	2.02	0.42
1:A:307:HIS:HB2	4:A:2561:HOH:O	2.19	0.42
1:A:583:MET:HB2	1:A:615:SER:HB2	2.02	0.41
1:A:20:HIS:HB3	1:A:605:LYS:HD3	2.01	0.41
1:A:257:PRO:O	1:A:289:GLU:HB2	2.20	0.41
1:A:6:TYR:HA	1:A:7:PRO:HD3	1.92	0.41
1:A:55:GLU:HG2	1:A:60:ARG:HD3	2.03	0.41
1:A:341:VAL:HG13	1:A:351:LEU:HD22	2.02	0.41
1:A:57:CYS:HB3	4:A:2131:HOH:O	2.21	0.40
1:A:347:ASN:HD22	1:A:347:ASN:N	2.08	0.40

There are no symmetry-related clashes.

## 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	708/710 (100%)	689 (97%)	17 (2%)	2 (0%)	50	20
2	I	5/9 (56%)	5 (100%)	0	0	100	100
All	All	713/719 (99%)	694 (97%)	17 (2%)	2 (0%)	50	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	THR
1	A	357	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	616/616 (100%)	610 (99%)	6 (1%)	85	65
2	I	3/4 (75%)	3 (100%)	0	100	100
All	All	619/620 (100%)	613 (99%)	6 (1%)	85	65

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	CYS
1	A	347	ASN
1	A	351	LEU
1	A	361	LEU
1	A	415	GLU
1	A	598	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	315	ASN
1	A	347	ASN
1	A	362	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z  > 2$
2	BE2	I	722	2	9,9,10	1.44	2 (22%)	8,11,13	0.77	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
2	BE2	I	722	2	-	0/0/2/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	722	BE2	C1-C	2.87	1.51	1.41
2	I	722	BE2	C6-C1	2.12	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

5 ligands are modelled in this entry.

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	GOL	A	790	-	5,5,5	0.18	0	5,5,5	0.28	0
3	GOL	A	791	-	5,5,5	0.33	0	5,5,5	0.31	0
3	GOL	A	792	-	5,5,5	0.09	0	5,5,5	0.23	0
3	GOL	A	793	-	5,5,5	0.09	0	5,5,5	0.22	0
3	GOL	A	794	-	5,5,5	0.35	0	5,5,5	0.36	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
3	GOL	A	790	-	-	0/4/4/4	0/0/0/0
3	GOL	A	791	-	-	0/4/4/4	0/0/0/0
3	GOL	A	792	-	-	0/4/4/4	0/0/0/0
3	GOL	A	793	-	-	0/4/4/4	0/0/0/0
3	GOL	A	794	-	-	0/4/4/4	0/0/0/0

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.