



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 04:22 pm BST

PDB ID : 1KN9  
Title : CRYSTAL STRUCTURE OF A BACTERIAL SIGNAL PEPTIDASE APO-  
ENZYME, IMPLICATIONS FOR SIGNAL PEPTIDE BINDING AND THE  
SER-LYS DYAD MECHANISM.  
Authors : Paetzel, M.; Dalbey, R.E.; Strynadka, N.C.J.  
Deposited on : 2001-12-18  
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

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

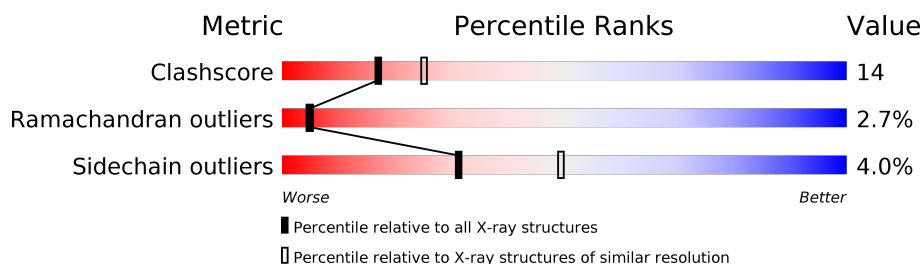
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	249	
1	B	249	
1	C	249	
1	D	249	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7154 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 Signal peptidase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1782	1132	306	337	7			
1	B	222	Total	C	N	O	S	0	0	0
			1688	1076	284	320	8			
1	C	234	Total	C	N	O	S	0	0	0
			1805	1156	303	339	7			
1	D	214	Total	C	N	O	S	0	0	0
			1623	1033	276	307	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	INITIATING METHIONINE	UNP P00803
B	75	MET	-	INITIATING METHIONINE	UNP P00803
C	75	MET	-	INITIATING METHIONINE	UNP P00803
D	75	MET	-	INITIATING METHIONINE	UNP P00803

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	64	Total	O	0	0
			64	64		
2	C	49	Total	O	0	0
			49	49		
2	D	49	Total	O	0	0
			49	49		



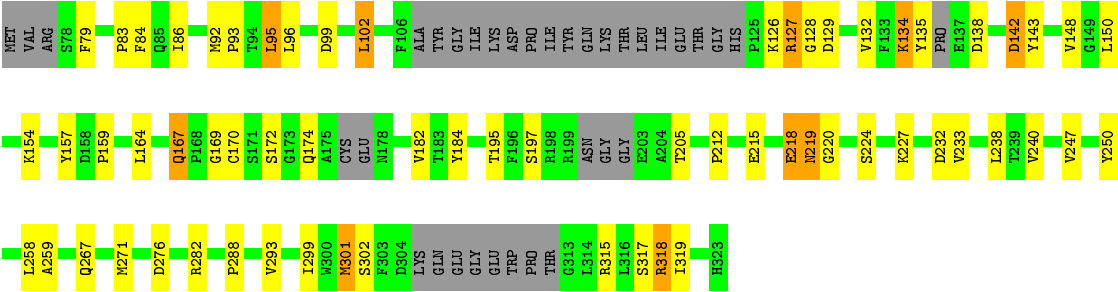
Chain D: 

60%

22%

•

14%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.44Å 112.44Å 198.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.05 – 2.40	Depositor
% Data completeness (in resolution range)	98.7 (40.05-2.40)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.239 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 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	0.39	0/1827	0.68	0/2472
1	B	0.39	0/1730	0.71	2/2344 (0.1%)
1	C	0.37	0/1852	0.63	0/2509
1	D	0.35	0/1660	0.66	0/2243
All	All	0.38	0/7069	0.67	2/9568 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	CYS	CA-CB-SG	-7.70	100.14	114.00
1	B	176	CYS	CA-CB-SG	-6.16	102.91	114.00

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	1782	0	1696	42	0
1	B	1688	0	1602	38	0
1	C	1805	0	1722	63	0
1	D	1623	0	1537	49	0
2	A	94	0	0	0	0
2	B	64	0	0	1	0
2	C	49	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	49	0	0	1	0
All	All	7154	0	6557	188	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 14.

The worst 5 of 188 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:C:197:SER:HB3	1:C:204:ALA:HB3	1.38	1.05
1:A:323:HIS:CD2	1:A:323:HIS:H	1.88	0.90
1:D:127:ARG:HH21	1:D:127:ARG:HB2	1.38	0.89
1:C:257:GLN:HE21	1:C:258:LEU:H	1.13	0.89
1:A:244:GLN:HE21	1:B:219:ASN:HD22	1.25	0.82

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	228/249 (92%)	214 (94%)	12 (5%)	2 (1%)	17	25
1	B	216/249 (87%)	199 (92%)	10 (5%)	7 (3%)	4	3
1	C	228/249 (92%)	209 (92%)	10 (4%)	9 (4%)	3	2
1	D	202/249 (81%)	185 (92%)	11 (5%)	6 (3%)	4	3
All	All	874/996 (88%)	807 (92%)	43 (5%)	24 (3%)	5	5

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PRO

*Continued on next page...*





### 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.