

# wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 08:54 AM EDT

PDB ID : 1SPB

Title : SUBTILISIN BPN' PROSEGMENT (77 RESIDUES) COMPLEXED

WITH A MUTANT SUBTILISIN BPN' (266 RESIDUES). CRYSTAL PH 4.6. CRYSTALLIZATION TEMPERATURE 20 C DIFFRACTION

TEMPERATURE-160 C

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Deposited on : 1995-06-21

Resolution : 2.00 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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)

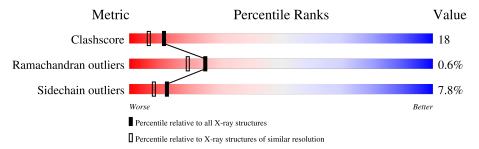
Validation Pipeline (wwPDB-VP) : 2.23.2

## 1 Overall quality at a glance (i)

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain						
1	Р	78	22%	47%	17%	5%	9%		
2	S	266	45%		41%	12'	% ••		



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2668 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 SUBTILISIN BPN' PROSEGMENT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Р	71	Total 557	C 354	N 93	O 108	S 2	0	0	0

• Molecule 2 is a protein called SUBTILISIN BPN'.

2 S 264 Total C N O S 0 1860 1159 321 376 4	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	32	ASN	ASP	engineered mutation	UNP P00782
S	43	ASN	LYS	engineered mutation	UNP P00782
S	50	PHE	MET	engineered mutation	UNP P00782
S	73	LEU	ALA	engineered mutation	UNP P00782
S	?	-	LEU	deletion	UNP P00782
S	?	-	ASN	deletion	UNP P00782
S	?	-	ASN	deletion	UNP P00782
S	?	-	SER	deletion	UNP P00782
S	?	-	ILE	deletion	UNP P00782
S	?	-	GLY	deletion	UNP P00782
S	?	-	VAL	deletion	UNP P00782
S	?	-	LEU	deletion	UNP P00782
S	?	-	GLY	deletion	UNP P00782
S	206	VAL	GLN	engineered mutation	UNP P00782
S	217	LYS	TYR	engineered mutation	UNP P00782
S	218	SER	ASN	engineered mutation	UNP P00782
S	221	ALA	SER	engineered mutation	UNP P00782

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	1	Total Na 1 1	0	0

## • Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Р	55	Total O 55 55	0	0
4	S	195	Total O 195 195	0	0

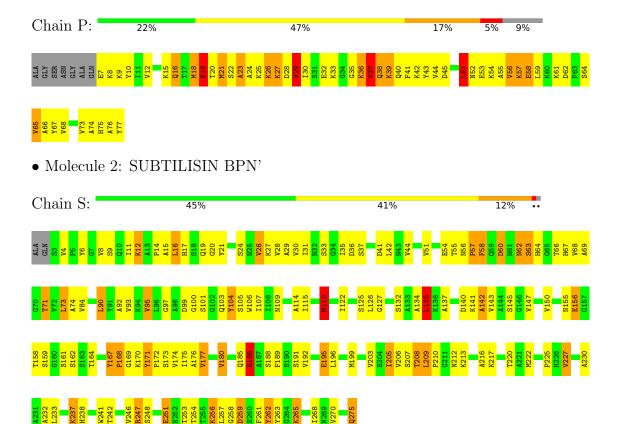


# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Note EDS was not executed.

• Molecule 1: SUBTILISIN BPN' PROSEGMENT





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 2	Depositor	
Cell constants	74.10Å 77.85Å 57.65Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	8.00 - 2.00	Depositor	
% Data completeness	(Not available) (8.00-2.00)	Depositor	
(in resolution range)	(1101 available) (0.00 2.00)		
$R_{merge}$	0.08	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	PROLSQ	Depositor	
$R, R_{free}$	0.204 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2668	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP	



# 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: NA

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	Bo	nd lengths	Bond angles		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	Р	1.29	1/565~(0.2%)	2.59	$45/752 \ (6.0\%)$	
2	S	1.35	$4/1898 \ (0.2\%)$	2.53	123/2592 (4.7%)	
All	All	1.34	5/2463 (0.2%)	2.54	168/3344 (5.0%)	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Р	0	4
2	S	0	13
All	All	0	17

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
2	S	20	GLY	N-CA	-7.84	1.34	1.46
1	Р	19	SER	CA-CB	7.19	1.63	1.52
2	S	54	GLU	CB-CG	-5.46	1.41	1.52
2	S	251	GLU	CG-CD	-5.25	1.44	1.51
2	S	54	GLU	CG-CD	-5.12	1.44	1.51

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathrm{Ideal}(^{o})$
2	S	247	ARG	NE-CZ-NH2	-16.88	111.86	120.30
2	S	186	ARG	CD-NE-CZ	16.00	146.00	123.60
2	S	247	ARG	NE-CZ-NH1	15.92	128.26	120.30
2	S	19	GLN	C-N-CA	14.33	152.38	122.30

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	S	104	TYR	CB-CG-CD1	12.68	128.61	121.00

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Р	23	ALA	Mainchain
1	Р	26	LYS	Mainchain
1	Р	29	VAL	Mainchain
1	Р	55	ALA	Mainchain
2	S	24	SER	Mainchain

### 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	Р	557	0	572	35	0
2	S	1860	0	1822	57	0
3	S	1	0	0	0	0
4	Р	55	0	0	3	0
4	S	195	0	0	12	0
All	All	2668	0	2394	85	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 18.

The worst 5 of 85 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:P:19:SER:CB	1:P:64:SER:HA	1.97	0.94
1:P:27:LYS:HG2	1:P:37:VAL:HG11	1.53	0.89
1:P:15:LYS:HD3	1:P:18:MET:HB3	1.55	0.85
2:S:35:ILE:HD12	2:S:92:ALA:HB2	1.59	0.85
1:P:36:LYS:HD3	1:P:38:GLN:HE22	1.48	0.79

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	Р	69/78 (88%)	64 (93%)	4 (6%)	1 (1%)	11 5
2	S	$262/266 \ (98\%)$	250 (95%)	11 (4%)	1 (0%)	34 30
All	All	331/344 (96%)	314 (95%)	15 (4%)	2 (1%)	25 19

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	63	SER
1	Р	19	SER

#### 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	Р	59/62 (95%)	49 (83%)	10 (17%)	2 1
2	S	197/198 (100%)	187 (95%)	10 (5%)	24 19
All	All	256/260~(98%)	236 (92%)	20 (8%)	12 8

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	180	VAL
2	S	222	MET
2	S	259	ASP
2	S	237	LYS

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Mol	Chain	Res	Type
1	Р	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	Р	38	GLN
1	Р	72	HIS
2	S	43	ASN
2	S	64	HIS
2	S	109	ASN

#### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

