



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:08 AM GMT

PDB ID : 3SIC  
Title : MOLECULAR RECOGNITION AT THE ACTIVE SITE OF SUBTILISIN BPN': CRYSTALLOGRAPHIC STUDIES USING GENETICALLY ENGINEERED PROTEINACEOUS INHIBITOR SSI (STREPTOMYCES SUBTILISIN INHIBITOR)  
Authors : Mitsui, Y.; Takeuchi, Y.; Nakamura, K.T.  
Deposited on : 1991-08-30  
Resolution : 1.80 Å(reported)

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

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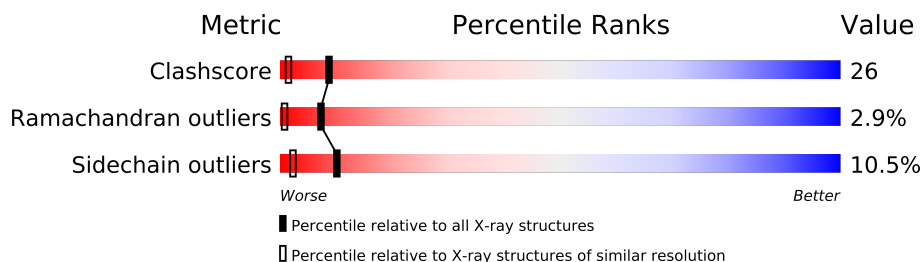
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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	E	275	
2	I	107	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2978 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 SUBTILISIN BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	275	Total	C	N	O	S	0	0	0
			1938	1204	335	394	5			

- Molecule 2 is a protein called STREPTOMYCES SUBTILISIN INHIBITOR (SSI).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	107	Total	C	N	O	S	0	0	0
			765	477	131	151	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	73	LYS	MET	CONFLICT	UNP P01006

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	169	Total	O	0	0
			169	169		
4	I	104	Total	O	0	0
			104	104		

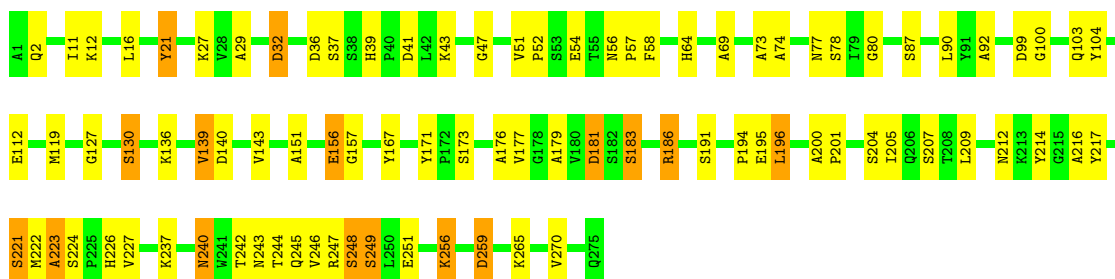
### 3 Residue-property plots

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.

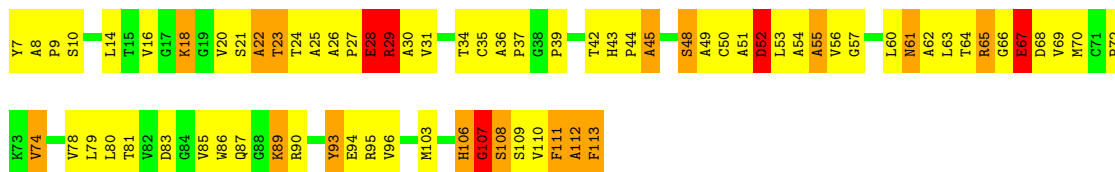
#### • Molecule 1: SUBTILISIN BPN'

Chain E: 



#### • Molecule 2: STREPTOMYCES SUBTILISIN INHIBITOR (SSI)

Chain I: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.20Å 185.90Å 69.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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: CA

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	E	1.04	0/1976	1.74	32/2697 (1.2%)
2	I	0.90	0/781	1.85	18/1066 (1.7%)
All	All	1.00	0/2757	1.77	50/3763 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	I	23	THR	C-N-CA	20.91	173.97	121.70
1	E	181	ASP	CB-CG-OD1	14.01	130.91	118.30
1	E	99	ASP	CB-CG-OD2	-11.72	107.75	118.30
2	I	52	ASP	CB-CG-OD1	-10.76	108.61	118.30
1	E	196	LEU	CA-CB-CG	10.32	139.04	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	186	ARG	Sidechain

## 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	E	1938	0	1899	53	1
2	I	765	0	742	94	1
3	E	2	0	0	0	0
4	E	169	0	0	12	1
4	I	104	0	0	12	2
All	All	2978	0	2641	136	4

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 26.

The worst 5 of 136 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:177:VAL:HG22	4:E:623:HOH:O	1.33	1.29
2:I:28:GLU:HG3	2:I:29:ARG:HD3	1.42	1.01
4:E:660:HOH:O	2:I:74:VAL:HB	1.59	1.01
2:I:109:SER:HA	2:I:112:ALA:HB2	1.39	1.00
2:I:31:VAL:HB	2:I:42:THR:O	1.68	0.93

All (4) 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	Distance(Å)	Clash(Å)
4:I:132:HOH:O	4:I:132:HOH:O[4_555]	1.39	0.81
2:I:23:THR:OG1	2:I:90:ARG:NE[2_555]	1.62	0.58
1:E:12:LYS:NZ	4:E:544:HOH:O[6_555]	2.03	0.17
4:I:122:HOH:O	4:I:122:HOH:O[3_555]	2.17	0.03

## 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	E	273/275 (99%)	260 (95%)	11 (4%)	2 (1%)	30	13
2	I	105/107 (98%)	79 (75%)	17 (16%)	9 (9%)	1	0
All	All	378/382 (99%)	339 (90%)	28 (7%)	11 (3%)	7	1

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	24	THR
2	I	65	ARG
2	I	61	ASN
2	I	108	SER
2	I	55	ALA

### 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	E	205/205 (100%)	188 (92%)	17 (8%)	16	4
2	I	80/80 (100%)	67 (84%)	13 (16%)	3	0
All	All	285/285 (100%)	255 (90%)	30 (10%)	10	2

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	249	SER
1	E	265	LYS
2	I	108	SER
1	E	259	ASP
2	I	18	LYS

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

Mol	Chain	Res	Type
1	E	59	GLN

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Mol	Chain	Res	Type
1	E	271	GLN
2	I	43	HIS
2	I	61	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are 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.

## 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.