



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:20 am BST

PDB ID : 2SEC  
Title : STRUCTURAL COMPARISON OF TWO SERINE PROTEINASE-  
PROTEIN INHIBITOR COMPLEXES. EGLIN-C-SUBTILISIN CARLS-  
BERG AND CI-2-SUBTILISIN NOVO  
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Deposited on : 1988-09-05  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure 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

<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

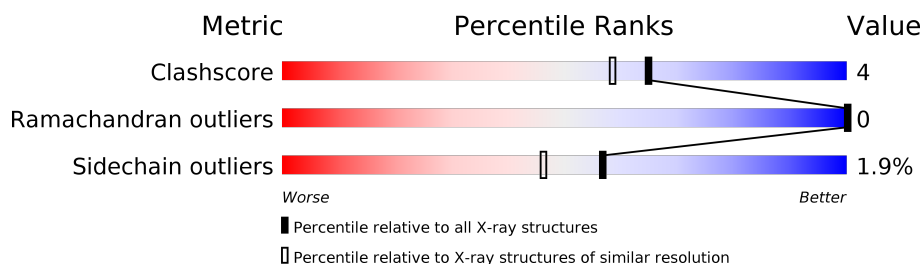
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 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	E	274	
2	I	70	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2623 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 CARLSBERG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	274	Total	C	N	O	S	0	0	0
			1920	1190	332	393	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	103	SER	THR	CONFLICT	UNP P00780
E	129	ALA	PRO	CONFLICT	UNP P00780
E	158	ASN	SER	CONFLICT	UNP P00780
E	161	SER	ASN	CONFLICT	UNP P00780
E	212	ASN	SER	CONFLICT	UNP P00780

- Molecule 2 is a protein called EGLIN C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	64	Total	C	N	O	0	0	0
			530	345	91	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	47	ASN	ASP	CONFLICT	UNP P01051

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	149	Total 149	O 149	0	0
4	I	21	Total 21	O 21	0	0

### 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. 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.

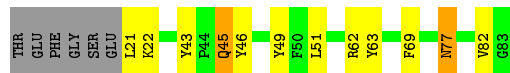
- Molecule 1: SUBTILISIN CARLSBERG

Chain E:  91% 9%



- Molecule 2: EGLIN C

Chain I:  74% 14% • 9%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.31Å 41.41Å 56.50Å 69.51° 83.67° 75.32°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.136 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	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	0.78	2/1952 (0.1%)	1.20	9/2662 (0.3%)
2	I	0.72	0/548	1.18	1/749 (0.1%)
All	All	0.77	2/2500 (0.1%)	1.20	10/3411 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	271	GLU	CD-OE2	6.25	1.32	1.25
1	E	112	GLU	CD-OE2	6.19	1.32	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	249	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	E	14	ASP	CB-CG-OD1	8.47	125.92	118.30
1	E	145	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	E	14	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	E	41	ASP	CB-CG-OD1	6.21	123.89	118.30
1	E	73	ALA	N-CA-CB	-5.96	101.76	110.10
2	I	62	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	E	140	ASP	CB-CG-OD1	5.75	123.48	118.30
1	E	120	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	247	ARG	NE-CZ-NH2	-5.29	117.66	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	E	1920	0	1880	10	0
2	I	530	0	511	11	0
3	E	3	0	0	0	0
4	E	149	0	0	3	0
4	I	21	0	0	0	0
All	All	2623	0	2391	20	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 4.

All (20) 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)
2:I:45:GLN:HE21	2:I:45:GLN:H	0.95	0.90
2:I:45:GLN:N	2:I:45:GLN:HE21	1.75	0.83
2:I:77:ASN:H	2:I:77:ASN:HD22	1.32	0.75
2:I:45:GLN:NE2	2:I:45:GLN:H	1.80	0.75
1:E:240:ASN:HB2	4:E:468:HOH:O	1.98	0.64
1:E:104:TYR:HE1	4:E:505:HOH:O	1.89	0.55
2:I:21:LEU:HD12	2:I:22:LYS:N	2.21	0.55
2:I:43:TYR:HB3	2:I:46:TYR:HD1	1.75	0.52
2:I:51:LEU:O	2:I:69:PHE:HA	2.10	0.51
1:E:99:SER:HB2	2:I:49:TYR:CE2	2.48	0.48
1:E:135:MET:HE3	1:E:171:TYR:HE2	1.79	0.48
1:E:156:SER:HB2	1:E:164:THR:HB	1.98	0.46
1:E:238:HIS:HD2	4:E:467:HOH:O	1.98	0.45
2:I:63:TYR:HA	2:I:82:VAL:CG1	2.47	0.45
1:E:238:HIS:HE1	1:E:274:ALA:O	2.00	0.45
2:I:63:TYR:HA	2:I:82:VAL:HG12	2.00	0.43
1:E:127:GLY:HA2	1:E:167:TYR:O	2.18	0.43
1:E:8:ILE:HB	1:E:9:PRO:HD3	2.02	0.41
2:I:77:ASN:N	2:I:77:ASN:HD22	2.04	0.41
1:E:104:TYR:O	1:E:108:VAL:HG23	2.21	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	E	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
2	I	62/70 (89%)	61 (98%)	1 (2%)	0	100	100
All	All	334/344 (97%)	327 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	198/198 (100%)	195 (98%)	3 (2%)	65	56
2	I	59/64 (92%)	57 (97%)	2 (3%)	37	22
All	All	257/262 (98%)	252 (98%)	5 (2%)	57	46

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	77	ASN
1	E	145	ARG
1	E	222	MET
2	I	45	GLN
2	I	77	ASN

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

Mol	Chain	Res	Type
1	E	238	HIS
1	E	240	ASN
2	I	45	GLN
2	I	47	ASN
2	I	77	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

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 ⓘ

### 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.