



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:01 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

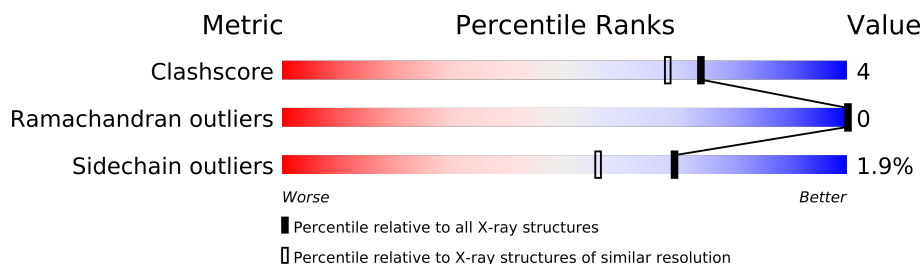
The following versions of software and data (see [references](#)) were used in the production of this report:

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 ≥ 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	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 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 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

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.

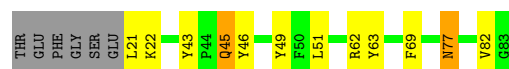
• Molecule 1: SUBTILISIN CARLSBERG

Chain E: 



• Molecule 2: EGLIN C

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	P 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	12.0	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: 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 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	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	1
4	I	21	0	0	0	1
All	All	2623	0	2391	20	1

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

Atom-1	Atom-2	Distance(Å)	Clash(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
2:I:77:ASN:N	2:I:77:ASN:HD22	2.04	0.41
1:E:8:ILE:HB	1:E:9:PRO:HD3	2.02	0.41
1:E:104:TYR:O	1:E:108:VAL:HG23	2.21	0.40

All (1) 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:E:398:HOH:O	4:I:605:HOH:O[1_655]	0.16	2.04

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%)	76	66
2	I	59/64 (92%)	57 (97%)	2 (3%)	49	29
All	All	257/262 (98%)	252 (98%)	5 (2%)	69	56

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 ⓘ

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 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.

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.