



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:50 PM GMT

PDB ID : 1CSE
Title : THE HIGH-RESOLUTION X-RAY CRYSTAL STRUCTURE OF THE COMPLEX FORMED BETWEEN SUBTILISIN CARLSBERG AND EGLIN C, AN ELASTASE INHIBITOR FROM THE LEECH HIRUDO MEDICINALIS. STRUCTURAL ANALYSIS, SUBTILISIN STRUCTURE AND INTERFACE GEOMETRY
Authors : Bode, W.
Deposited on : 1988-06-03
Resolution : 1.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

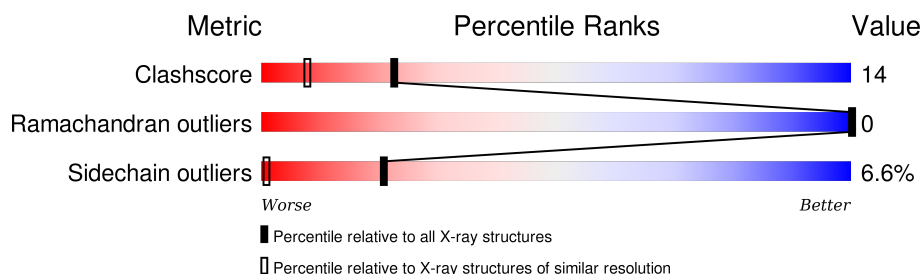
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	102246	1607 (1.26-1.14)
Ramachandran outliers	100387	1540 (1.26-1.14)
Sidechain outliers	100360	1538 (1.26-1.14)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 2876 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	63	Total	C	N	O	0	0	0
			522	339	90	93			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	33	ASN	ASP	CONFLICT	UNP P01051

- 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.

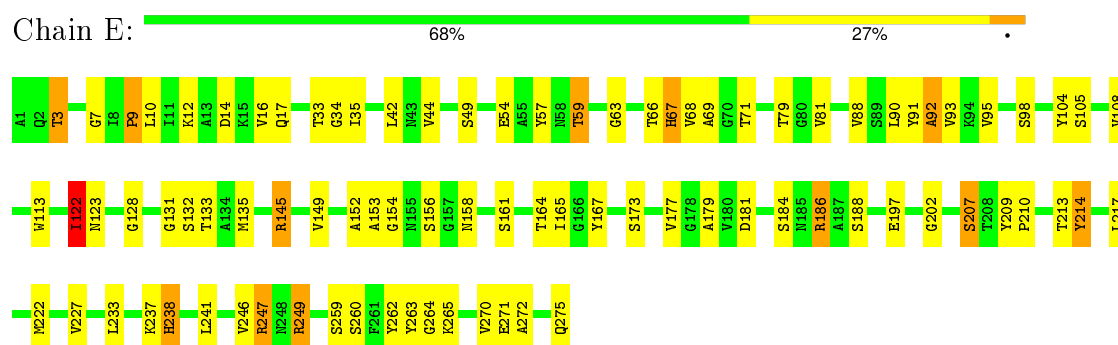
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	312	Total 312	O 312	0	0
4	I	120	Total 120	O 120	0	0

3 Residue-property plots [i](#)

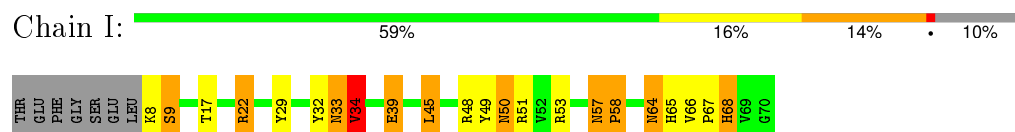
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



• Molecule 2: EGLIN C



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	38.30 Å 41.50 Å 57.00 Å 111.80° 85.80° 104.70°	Depositor
Resolution (Å)	10.00 – 1.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2876	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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	1.37	8/1952 (0.4%)	1.78	27/2662 (1.0%)
2	I	1.21	1/540 (0.2%)	1.88	14/738 (1.9%)
All	All	1.33	9/2492 (0.4%)	1.80	41/3400 (1.2%)

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	11
2	I	0	3
All	All	0	14

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	207	SER	CA-CB	6.75	1.63	1.52
1	E	113	TRP	NE1-CE2	-6.64	1.28	1.37
1	E	186	ARG	NE-CZ	5.62	1.40	1.33
1	E	7	GLY	N-CA	5.44	1.54	1.46
1	E	67	HIS	CE1-NE2	5.41	1.45	1.32
1	E	49	SER	CB-OG	5.20	1.49	1.42
1	E	92	ALA	CA-CB	5.19	1.63	1.52
1	E	238	HIS	ND1-CE1	5.15	1.47	1.34
2	I	51	ARG	NE-CZ	5.11	1.39	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	ARG	NE-CZ-NH2	-29.79	105.41	120.30
1	E	145	ARG	NE-CZ-NH1	21.40	131.00	120.30
2	I	51	ARG	NE-CZ-NH1	-15.48	112.56	120.30
1	E	145	ARG	CD-NE-CZ	10.69	138.57	123.60
2	I	34	VAL	CG1-CB-CG2	10.03	126.94	110.90
2	I	48	ARG	NE-CZ-NH1	8.95	124.77	120.30
2	I	51	ARG	NH1-CZ-NH2	8.70	128.97	119.40
2	I	53	ARG	NE-CZ-NH1	-8.60	116.00	120.30
2	I	53	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	E	122	ILE	CG1-CB-CG2	-7.90	94.02	111.40
1	E	263	TYR	CB-CG-CD1	-6.90	116.86	121.00
2	I	53	ARG	NH1-CZ-NH2	6.90	126.99	119.40
1	E	81	VAL	CA-CB-CG1	-6.87	100.60	110.90
1	E	214	TYR	CB-CG-CD2	-6.83	116.90	121.00
2	I	39	GLU	N-CA-CB	-6.74	98.47	110.60
1	E	184	SER	N-CA-CB	-6.72	100.42	110.50
1	E	88	VAL	CG1-CB-CG2	6.42	121.18	110.90
1	E	181	ASP	CB-CG-OD1	6.31	123.98	118.30
1	E	249	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	E	153	ALA	CB-CA-C	-6.26	100.71	110.10
1	E	68	VAL	O-C-N	6.06	132.40	122.70
1	E	262	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	E	91	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	E	177	VAL	CA-CB-CG2	-5.85	102.12	110.90
1	E	95	VAL	CG1-CB-CG2	5.61	119.88	110.90
2	I	48	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	I	9	SER	N-CA-CB	-5.43	102.36	110.50
1	E	14	ASP	CB-CG-OD2	5.42	123.18	118.30
2	I	58	PRO	C-N-CA	-5.42	110.91	122.30
1	E	165	ILE	CA-CB-CG1	-5.38	100.78	111.00
1	E	247	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	E	113	TRP	N-CA-CB	-5.33	101.01	110.60
2	I	68	HIS	CB-CA-C	-5.30	99.79	110.40
1	E	42	LEU	CB-CG-CD1	5.29	119.99	111.00
1	E	67	HIS	N-CA-CB	-5.26	101.13	110.60
2	I	22	ARG	N-CA-CB	-5.26	101.13	110.60
1	E	71	THR	CA-CB-CG2	5.17	119.64	112.40
2	I	45	LEU	O-C-N	5.13	130.91	122.70
1	E	249	ARG	CD-NE-CZ	-5.05	116.53	123.60
1	E	122	ILE	CB-CG1-CD1	-5.03	99.81	113.90
1	E	88	VAL	CA-CB-CG1	5.01	118.42	110.90

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	LEU	Mainchain
1	E	105	SER	Mainchain
1	E	17	GLN	Mainchain
1	E	186	ARG	Sidechain
1	E	197	GLU	Mainchain
1	E	214	TYR	Sidechain
1	E	227	VAL	Mainchain
1	E	265	LYS	Mainchain
1	E	54	GLU	Mainchain
1	E	59	THR	Mainchain
1	E	93	VAL	Mainchain
2	I	32	TYR	Mainchain
2	I	49	TYR	Mainchain
2	I	58	PRO	Mainchain

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	1881	51	1
2	I	522	0	500	17	0
3	E	2	0	0	0	0
4	E	312	0	0	37	1
4	I	120	0	0	9	0
All	All	2876	0	2381	66	1

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.

All (66) 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:E:213:THR:HG23	4:E:816:HOH:O	1.72	0.89
1:E:209:TYR:HA	4:E:812:HOH:O	1.78	0.82
1:E:249:ARG:HD2	4:E:572:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:GLN:HG3	4:E:591:HOH:O	1.83	0.78
1:E:233:LEU:HD12	4:E:588:HOH:O	1.84	0.78
1:E:241:LEU:HD13	4:E:572:HOH:O	1.85	0.74
1:E:98:SER:HA	4:E:514:HOH:O	1.88	0.74
1:E:217:LEU:HD22	4:I:502:HOH:O	1.89	0.72
1:E:33:THR:HB	4:E:514:HOH:O	1.92	0.69
2:I:64:ASN:H	2:I:64:ASN:HD22	1.43	0.65
1:E:249:ARG:HG2	4:E:550:HOH:O	1.99	0.63
1:E:90:LEU:HG	4:E:592:HOH:O	1.98	0.62
1:E:270:VAL:HG21	4:E:588:HOH:O	1.98	0.62
1:E:167:TYR:HB2	4:E:471:HOH:O	1.99	0.61
1:E:173:SER:HB3	4:E:791:HOH:O	2.00	0.61
1:E:34:GLY:HA2	4:E:563:HOH:O	2.01	0.59
2:I:39:GLU:OE1	2:I:65:HIS:HE1	1.86	0.59
1:E:209:TYR:HB3	4:E:816:HOH:O	2.02	0.59
2:I:22:ARG:HG2	4:I:852:HOH:O	2.02	0.59
2:I:17:THR:HG22	4:I:652:HOH:O	2.03	0.58
1:E:247:ARG:NH1	4:E:482:HOH:O	2.35	0.58
2:I:33:ASN:HB2	4:I:778:HOH:O	2.05	0.57
2:I:9:SER:HB2	4:I:855:HOH:O	2.04	0.56
1:E:16:VAL:HG11	4:E:599:HOH:O	2.05	0.55
1:E:66:THR:HG23	4:E:574:HOH:O	2.07	0.55
1:E:152:ALA:HB3	2:I:45:LEU:HD12	1.88	0.55
1:E:104:TYR:HB3	4:E:781:HOH:O	2.05	0.55
1:E:104:TYR:HE1	4:E:765:HOH:O	1.90	0.54
1:E:154:GLY:HA2	2:I:45:LEU:HD13	1.90	0.54
1:E:35:ILE:HB	4:E:581:HOH:O	2.08	0.53
1:E:246:VAL:HA	4:E:572:HOH:O	2.09	0.52
1:E:12:LYS:HD3	4:E:571:HOH:O	2.10	0.51
1:E:237:LYS:HB2	4:E:615:HOH:O	2.11	0.51
1:E:67:HIS:HB3	4:E:522:HOH:O	2.11	0.50
1:E:210:PRO:HD3	4:E:812:HOH:O	2.13	0.49
2:I:8:LYS:HZ3	2:I:29:TYR:HE2	1.60	0.49
1:E:66:THR:HB	4:E:812:HOH:O	2.13	0.47
1:E:122:ILE:HG13	1:E:149:VAL:HG13	1.96	0.47
1:E:44:VAL:HG13	4:E:592:HOH:O	2.14	0.46
1:E:135:MET:HB2	4:E:781:HOH:O	2.14	0.46
1:E:156:SER:HB2	1:E:164:THR:HB	1.98	0.46
1:E:249:ARG:HH11	1:E:249:ARG:HD3	1.47	0.46
2:I:50:ASN:H	2:I:50:ASN:HD22	1.62	0.46
2:I:57:ASN:HD22	2:I:57:ASN:C	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:8:LYS:N	4:I:461:HOH:O	2.50	0.45
1:E:131:GLY:N	4:E:471:HOH:O	2.47	0.44
1:E:128:GLY:HA3	4:E:766:HOH:O	2.17	0.43
1:E:238:HIS:HB2	1:E:241:LEU:CD1	2.48	0.43
1:E:179:ALA:HB1	1:E:202:GLY:HA3	2.01	0.43
1:E:63:GLY:HA2	1:E:210:PRO:CG	2.48	0.43
1:E:67:HIS:CD2	1:E:207:SER:HB3	2.53	0.43
1:E:9:PRO:HG3	4:E:601:HOH:O	2.18	0.43
1:E:69:ALA:HB3	4:E:589:HOH:O	2.19	0.43
2:I:64:ASN:HD22	2:I:64:ASN:N	2.11	0.42
1:E:57:TYR:HD1	1:E:92:ALA:HB3	1.84	0.42
1:E:188:SER:HB3	4:E:875:HOH:O	2.19	0.42
2:I:34:VAL:CB	4:I:466:HOH:O	2.68	0.42
2:I:39:GLU:HB3	4:I:458:HOH:O	2.20	0.41
1:E:123:ASN:CB	4:E:551:HOH:O	2.68	0.41
2:I:66:VAL:HA	2:I:67:PRO:HD3	1.90	0.41
2:I:29:TYR:HB2	4:I:714:HOH:O	2.21	0.41
1:E:271:GLU:HB2	4:E:827:HOH:O	2.19	0.41
1:E:3:THR:HG23	4:E:427:HOH:O	2.19	0.41
1:E:260:SER:HA	1:E:264:GLY:O	2.21	0.41
1:E:272:ALA:O	1:E:275:GLN:HG2	2.21	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	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:THR:CB	4:E:413:HOH:O[1_565]	1.47	0.73

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	E	272/274 (99%)	265 (97%)	7 (3%)	0	100	100
2	I	61/70 (87%)	60 (98%)	1 (2%)	0	100	100
All	All	333/344 (97%)	325 (98%)	8 (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%)	187 (94%)	11 (6%)	26	2
2	I	58/64 (91%)	52 (90%)	6 (10%)	9	0
All	All	256/262 (98%)	239 (93%)	17 (7%)	21	1

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	THR
1	E	9	PRO
1	E	79	THR
1	E	122	ILE
1	E	132	SER
1	E	133	THR
1	E	145	ARG
1	E	158	ASN
1	E	161	SER
1	E	222	MET
1	E	259	SER
2	I	33	ASN
2	I	34	VAL
2	I	50	ASN
2	I	57	ASN
2	I	64	ASN
2	I	68	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	123	ASN
1	E	141	ASN
1	E	185	ASN
2	I	50	ASN
2	I	57	ASN
2	I	64	ASN
2	I	68	HIS

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 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.

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 ⓘ

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.