



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2021 – 12:50 AM EDT

PDB ID : 2ABZ  
Title : Crystal structure of C19A/C43A mutant of leech carboxypeptidase inhibitor in complex with bovine carboxypeptidase A  
Authors : Arolas, J.L.; Popowicz, G.M.; Bronsoms, S.; Aviles, F.X.; Huber, R.; Holak, T.A.; Ventura, S.  
Deposited on : 2005-07-18  
Resolution : 2.16 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](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) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

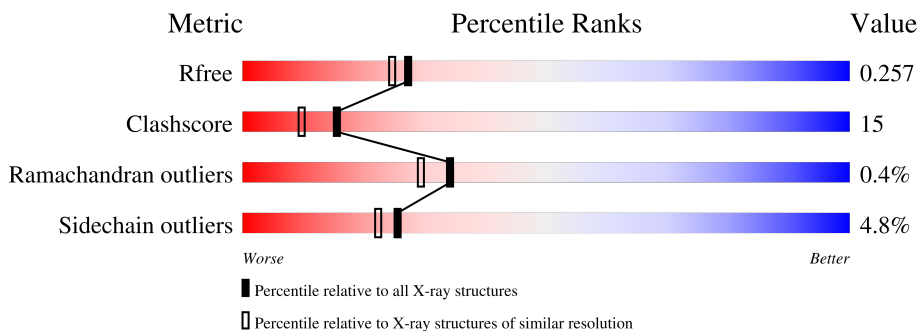
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	309	
1	B	309	
2	C	67	
2	D	67	
2	E	67	
2	F	67	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6504 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 Carboxypeptidase A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	299	2379	1531	390	453	5	0	0	0
1	B	301	2392	1538	392	457	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ALA	GLU	SEE REMARK 999	UNP P00730
A	305	VAL	LEU	SEE REMARK 999	UNP P00730
B	228	ALA	GLU	SEE REMARK 999	UNP P00730
B	305	VAL	LEU	SEE REMARK 999	UNP P00730

- Molecule 2 is a protein called Metallocoarboxypeptidase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	62	476	301	79	90	6	0	0	0
2	D	46	345	214	58	67	6	0	0	0
2	E	60	463	293	77	87	6	0	0	0
2	F	58	447	283	75	83	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	cloning artifact	UNP P81511
C	19	ALA	CYS	engineered mutation	UNP P81511
C	43	ALA	CYS	engineered mutation	UNP P81511
D	1	GLY	-	cloning artifact	UNP P81511

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	ALA	CYS	engineered mutation	UNP P81511
D	43	ALA	CYS	engineered mutation	UNP P81511
E	1	GLY	-	cloning artifact	UNP P81511
E	19	ALA	CYS	engineered mutation	UNP P81511
E	43	ALA	CYS	engineered mutation	UNP P81511
F	1	GLY	-	cloning artifact	UNP P81511
F	19	ALA	CYS	engineered mutation	UNP P81511
F	43	ALA	CYS	engineered mutation	UNP P81511

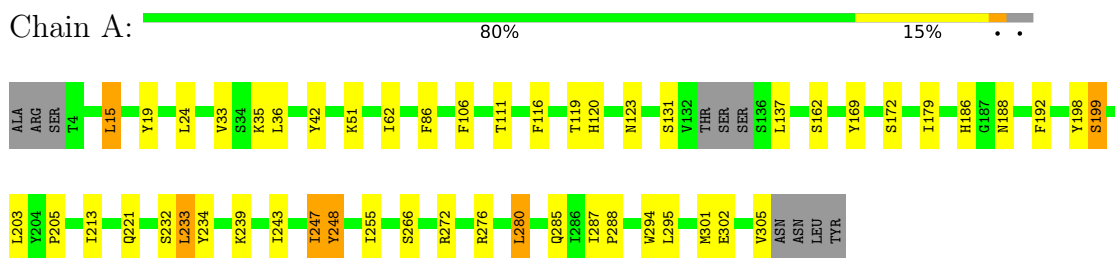
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

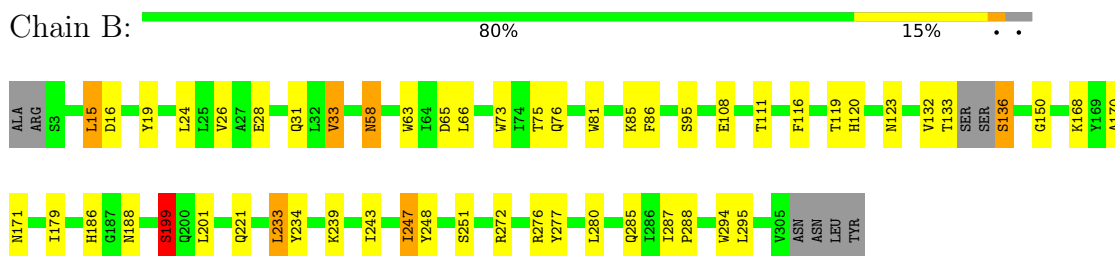
### 3 Residue-property plots

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.

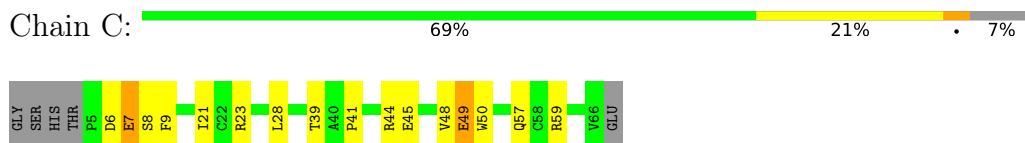
- Molecule 1: Carboxypeptidase A1



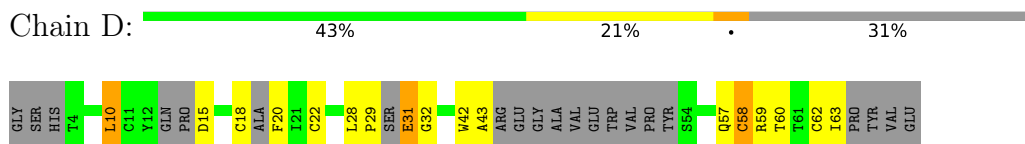
- Molecule 1: Carboxypeptidase A1



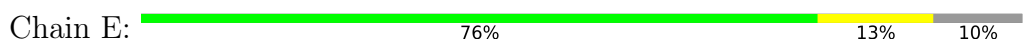
- Molecule 2: Metallocoarboxypeptidase inhibitor



- Molecule 2: Metallocoarboxypeptidase inhibitor



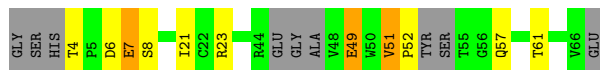
- Molecule 2: Metallocoarboxypeptidase inhibitor





- Molecule 2: Metalloprotease inhibitor

Chain F: 70% 12% 13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.93Å 124.93Å 154.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.16 97.26 – 2.16	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.16) 99.8 (97.26-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.1.2	Depositor
R, $R_{free}$	0.189 , 0.234 0.241 , 0.257	Depositor DCC
$R_{free}$ test set	3360 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtrriage
Anisotropy	0.335	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 26.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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:  
ZN

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	A	0.47	0/2444	0.62	0/3322
1	B	0.50	1/2457 (0.0%)	0.63	0/3340
2	C	0.46	0/494	0.70	0/680
2	D	0.52	0/352	0.64	0/477
2	E	0.56	0/479	0.68	0/658
2	F	0.52	0/462	0.75	0/635
All	All	0.49	1/6688 (0.0%)	0.64	0/9112

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	SER	N-CA	6.76	1.59	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2379	0	2290	60	1
1	B	2392	0	2302	81	0
2	C	476	0	431	34	0
2	D	345	0	306	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	463	0	417	22	1
2	F	447	0	407	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	6504	0	6153	187	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 15.

The worst 5 of 187 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:A:276:ARG:HH12	1:B:295:LEU:CD2	1.36	1.38
1:B:133:THR:HG22	1:B:168:LYS:NZ	1.38	1.34
1:B:276:ARG:NH2	1:B:277:TYR:HE2	1.35	1.24
1:A:15:LEU:O	1:A:15:LEU:HD23	1.13	1.22
1:B:15:LEU:C	1:B:15:LEU:HD23	1.60	1.17

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:A:137:LEU:CD2	2:E:7:GLU:OE2[6_555]	1.63	0.57

## 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	A	295/309 (96%)	282 (96%)	12 (4%)	1 (0%)	41	37
1	B	297/309 (96%)	285 (96%)	11 (4%)	1 (0%)	41	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	60/67 (90%)	59 (98%)	1 (2%)	0	100	100
2	D	36/67 (54%)	34 (94%)	2 (6%)	0	100	100
2	E	56/67 (84%)	56 (100%)	0	0	100	100
2	F	52/67 (78%)	51 (98%)	0	1 (2%)	8	2
All	All	796/886 (90%)	767 (96%)	26 (3%)	3 (0%)	34	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	B	199	SER
2	F	51	VAL

### 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	A	256/265 (97%)	248 (97%)	8 (3%)	40	39
1	B	258/265 (97%)	249 (96%)	9 (4%)	36	34
2	C	52/56 (93%)	48 (92%)	4 (8%)	13	8
2	D	39/56 (70%)	33 (85%)	6 (15%)	2	1
2	E	50/56 (89%)	47 (94%)	3 (6%)	19	14
2	F	50/56 (89%)	46 (92%)	4 (8%)	12	7
All	All	705/754 (94%)	671 (95%)	34 (5%)	25	22

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	39	THR
2	E	49	GLU
2	F	49	GLU
1	B	199	SER

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Mol	Chain	Res	Type
1	B	95	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	285	GLN
2	E	35	ASN
2	D	57	GLN
1	B	37	GLN
1	B	249	GLN

### 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 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.