



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:30 AM UTC

PDB ID : 1K9X / pdb_00001k9x
Title : Structure of Pyrococcus furiosus carboxypeptidase Apo-Yb
Authors : Arndt, J.W.; Hao, B.; Ramakrishnan, V.; Cheng, T.; Chan, S.I.; Chan, M.K.
Deposited on : 2001-10-31
Resolution : 2.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

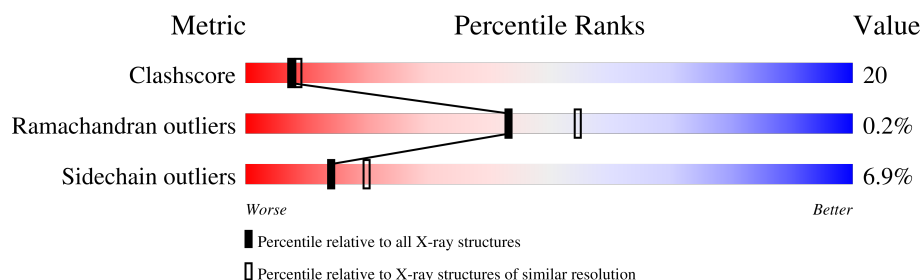
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 ≥ 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	A	499	62% 33% 5%
1	B	499	57% 37% 5%
1	C	499	62% 33% .
1	D	499	55% 39% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17261 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 M32 carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			4163	2700	699	755	9			
1	B	497	Total	C	N	O	S	0	0	0
			4163	2700	699	755	9			
1	C	497	Total	C	N	O	S	0	0	0
			4163	2700	699	755	9			
1	D	497	Total	C	N	O	S	0	0	0
			4163	2700	699	755	9			

- Molecule 2 is water.

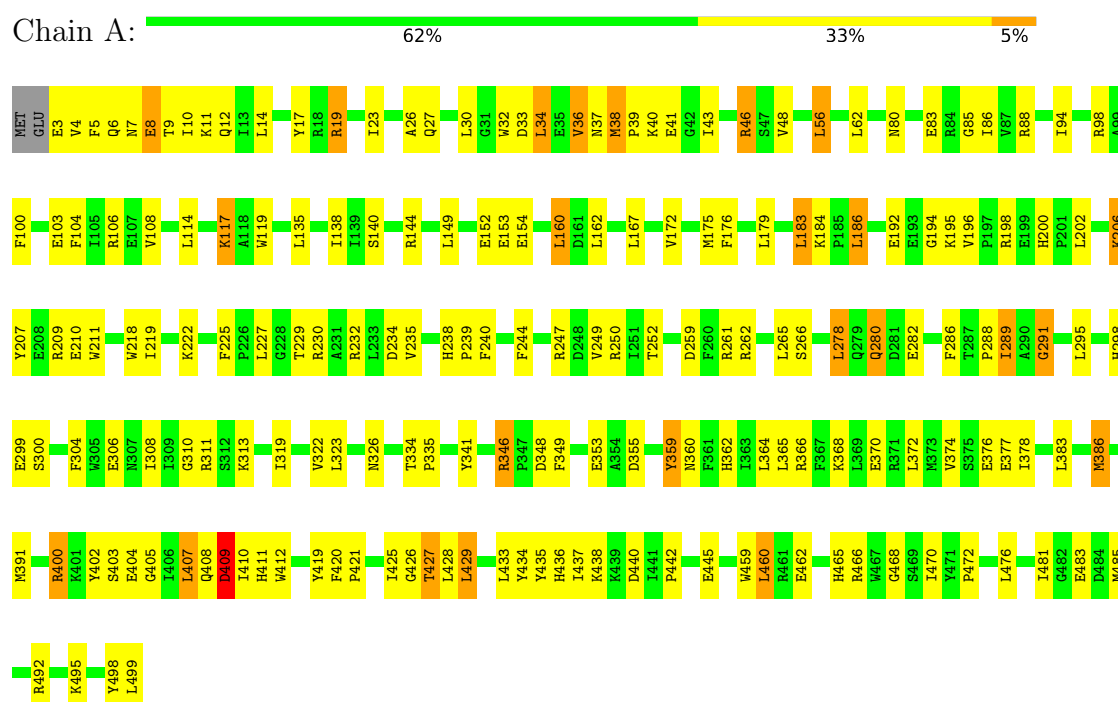
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	182	Total	O	0	0
			182	182		
2	B	109	Total	O	0	0
			109	109		
2	C	147	Total	O	0	0
			147	147		
2	D	171	Total	O	0	0
			171	171		

3 Residue-property plots

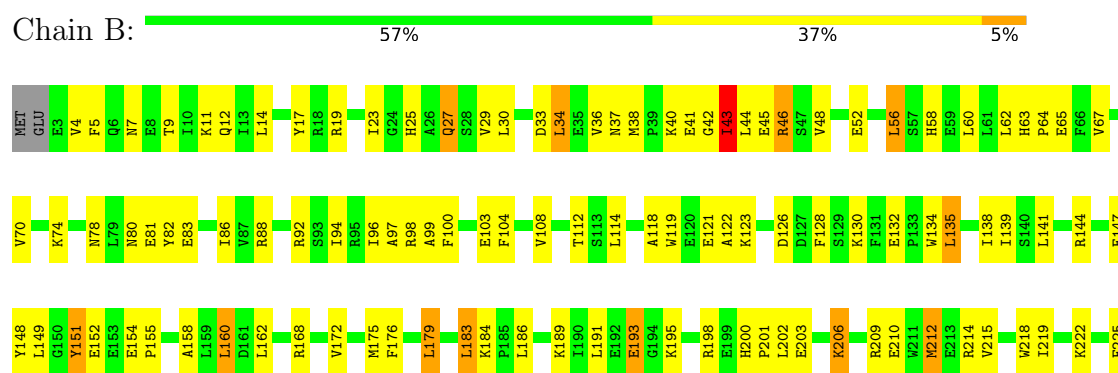
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

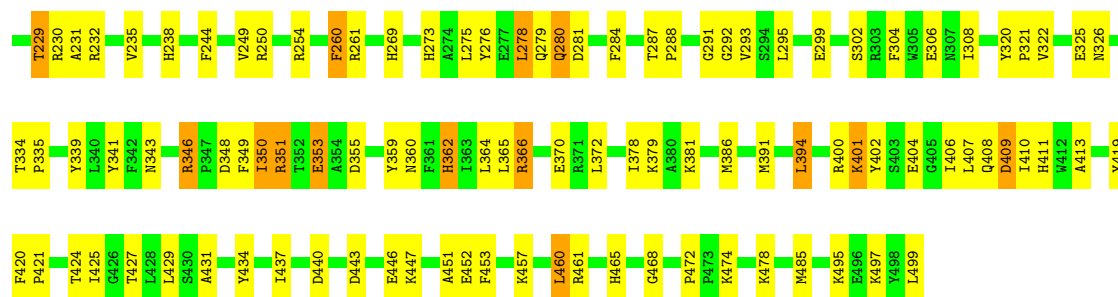
Note EDS was not executed.

• Molecule 1: M32 carboxypeptidase

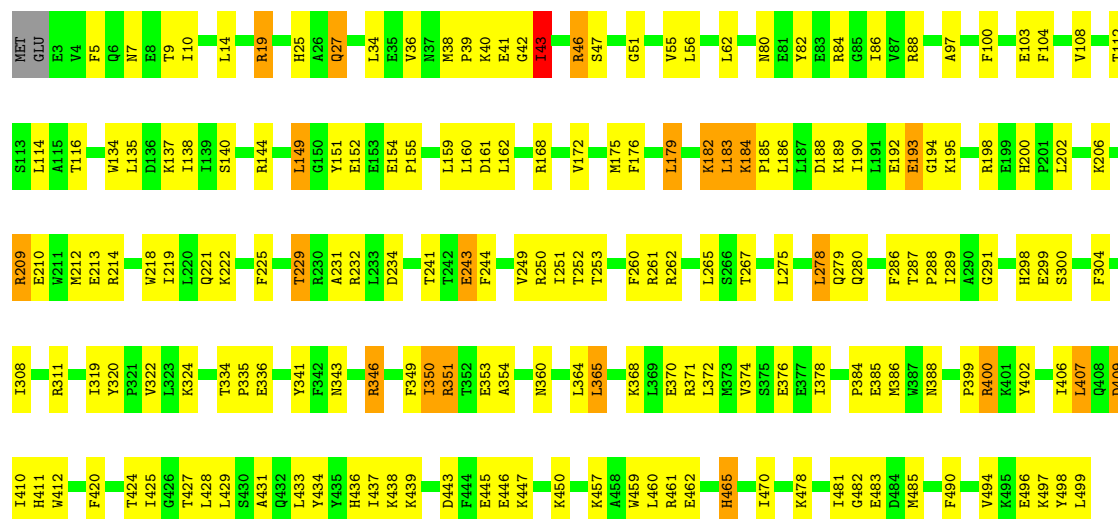


• Molecule 1: M32 carboxypeptidase

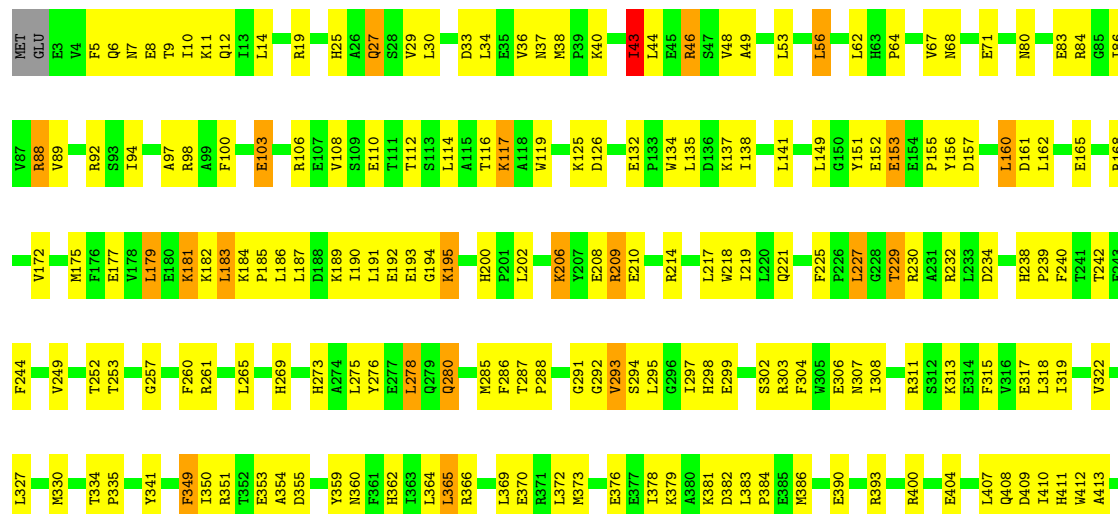




- Molecule 1: M32 carboxypeptidase



- Molecule 1: M32 carboxypeptidase



Y419	F420	G426	T427	L428	L429	S430	A431	Y434	Y435	H436	I437	K438	K439	D440	I441	V448	A449	K450	A451	E452	F453	D454	P455	I456	K457	A458	W459	L460	H465	R466	W467	G468	S469	P472	R492	W493	K497	Y498	L499
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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, α , β , γ	66.34Å 86.78Å 107.89Å 88.64° 78.54° 69.44°	Depositor
Resolution (Å)	48.78 – 2.30	Depositor
% Data completeness (in resolution range)	93.8 (48.78-2.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17261	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/4271	0.91	14/5770 (0.2%)
1	B	0.44	1/4271 (0.0%)	0.94	15/5770 (0.3%)
1	C	0.44	0/4271	0.90	9/5770 (0.2%)
1	D	0.44	0/4271	0.96	15/5770 (0.3%)
All	All	0.44	1/17084 (0.0%)	0.93	53/23080 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	TYR	C-N	-5.71	1.26	1.33

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	VAL	N-CA-C	11.90	122.05	111.81
1	B	36	VAL	N-CA-C	10.09	120.48	111.81
1	A	36	VAL	N-CA-C	9.02	120.24	111.67
1	D	349	PHE	N-CA-C	8.13	121.69	111.69
1	C	36	VAL	N-CA-C	7.72	119.76	111.58

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	4163	0	4144	156	0
1	B	4163	0	4144	192	0
1	C	4163	0	4144	158	0
1	D	4163	0	4144	183	0
2	A	182	0	0	9	0
2	B	109	0	0	10	0
2	C	147	0	0	8	0
2	D	171	0	0	6	0
All	All	17261	0	16576	675	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 20.

The worst 5 of 675 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:429:LEU:HD13	1:A:485:MET:HE3	1.28	1.07
1:A:117:LYS:HE3	1:A:117:LYS:HA	1.37	1.05
1:C:116:THR:HG23	1:C:410:ILE:HD11	1.34	1.05
1:C:385:GLU:OE2	2:C:559:HOH:O	1.76	1.03
1:A:409:ASP:HB2	1:A:411:HIS:HD2	1.24	1.03

There are no symmetry-related clashes.

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	495/499 (99%)	480 (97%)	15 (3%)	0	100	100
1	B	495/499 (99%)	479 (97%)	14 (3%)	2 (0%)	30	38
1	C	495/499 (99%)	474 (96%)	21 (4%)	0	100	100
1	D	495/499 (99%)	477 (96%)	16 (3%)	2 (0%)	30	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1980/1996 (99%)	1910 (96%)	66 (3%)	4 (0%)	43 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	ASN
1	D	153	GLU
1	B	401	LYS
1	D	195	LYS

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	A	444/446 (100%)	408 (92%)	36 (8%)	11 14
1	B	444/446 (100%)	422 (95%)	22 (5%)	22 33
1	C	444/446 (100%)	410 (92%)	34 (8%)	12 16
1	D	444/446 (100%)	414 (93%)	30 (7%)	14 20
All	All	1776/1784 (100%)	1654 (93%)	122 (7%)	14 20

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	460	LEU
1	D	209	ARG
1	C	184	LYS
1	D	206	LYS
1	D	407	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	411	HIS

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Mol	Chain	Res	Type
1	D	200	HIS
1	C	414	HIS
1	D	12	GLN
1	D	360	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.