



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:06 PM GMT

PDB ID : 1WGZ
Title : Crystal structure of carboxypeptidase 1 from *Thermus thermophilus*
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(RSGI)
Deposited on : 2004-05-28
Resolution : 2.60 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
<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

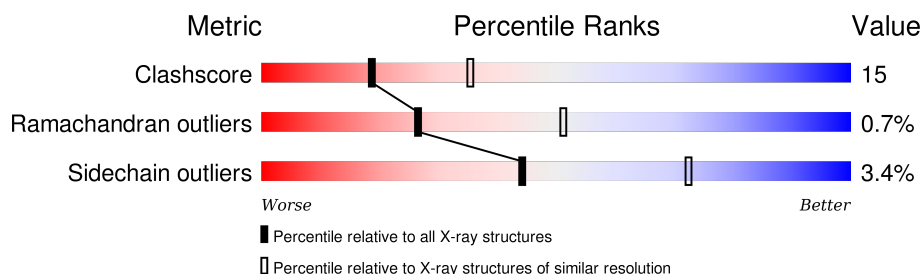
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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	A	510	
1	B	510	
1	C	510	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1001	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	1002	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12641 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4112	2636	722	746	8			
1	B	510	Total	C	N	O	S	0	0	0
			4112	2636	722	746	8			
1	C	510	Total	C	N	O	S	0	0	0
			4112	2636	722	746	8			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

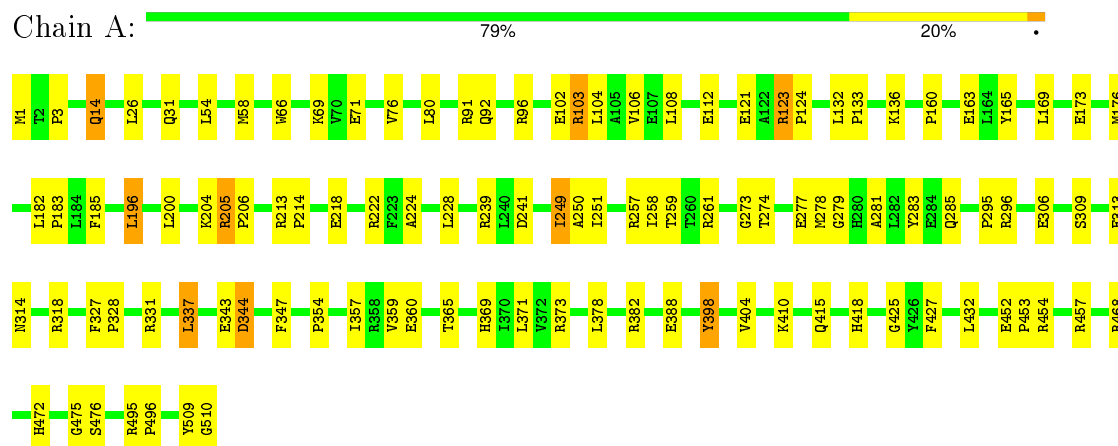
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		
4	B	59	Total	O	0	0
			59	59		
4	C	84	Total	O	0	0
			84	84		

3 Residue-property plots

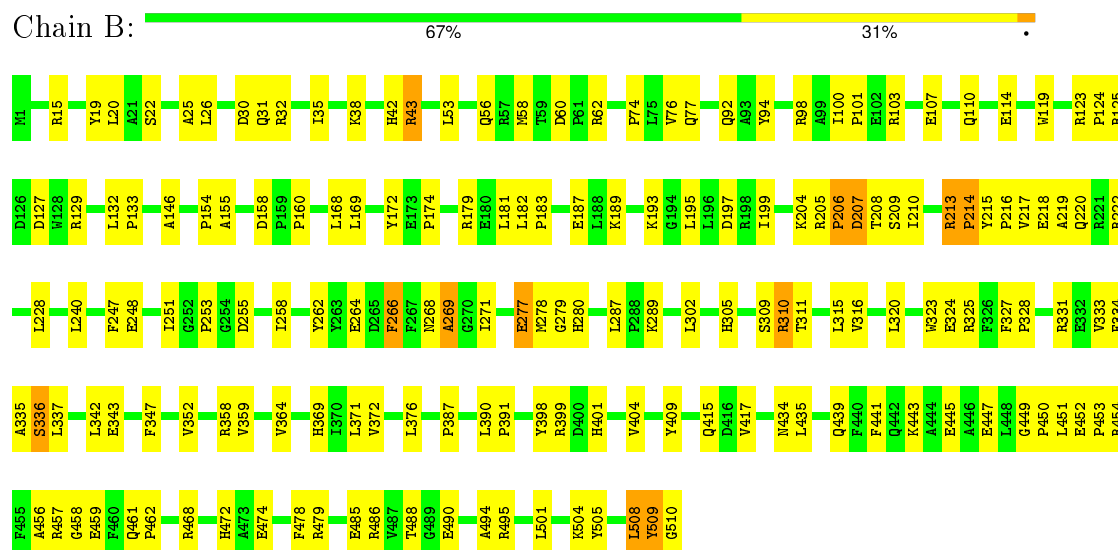
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: carboxypeptidase 1



- Molecule 1: carboxypeptidase 1



- Molecule 1: carboxypeptidase 1



E485	E488	E492	E493	E494	E504	E505	E508	E509	E510	L374	E375	L376	E377	L378	R382	P387	E388	D389	L390	P391	Y398	L402	Y409	V413	M414	Q415	D416	V417	H418	L423	Y426	N434	Q439	K443	E447	E452	P453	R454	E459	F460	Q461	P462	W466	T467	R468	A469	R470	I471	H472	R477	R481	T259	T260	R261	E264	D265	F266	F267	I268	A269	G270	I271	G279	Y283	L287	E290	P295	R296	G297	V300	S301	R305	Q308	S309	R310	L320	E324	F327	P328	V333	F334	V340	V352	I357	R358	V359	E360	V364	R369	L370	L371	V372	R373	R137	V138	T142	K143	E147	V148	L149	P160	E163	A167	R179	L182	P183	L184	L188	L192	K193	G194	L196	L199	K204	R205	P206	R103	L104	A105	V106	E107	L108	P216	V217	E218	A219	R222	E226	L227	L228	Y233	E236	I249	G252	I258	R1	T2	P3	E4	L10	Q14	R15	A25	D30	R43	A44	R45	Q46	Q77	D82	N86	V87	R88	Y94	R98	A99	I100	P101	E102	R103	L104	A105	V106	E107	L108	A109	Q110	A111	E112	F118	E121	A122	R123	P124	R125	D126	R129	L132	P133	K136
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4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	170.10 Å 233.70 Å 124.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.20 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (41.20-2.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12641	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: GOL, 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	0.40	0/4230	0.60	0/5741
1	B	0.34	0/4230	0.56	1/5741 (0.0%)
1	C	0.37	0/4230	0.57	0/5741
All	All	0.37	0/12690	0.58	1/17223 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	509	TYR	CB-CA-C	5.30	121.00	110.40

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	4112	0	3999	100	0
1	B	4112	0	3999	152	0
1	C	4112	0	3999	127	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	6	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	4	0	0
4	A	147	0	0	4	0
4	B	59	0	0	5	0
4	C	84	0	0	1	0
All	All	12641	0	12005	374	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 15.

The worst 5 of 374 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:205:ARG:HB3	1:A:206:PRO:HA	1.26	1.14
1:C:468:ARG:HD3	1:C:472:HIS:HD1	1.26	0.99
1:A:468:ARG:HD3	1:A:472:HIS:HD1	1.29	0.98
1:C:310:ARG:HE	1:C:434:ASN:HD21	1.13	0.94
1:A:205:ARG:HB3	1:A:206:PRO:CA	1.95	0.93

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	508/510 (100%)	487 (96%)	20 (4%)	1 (0%)	52	77
1	B	508/510 (100%)	459 (90%)	42 (8%)	7 (1%)	14	28
1	C	508/510 (100%)	490 (96%)	16 (3%)	2 (0%)	39	65
All	All	1524/1530 (100%)	1436 (94%)	78 (5%)	10 (1%)	26	51

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ARG
1	B	207	ASP
1	C	205	ARG
1	B	206	PRO
1	B	213	ARG

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	412/412 (100%)	401 (97%)	11 (3%)	52	79
1	B	412/412 (100%)	404 (98%)	8 (2%)	65	86
1	C	412/412 (100%)	389 (94%)	23 (6%)	26	50
All	All	1236/1236 (100%)	1194 (97%)	42 (3%)	44	72

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	310	ARG
1	C	106	VAL
1	C	378	LEU
1	C	15	ARG
1	C	77	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	276	HIS
1	B	415	GLN
1	C	415	GLN
1	B	369	HIS
1	B	434	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	1001	-	5,5,5	4.68	5 (100%)	5,5,5	5.63	3 (60%)
3	GOL	C	1002	-	5,5,5	4.82	5 (100%)	5,5,5	5.62	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1001	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1002	-	-	0/4/4/4	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	GOL	C3-C2	-8.20	1.21	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	GOL	C3-C2	-7.82	1.22	1.52
3	C	1002	GOL	C1-C2	-3.38	1.39	1.52
3	A	1001	GOL	C1-C2	-2.94	1.41	1.52
3	C	1002	GOL	O2-C2	-2.81	1.35	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	GOL	O1-C1-C2	3.07	125.08	110.18
3	A	1001	GOL	O1-C1-C2	3.32	126.26	110.18
3	A	1001	GOL	O2-C2-C3	6.35	137.78	108.65
3	C	1002	GOL	O2-C2-C3	6.43	138.15	108.65
3	C	1002	GOL	O3-C3-C2	10.32	160.25	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	GOL	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.