



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 07:09 PM UTC

PDB ID : 1KP0 / pdb_00001kp0
Title : The Crystal Structure Analysis of Creatine Amidinohydrolase from Actinobacillus
Authors : Padmanabhan, B.; Paehler, A.; Horikoshi, M.
Deposited on : 2001-12-26
Resolution : 2.70 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)	:	2.0
EDS	:	FAILED
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

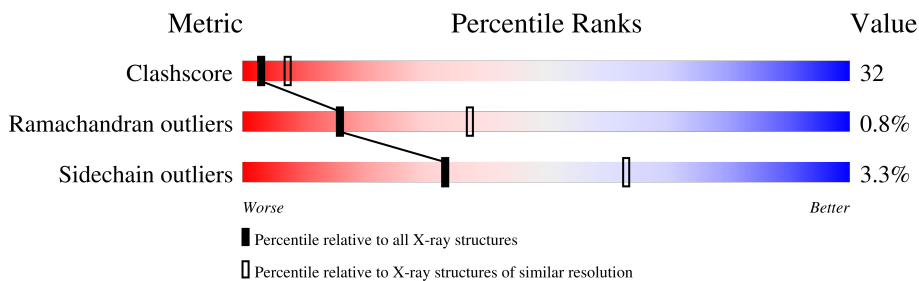
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	402	
1	B	402	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6586 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 CREATINE AMIDINOHYDROLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	X	0	0	0
			3234	2050	547	547	16	74			
1	B	402	Total	C	N	O	S	X	0	0	0
			3234	2050	547	547	16	74			

- Molecule 2 is water.

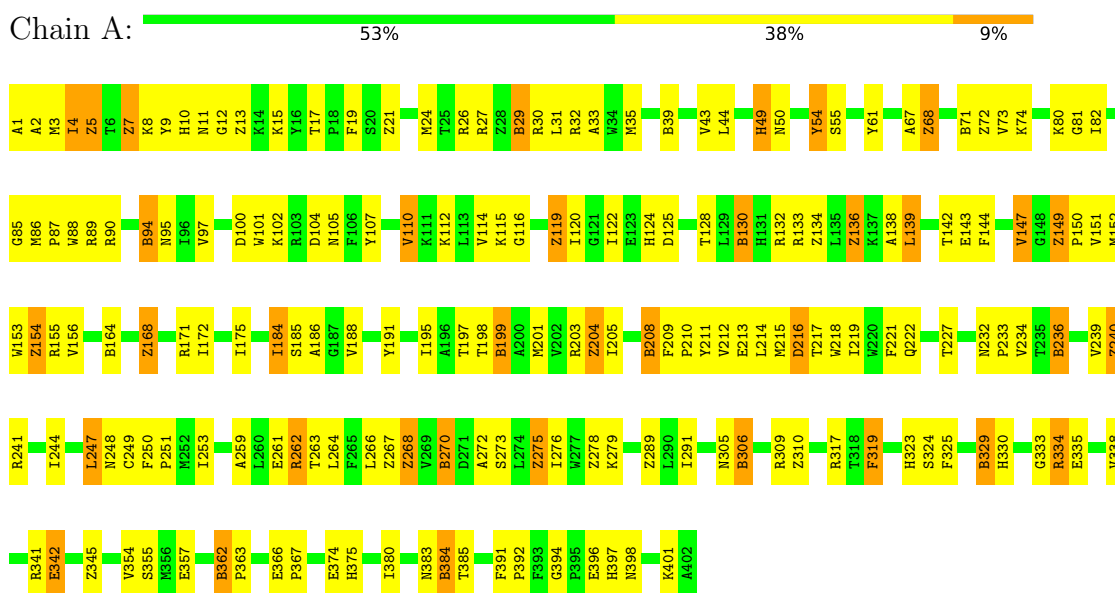
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	57	Total	O	0	0
			57	57		
2	B	61	Total	O	0	0
			61	61		

3 Residue-property plots

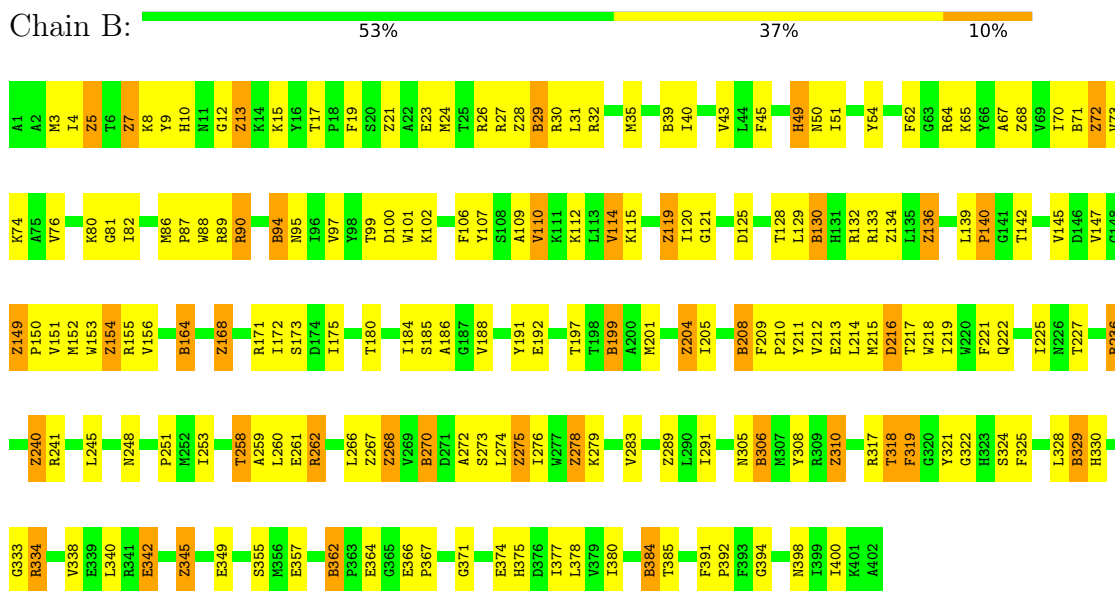
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

• Molecule 1: CREATINE AMIDINOHYDROLASE



• Molecule 1: CREATINE AMIDINOHYDROLASE



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	111.26Å 113.62Å 191.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.6 (30.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.12 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.188 , 0.222	Depositor
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.317	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
Total number of atoms	6586	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	1.14	33/2993 (1.1%)	0.95	14/4053 (0.3%)
1	B	1.15	33/2993 (1.1%)	0.92	11/4053 (0.3%)
All	All	1.15	66/5986 (1.1%)	0.93	25/8106 (0.3%)

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	GLX	C-N	-11.08	1.32	1.43
1	B	208	ASX	C-N	-10.76	1.32	1.43
1	B	275	GLX	C-N	-10.76	1.32	1.43
1	A	68	GLX	C-N	-10.72	1.32	1.43
1	B	164	ASX	C-N	-10.67	1.32	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ASN	N-CA-C	10.08	123.96	112.57
1	B	398	ASN	N-CA-C	8.22	121.86	112.57
1	A	139	LEU	CA-C-N	7.62	129.37	119.84
1	A	139	LEU	C-N-CA	7.62	129.37	119.84
1	A	394	GLY	CA-C-N	6.97	126.95	119.28

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	3234	0	3106	206	0
1	B	3234	0	3106	212	0
2	A	57	0	0	5	0
2	B	61	0	0	4	0
All	All	6586	0	6212	401	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 32.

The worst 5 of 401 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:B:71:ASX:XD1	1:B:74:LYS:H	1.61	1.13
1:A:201:MET:HE2	1:A:219:ILE:HD11	1.39	1.05
1:A:71:ASX:XD1	1:A:74:LYS:H	1.74	1.01
1:A:380:ILE:HA	1:A:385:THR:HG22	1.39	1.01
1:B:171:ARG:HH22	1:B:204:GLX:XE2	1.73	1.01

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	363/402 (90%)	347 (96%)	13 (4%)	3 (1%)	16	37
1	B	363/402 (90%)	353 (97%)	7 (2%)	3 (1%)	16	37
All	All	726/804 (90%)	700 (96%)	20 (3%)	6 (1%)	16	37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	140	PRO
1	B	216	ASP
1	A	334	ARG
1	B	334	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	301/301 (100%)	294 (98%)	7 (2%)	44	73
1	B	301/301 (100%)	288 (96%)	13 (4%)	26	54
All	All	602/602 (100%)	582 (97%)	20 (3%)	33	63

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	140	PRO
1	B	318	THR
1	B	349	GLU
1	B	328	LEU
1	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	ASN
1	B	124	HIS
1	B	305	ASN
1	B	231	HIS
1	A	397	HIS

5.3.3 RNA ⓘ

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 [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.