



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:30 AM UTC

PDB ID : 1CHM / pdb_00001chm
Title : ENZYMATIC MECHANISM OF CREATINE AMIDINOHYDROLASE AS DEDUCED FROM CRYSTAL STRUCTURES
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Deposited on : 1993-07-19
Resolution : 1.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

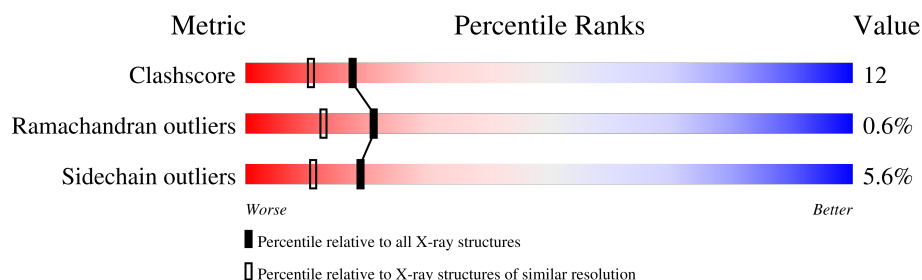
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	401	
1	B	401	

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
2	CMS	A	404	-	X	-	-

2 Entry composition [i](#)

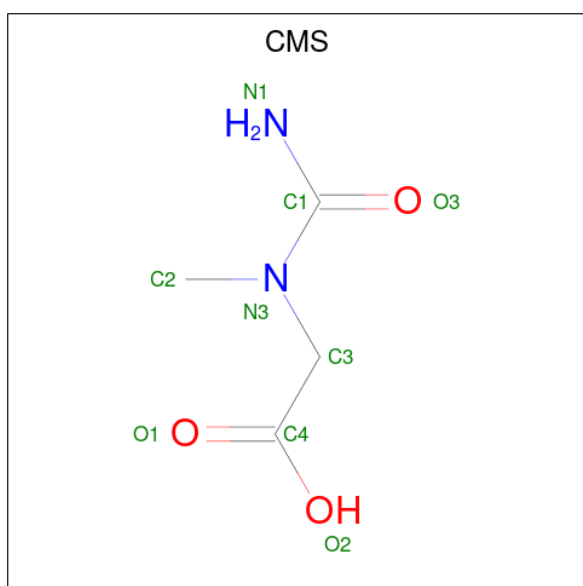
There are 3 unique types of molecules in this entry. The entry contains 6786 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	401	Total	C	N	O	S	89	0	0
			3187	2004	568	598	17			
1	B	401	Total	C	N	O	S	96	0	0
			3187	2004	568	598	17			

- Molecule 2 is CARBAMOYL SARCOSINE (CCD ID: CMS) (formula: $C_4H_8N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	2	3		
2	B	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 3 is water.

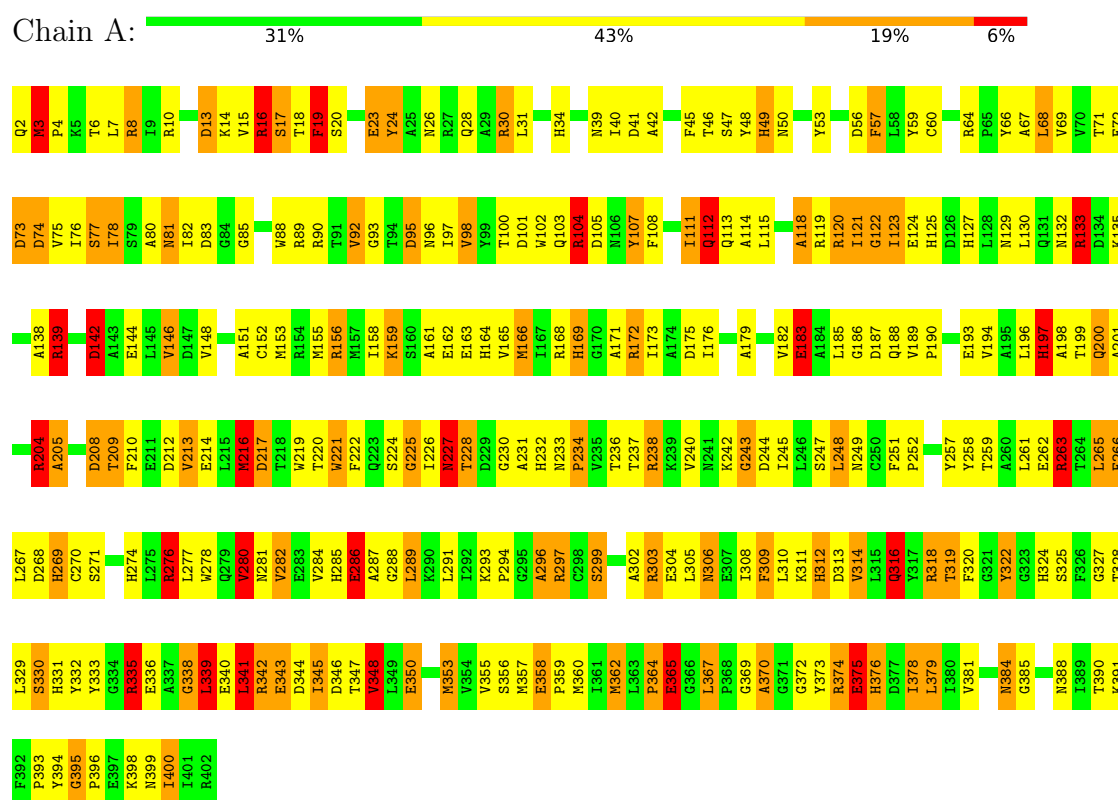
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total 198	O 198	0	0
3	B	196	Total 196	O 196	0	0

3 Residue-property plots

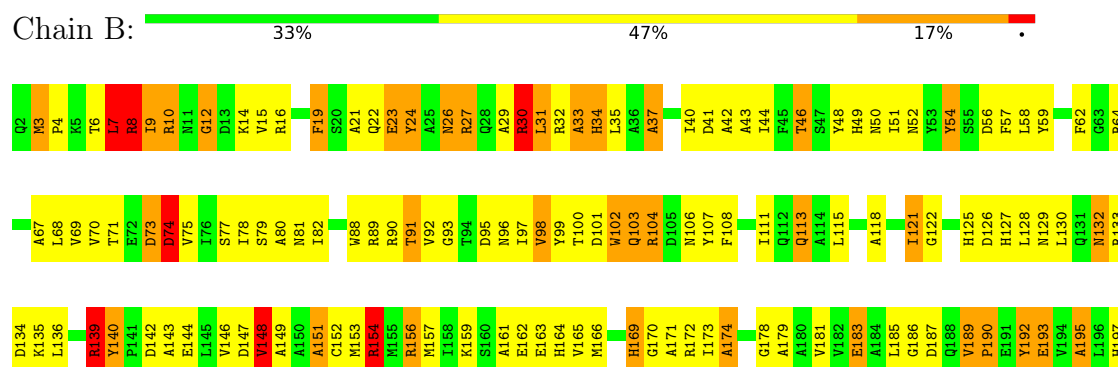
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: CREATINE AMIDINOHYDROLASE



• Molecule 1: CREATINE AMIDINOHYDROLASE



A198	T199	Q200	A201	M202	V203	R204	A205	I206	A207	D208	T209	F210	V213	E214	L215	M216	D217	T218	W219	T220	W221	F222	G225	I226	N227	T228	A231	H232	N233	P234	V235	R238	K242	G243	D244	S247	L248	F251	P252	M253	I254	A255	G256	Y257	T258	A260	L261	E262	R263	T264	L265	
F266	L267	D268	H269	C270	S271	D272	D273	H274	L275	R276	L277	W278	Q279	V280	N281	V284	H285	E286	G287	G288	L291	I292	K293	P294	R297	C298	I301	A302	R303	N306	K311	H312	D313	V314	Y317	R318	T319	F320	G321	Y322	G323	H324	S325	F326	G327	T328	L329	S330	H331	Y332	Y333	G334
R335	E336	A337	G338	L339	E340	L341	R342	D346	E350	M353	V354	V355	S356	M357	E358	P359	M360	I361	M362	L363	P364	E365	G366	L367	F368	G369	A370	G371	G372	E375	H376	D377	I378	L379	N382	E383	N384	K391	F392	P393	Y394	G395	K398	N399	I400	I401	R402					

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.83Å 110.55Å 62.63Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6786	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: CMS

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	2.47	166/3257 (5.1%)	2.79	240/4416 (5.4%)
1	B	2.42	152/3257 (4.7%)	2.65	255/4416 (5.8%)
All	All	2.44	318/6514 (4.9%)	2.72	495/8832 (5.6%)

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	A	6	69
1	B	5	44
All	All	11	113

The worst 5 of 318 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	324	HIS	ND1-CE1	18.14	1.50	1.32
1	B	197	HIS	CE1-NE2	17.37	1.50	1.32
1	A	34	HIS	CE1-NE2	16.90	1.49	1.32
1	A	312	HIS	ND1-CE1	16.20	1.48	1.32
1	A	274	HIS	ND1-CE1	15.40	1.48	1.32

The worst 5 of 495 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	GLN	OE1-CD-NE2	46.97	169.56	122.60
1	A	263	ARG	NE-CZ-NH2	-28.11	93.91	119.20
1	A	200	GLN	CG-CD-OE1	-21.48	77.85	120.80
1	B	89	ARG	NE-CZ-NH1	-21.00	100.50	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	NE-CZ-NH1	-20.96	100.54	121.50

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2	GLN	CA
1	A	71	THR	CB
1	A	104	ARG	CA
1	A	228	THR	CB
1	A	319	THR	CB

5 of 113 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASP	Mainchain
1	A	14	LYS	Mainchain
1	A	16	ARG	Mainchain
1	A	6	THR	Mainchain
1	A	8	ARG	Sidechain

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	A	3187	0	3097	77	0
1	B	3187	0	3097	75	0
2	A	9	0	7	1	0
2	B	9	0	7	2	0
3	A	198	0	0	3	0
3	B	196	0	0	5	0
All	All	6786	0	6208	151	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 12.

The worst 5 of 151 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:263:ARG:HD3	1:A:393:PRO:O	1.81	0.80
1:B:71:THR:HG23	1:B:73:ASP:H	1.46	0.80
1:A:71:THR:HG23	1:A:73:ASP:H	1.46	0.80
1:A:225:GLY:O	1:A:228:THR:HG22	1.82	0.78
1:B:263:ARG:HD3	1:B:393:PRO:O	1.85	0.75

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	399/401 (100%)	377 (94%)	19 (5%)	3 (1%)	16	8
1	B	399/401 (100%)	377 (94%)	20 (5%)	2 (0%)	24	16
All	All	798/802 (100%)	754 (94%)	39 (5%)	5 (1%)	21	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	ASP
1	A	3	MET
1	A	217	ASP
1	A	335	ARG
1	B	335	ARG

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	333/333 (100%)	312 (94%)	21 (6%)	16	8
1	B	333/333 (100%)	317 (95%)	16 (5%)	23	15
All	All	666/666 (100%)	629 (94%)	37 (6%)	19	11

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	204	ARG
1	B	363	LEU
1	B	208	ASP
1	B	268	ASP
1	A	263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	GLN
1	B	169	HIS
1	B	132	ASN
1	B	188	GLN
1	A	169	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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
2	CMS	A	404	-	8,8,8	2.28	3 (37%)	9,10,10	4.89	5 (55%)
2	CMS	B	404	-	8,8,8	1.45	1 (12%)	9,10,10	3.09	2 (22%)

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
2	CMS	A	404	-	-	5/8/8/8	-
2	CMS	B	404	-	-	5/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	404	CMS	C1-N3	5.07	1.41	1.34
2	A	404	CMS	C3-N3	2.95	1.51	1.46
2	B	404	CMS	C1-N1	2.66	1.38	1.34
2	A	404	CMS	O2-C4	-2.13	1.23	1.30

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	404	CMS	C2-N3-C3	-12.37	98.65	116.89
2	B	404	CMS	C2-N3-C3	-8.23	104.76	116.89
2	A	404	CMS	O3-C1-N1	-4.96	112.97	122.63
2	A	404	CMS	C4-C3-N3	4.51	121.43	113.16
2	A	404	CMS	N1-C1-N3	-3.51	116.14	119.79

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	404	CMS	N1-C1-N3-C2
2	A	404	CMS	N1-C1-N3-C3
2	A	404	CMS	O3-C1-N3-C2
2	A	404	CMS	O3-C1-N3-C3
2	A	404	CMS	C4-C3-N3-C1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	CMS	1	0
2	B	404	CMS	2	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

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.