wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:47 PM GMT

PDB ID	:	1CHM
Title	:	ENZYMATIC MECHANISM OF CREATINE AMIDINOHYDROLASE AS DEDUCED FROM CRYSTAL STRUCTURES
Authors	:	Hoeffken, H.W.; Knof, S.H.; Bartlett, P.A.; Huber, R.; Moellering, H.; Schumacher, G.
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

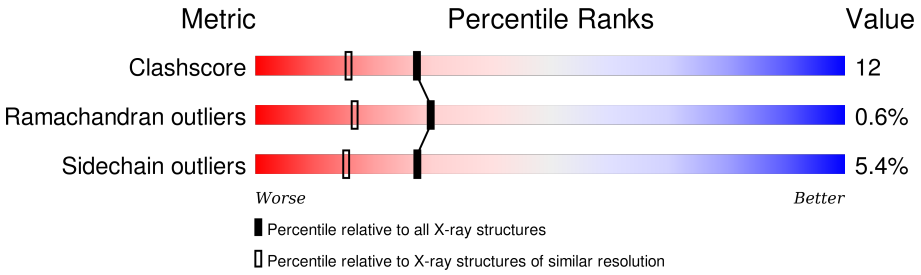
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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 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 <=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	401	51% 31% 15% •
1	B	401	56% 34% 7% •

2 Entry composition (i)

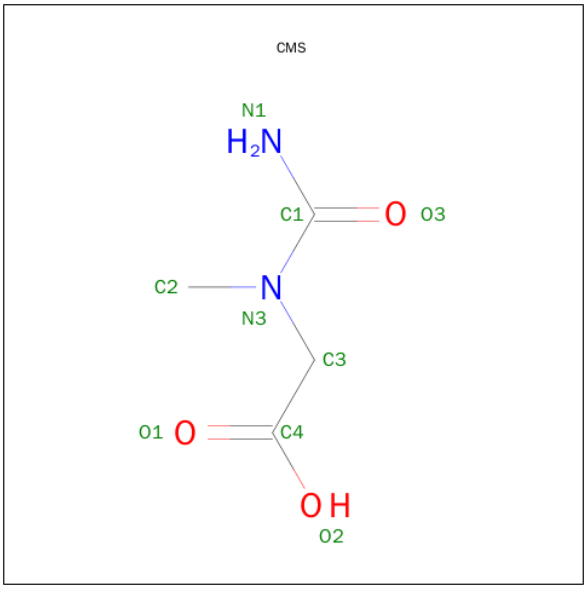
There are 3 unique types of molecules in this entry. The entry contains 6786 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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 O 198 198	0	0
3	B	196	Total O 196 196	0	0

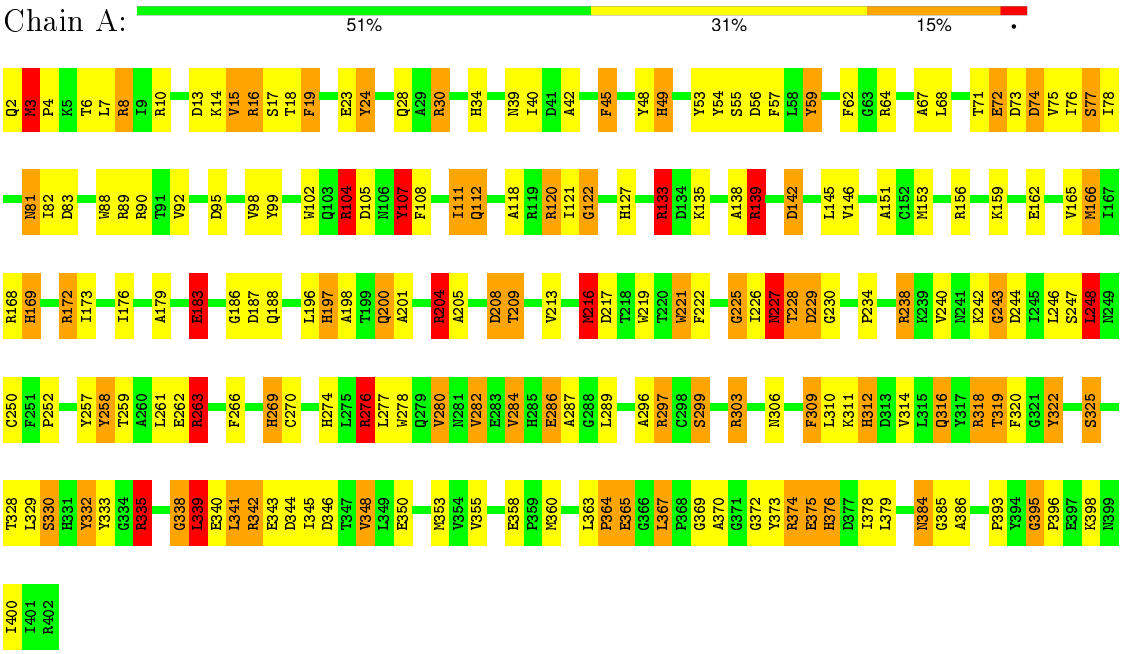
3 Residue-property plots (i)

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 (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.

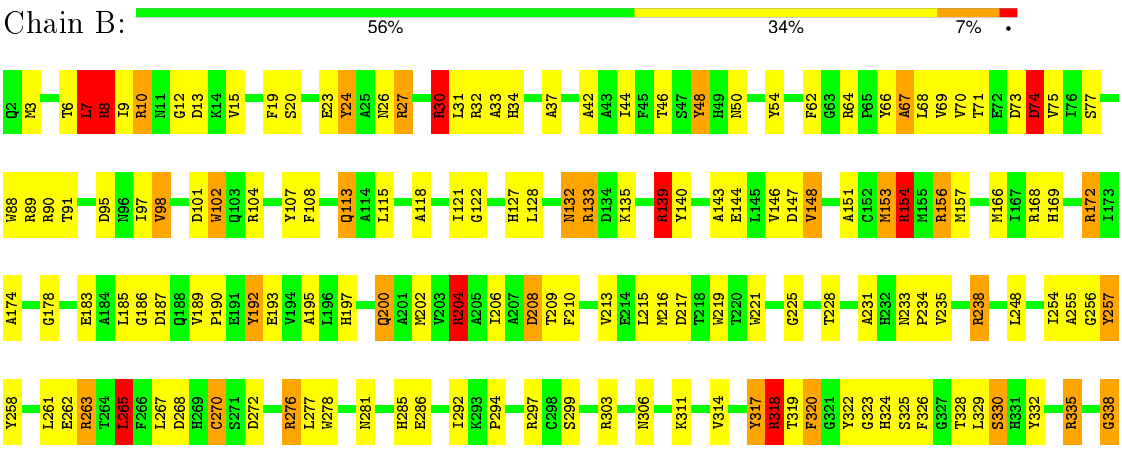
- Molecule 1: CREATINE AMIDINOHYDROLASE

Chain A:



- Molecule 1: CREATINE AMIDINOHYDROLASE

Chain B:




L339
R342
D346
V355
S356
M357
E358
L363
P364
E365
G366
L367
A370
G371
G372
Y373
R374
E375
H376
D377
I378
L379
N382
E383
A386
K391
F392
P393
N399
T400
T401
R402

4 Data and refinement statistics (i)

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

5.1 Standard geometry

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	1.76	48/3257 (1.5%)	2.62	122/4416 (2.8%)
1	B	1.72	36/3257 (1.1%)	2.37	115/4416 (2.6%)
All	All	1.74	84/6514 (1.3%)	2.50	237/8832 (2.7%)

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 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	GLU	CD-OE1	9.84	1.36	1.25
1	A	276	ARG	NE-CZ	9.07	1.44	1.33
1	A	263	ARG	NE-CZ	-8.96	1.21	1.33
1	A	365	GLU	CD-OE2	8.52	1.35	1.25
1	B	219	TRP	NE1-CE2	-8.00	1.27	1.37

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	263	ARG	NE-CZ-NH2	-52.79	93.91	120.30
1	B	89	ARG	NE-CZ-NH1	-39.61	100.50	120.30
1	A	64	ARG	NE-CZ-NH1	-39.52	100.54	120.30
1	A	263	ARG	NE-CZ-NH1	38.24	139.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	ARG	NE-CZ-NH1	-36.95	101.82	120.30

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 (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	3187	0	3097	72	0
1	B	3187	0	3096	74	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	6207	145	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 145 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%)	24	11
1	B	399/401 (100%)	377 (94%)	20 (5%)	2 (0%)	34	21
All	All	798/802 (100%)	754 (94%)	39 (5%)	5 (1%)	30	17

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%)	311 (93%)	22 (7%)	21 10
1	B	333/333 (100%)	319 (96%)	14 (4%)	36 24
All	All	666/666 (100%)	630 (95%)	36 (5%)	27 15

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	SER
1	A	339	LEU
1	B	329	LEU
1	A	314	VAL
1	A	341	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	B	26	ASN
1	B	169	HIS
1	A	197	HIS
1	A	306	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	-	4,8,8	0.83	0	3,10,10	4.36	3 (100%)
2	CMS	B	404	-	4,8,8	1.61	1 (25%)	3,10,10	1.73	1 (33%)

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	-	-	0/6/8/8	0/0/0/0
2	CMS	B	404	-	-	1/6/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	404	CMS	C1-N1	2.90	1.38	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	404	CMS	O3-C1-N1	-5.64	112.97	122.88
2	A	404	CMS	C2-N3-C3	-3.58	98.65	116.43
2	B	404	CMS	C2-N3-C3	-2.35	104.76	116.43
2	A	404	CMS	C4-C3-N3	3.52	121.43	113.84

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	404	CMS	N1-C1-N3-C3

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 will therefore be empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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