



# wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 07:02 PM GMT

PDB ID : 1HQH  
Title : CRYSTAL STRUCTURE OF THE BINUCLEAR MANGANESE METALLOENZYME ARGINASE COMPLEXED WITH NOR-N-HYDROXY-L-ARGININE  
Authors : Cox, J.D.; Cama, E.; Colleluori, D.M.; Ash, D.E.; Christianson, D.W.  
Deposited on : 2000-12-16  
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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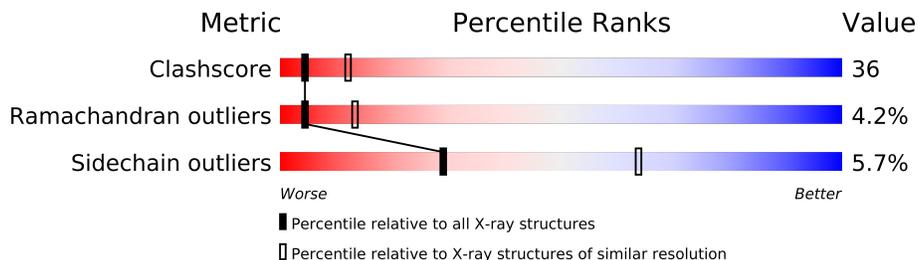
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	
1	C	323	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7248 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

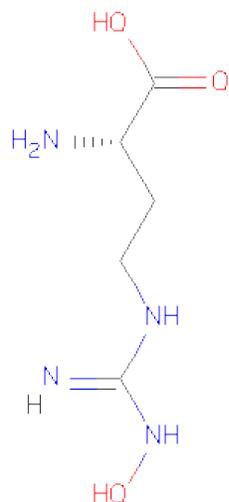
- Molecule 1 is a protein called ARGINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2395	1528	405	455	7	0	0	0
1	B	314	2395	1528	405	455	7	0	0	0
1	C	314	2395	1528	405	455	7	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is NOR-N-OMEGA-HYDROXY-L-ARGININE (three-letter code: NNH) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	5	4	3	0	0
3	B	1	12	5	4	3	0	0
3	C	1	12	5	4	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	5	5	5	0	0
4	B	8	8	8	0	0
4	C	8	8	8	0	0

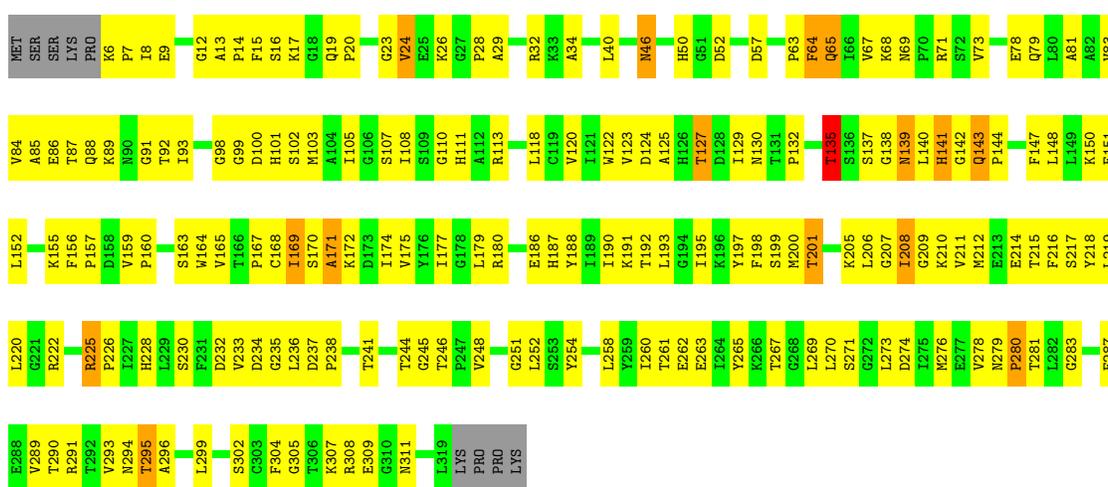
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

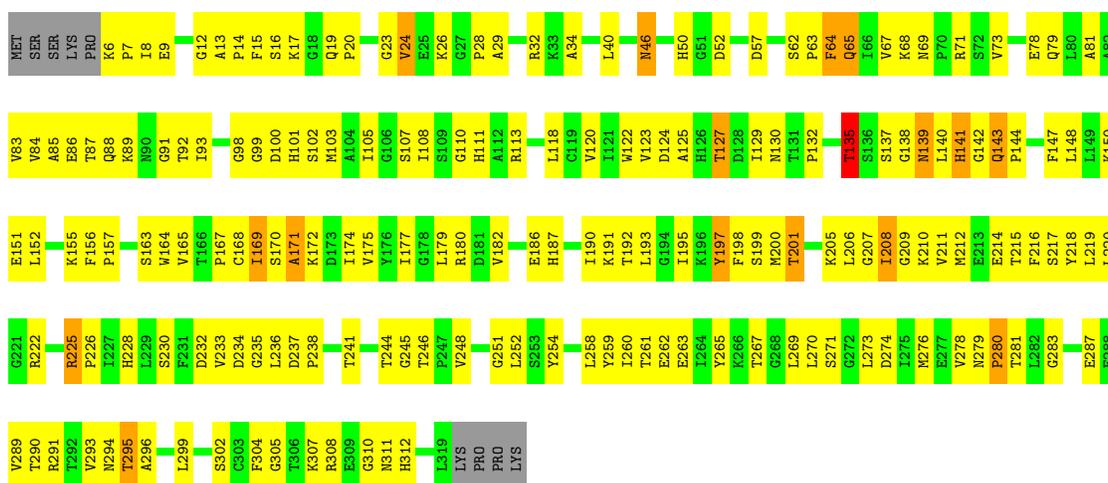
- Molecule 1: ARGINASE 1

Chain A:



- Molecule 1: ARGINASE 1

Chain B:



- Molecule 1: ARGINASE 1

Chain C: 

MET	V63	E151	Y218	E287
SER	V64	L152	L219	E288
SER	A85	K155	L220	V289
LYS	A86	G221	G221	T290
PRO	T87	F156	R222	R291
K6	Q88	P157	R225	T292
P7	K89	D158	P226	V293
I8	R90	V159	P227	M294
E9	G91	P160	L227	T295
G12	T92	S163	H228	A296
A13	I93	W164	L229	L299
P14	G98	V165	S230	S302
F15	G99	T166	D232	C303
S16	G99	P167	V233	F304
K17	D100	C168	D234	G305
G18	H101	I169	G235	T306
Q19	S102	S170	L236	K307
P20	M103	A171	D237	R308
P20	A104	K172	P238	N311
G23	I105	D173	T241	H312
V24	G106	I174	T244	K313
E25	S107	W175	G245	P314
K26	I108	Y176	T246	D317
G27	S109	I177	T247	Y318
P28	G110	G176	V248	L319
A29	H111	L179	G251	LYS
R32	A112	R180	L252	PRO
K33	L118	E186	S253	PRO
A34	C119	H187	Y254	LYS
L40	V120	Y188	L258	
L40	I121	I189	Y259	
M46	W122	I190	L260	
H50	V123	K191	T261	
G51	D124	L192	E262	
D52	A125	L193	E263	
D57	H126	G194	I264	
S62	I127	I195	Y265	
P63	D128	K196	K266	
F64	I129	F198	T267	
Q65	N130	S199	G268	
V67	T131	M200	L269	
K68	P132	T201	L270	
M69	T136	D204	S271	
F70	S136	K205	G272	
S72	G138	L206	L273	
V73	N139	G207	D274	
R71	L140	I208	I275	
G72	H141	G209	M276	
V73	G142	K210	E277	
E78	Q143	V211	V278	
Q79	P144	N212	N279	
L80	F147	E214	P280	
A81	L148	T215	T281	
A82	L149	F216	L282	
	K150	S217	G283	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.00Å 88.00Å 112.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.80)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.286 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	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: MN, NNH

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	0.41	0/2448	0.69	0/3325
1	B	0.41	0/2448	0.69	0/3325
1	C	0.41	0/2448	0.69	0/3325
All	All	0.41	0/7344	0.69	0/9975

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2395	0	2420	174	0
1	B	2395	0	2420	177	0
1	C	2395	0	2420	189	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	12	0	10	0	0
3	B	12	0	10	0	0
3	C	12	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
All	All	7248	0	7290	517	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

The worst 5 of 517 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:175:VAL:HG11	1:B:215:THR:HG22	1.45	0.98
1:C:175:VAL:HG11	1:C:215:THR:HG22	1.45	0.97
1:A:175:VAL:HG11	1:A:215:THR:HG22	1.45	0.96
1:B:143:GLN:H	1:B:144:PRO:CD	1.88	0.86
1:B:140:LEU:O	1:B:144:PRO:HD3	1.75	0.86

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	312/323 (97%)	245 (78%)	54 (17%)	13 (4%)	4	13
1	B	312/323 (97%)	244 (78%)	55 (18%)	13 (4%)	4	13
1	C	312/323 (97%)	245 (78%)	54 (17%)	13 (4%)	4	13
All	All	936/969 (97%)	734 (78%)	163 (17%)	39 (4%)	4	13

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PHE
1	A	143	GLN
1	B	64	PHE

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Mol	Chain	Res	Type
1	B	143	GLN
1	C	64	PHE

### 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	264/273 (97%)	249 (94%)	15 (6%)	29	64
1	B	264/273 (97%)	249 (94%)	15 (6%)	29	64
1	C	264/273 (97%)	249 (94%)	15 (6%)	29	64
All	All	792/819 (97%)	747 (94%)	45 (6%)	29	64

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	141	HIS
1	B	225	ARG
1	C	238	PRO
1	B	169	ILE
1	B	238	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	143	GLN
1	C	139	ASN
1	B	79	GLN
1	C	143	GLN

### 5.3.3 RNA (i)

There are no RNA chains 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)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	NNH	A	901	2	11,11,11	2.13	2 (18%)	13,13,13	1.92	5 (38%)
3	NNH	B	902	2	11,11,11	2.13	2 (18%)	13,13,13	1.92	5 (38%)
3	NNH	C	903	2	11,11,11	2.13	2 (18%)	13,13,13	1.91	5 (38%)

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	NNH	A	901	2	-	0/11/12/12	0/0/0/0
3	NNH	B	902	2	-	0/11/12/12	0/0/0/0
3	NNH	C	903	2	-	0/11/12/12	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	NNH	OH1-NH1	-5.30	1.30	1.39
3	C	903	NNH	OH1-NH1	-5.30	1.30	1.39
3	A	901	NNH	OH1-NH1	-5.30	1.30	1.39
3	B	902	NNH	CE-NH1	3.76	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NNH	CE-NH1	3.75	1.44	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	NNH	CG-ND-CE	3.21	129.66	124.03
3	C	903	NNH	CG-ND-CE	3.21	129.66	124.03
3	B	902	NNH	CG-ND-CE	3.20	129.65	124.03
3	C	903	NNH	O-C-CA	2.82	126.49	118.36
3	B	902	NNH	O-C-CA	2.82	126.49	118.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.