



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2016 – 11:30 AM EDT

PDB ID : 5K1S  
Title : crystal structure of AibC  
Authors : Bock, T.; Mueller, R.; Blankenfeldt, W.  
Deposited on : 2016-05-18  
Resolution : 2.55 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](mailto: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.

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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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

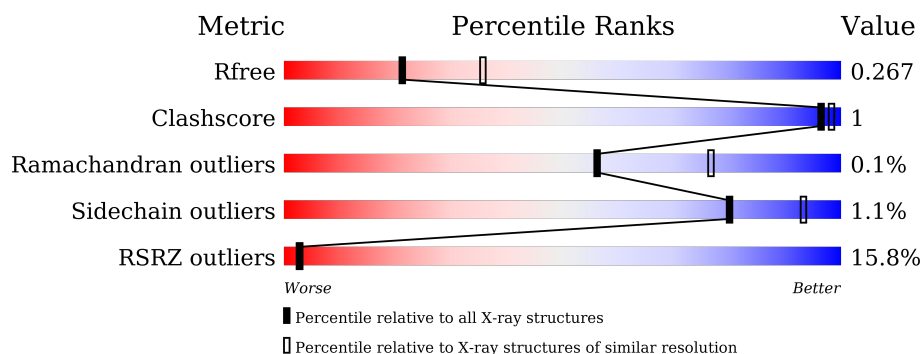
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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. 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.

Mol	Chain	Length	Quality of chain
1	A	362	<div> <div>8%</div> <div>94%</div> <div>5%</div> </div>
1	B	362	<div> <div>24%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>
1	C	362	<div> <div>8%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
1	D	362	<div> <div>20%</div> <div>90%</div> <div>.</div> <div>8%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	C	402	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19587 atoms, of which 9631 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 Oxidoreductase, zinc-binding dehydrogenase family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	358	Total	C	H	N	O	S	0	1	0
			5116	1607	2529	476	488	16			
1	C	358	Total	C	H	N	O	S	0	0	0
			5033	1588	2480	469	480	16			
1	B	333	Total	C	H	N	O	S	0	0	0
			4641	1453	2298	426	449	15			
1	D	333	Total	C	H	N	O	S	0	0	0
			4682	1467	2324	423	452	16			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q1D4I2
A	-15	GLY	-	expression tag	UNP Q1D4I2
A	-14	HIS	-	expression tag	UNP Q1D4I2
A	-13	HIS	-	expression tag	UNP Q1D4I2
A	-12	HIS	-	expression tag	UNP Q1D4I2
A	-11	HIS	-	expression tag	UNP Q1D4I2
A	-10	HIS	-	expression tag	UNP Q1D4I2
A	-9	HIS	-	expression tag	UNP Q1D4I2
A	-8	ALA	-	expression tag	UNP Q1D4I2
A	-7	GLU	-	expression tag	UNP Q1D4I2
A	-6	ASN	-	expression tag	UNP Q1D4I2
A	-5	LEU	-	expression tag	UNP Q1D4I2
A	-4	TYR	-	expression tag	UNP Q1D4I2
A	-3	PHE	-	expression tag	UNP Q1D4I2
A	-2	GLN	-	expression tag	UNP Q1D4I2
A	-1	GLY	-	expression tag	UNP Q1D4I2
A	0	HIS	-	expression tag	UNP Q1D4I2
C	-16	MET	-	initiating methionine	UNP Q1D4I2
C	-15	GLY	-	expression tag	UNP Q1D4I2
C	-14	HIS	-	expression tag	UNP Q1D4I2
C	-13	HIS	-	expression tag	UNP Q1D4I2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q1D4I2
C	-11	HIS	-	expression tag	UNP Q1D4I2
C	-10	HIS	-	expression tag	UNP Q1D4I2
C	-9	HIS	-	expression tag	UNP Q1D4I2
C	-8	ALA	-	expression tag	UNP Q1D4I2
C	-7	GLU	-	expression tag	UNP Q1D4I2
C	-6	ASN	-	expression tag	UNP Q1D4I2
C	-5	LEU	-	expression tag	UNP Q1D4I2
C	-4	TYR	-	expression tag	UNP Q1D4I2
C	-3	PHE	-	expression tag	UNP Q1D4I2
C	-2	GLN	-	expression tag	UNP Q1D4I2
C	-1	GLY	-	expression tag	UNP Q1D4I2
C	0	HIS	-	expression tag	UNP Q1D4I2
B	-16	MET	-	initiating methionine	UNP Q1D4I2
B	-15	GLY	-	expression tag	UNP Q1D4I2
B	-14	HIS	-	expression tag	UNP Q1D4I2
B	-13	HIS	-	expression tag	UNP Q1D4I2
B	-12	HIS	-	expression tag	UNP Q1D4I2
B	-11	HIS	-	expression tag	UNP Q1D4I2
B	-10	HIS	-	expression tag	UNP Q1D4I2
B	-9	HIS	-	expression tag	UNP Q1D4I2
B	-8	ALA	-	expression tag	UNP Q1D4I2
B	-7	GLU	-	expression tag	UNP Q1D4I2
B	-6	ASN	-	expression tag	UNP Q1D4I2
B	-5	LEU	-	expression tag	UNP Q1D4I2
B	-4	TYR	-	expression tag	UNP Q1D4I2
B	-3	PHE	-	expression tag	UNP Q1D4I2
B	-2	GLN	-	expression tag	UNP Q1D4I2
B	-1	GLY	-	expression tag	UNP Q1D4I2
B	0	HIS	-	expression tag	UNP Q1D4I2
D	-16	MET	-	initiating methionine	UNP Q1D4I2
D	-15	GLY	-	expression tag	UNP Q1D4I2
D	-14	HIS	-	expression tag	UNP Q1D4I2
D	-13	HIS	-	expression tag	UNP Q1D4I2
D	-12	HIS	-	expression tag	UNP Q1D4I2
D	-11	HIS	-	expression tag	UNP Q1D4I2
D	-10	HIS	-	expression tag	UNP Q1D4I2
D	-9	HIS	-	expression tag	UNP Q1D4I2
D	-8	ALA	-	expression tag	UNP Q1D4I2
D	-7	GLU	-	expression tag	UNP Q1D4I2
D	-6	ASN	-	expression tag	UNP Q1D4I2
D	-5	LEU	-	expression tag	UNP Q1D4I2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	TYR	-	expression tag	UNP Q1D4I2
D	-3	PHE	-	expression tag	UNP Q1D4I2
D	-2	GLN	-	expression tag	UNP Q1D4I2
D	-1	GLY	-	expression tag	UNP Q1D4I2
D	0	HIS	-	expression tag	UNP Q1D4I2

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

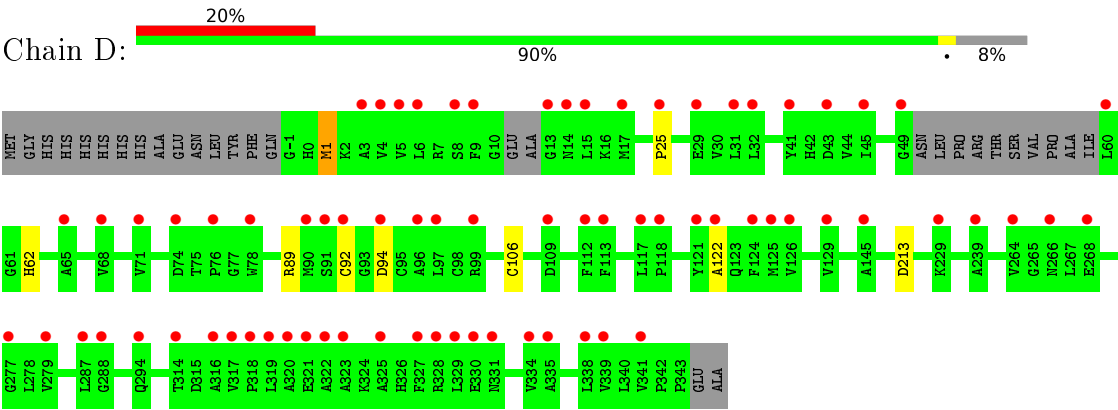
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total 42	O 42	0	0
3	C	35	Total 35	O 35	0	0
3	B	18	Total 18	O 18	0	0
3	D	12	Total 12	O 12	0	0



● Molecule 1: Oxidoreductase, zinc-binding dehydrogenase family





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.29Å 77.43Å 309.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.94 – 2.55 44.67 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.94-2.55) 100.0 (44.67-2.55)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.234 , 0.269 0.228 , 0.267	Depositor DCC
$R_{free}$ test set	3084 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/2633	0.42	0/3582
1	B	0.25	0/2374	0.43	0/3230
1	C	0.25	0/2596	0.42	0/3537
1	D	0.25	0/2390	0.43	0/3248
All	All	0.25	0/9993	0.43	0/13597

There are no bond length outliers.

There are no bond angle outliers.

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	2587	2529	2543	9	1
1	B	2343	2298	2297	10	0
1	C	2553	2480	2481	6	2
1	D	2358	2324	2323	3	0
2	A	2	0	0	0	1
2	B	2	0	0	0	0
2	C	2	0	0	0	2
2	D	2	0	0	0	0
3	A	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	0	0	0
3	C	35	0	0	1	0
3	D	12	0	0	0	0
All	All	9956	9631	9644	27	3

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 1.

The worst 5 of 27 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:89:ARG:NH2	1:B:106:CYS:O	2.10	0.84
1:C:75:THR:O	3:C:501:HOH:O	2.01	0.79
1:A:10:GLY:O	1:A:47:ARG:NH1	2.16	0.78
1:C:77:GLY:O	1:C:134:ARG:NH1	2.21	0.73
1:C:24:ARG:NH2	1:C:70:GLU:OE2	2.27	0.67

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:HIS:HE2	2:C:402:ZN:ZN[3_545]	1.43	0.17
1:C:149:CYS:HG	2:C:402:ZN:ZN[3_545]	1.54	0.06
1:A:-9:HIS:HE2	2:A:402:ZN:ZN[4_556]	1.56	0.04

## 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	357/362 (99%)	340 (95%)	17 (5%)	0	100	100
1	B	329/362 (91%)	312 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	356/362 (98%)	339 (95%)	16 (4%)	1 (0%)	46	66
1	D	327/362 (90%)	309 (94%)	17 (5%)	1 (0%)	46	66
All	All	1369/1448 (94%)	1300 (95%)	67 (5%)	2 (0%)	56	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-1	GLY
1	D	25	PRO

### 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	261/277 (94%)	259 (99%)	2 (1%)	86	96
1	B	232/277 (84%)	228 (98%)	4 (2%)	68	88
1	C	251/277 (91%)	250 (100%)	1 (0%)	93	98
1	D	236/277 (85%)	232 (98%)	4 (2%)	68	88
All	All	980/1108 (88%)	969 (99%)	11 (1%)	80	93

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	92	CYS
1	D	62	HIS
1	B	17	MET
1	D	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	358/362 (98%)	0.74	29 (8%) 15 16	35, 61, 99, 127	0
1	B	333/362 (91%)	1.55	86 (25%) 1 1	41, 85, 141, 180	0
1	C	358/362 (98%)	0.74	29 (8%) 15 16	41, 64, 106, 132	0
1	D	333/362 (91%)	1.36	74 (22%) 1 1	36, 79, 133, 166	0
All	All	1382/1448 (95%)	1.09	218 (15%) 3 3	35, 69, 124, 180	0

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	VAL	12.9
1	D	320	ALA	11.4
1	B	329	LEU	8.8
1	B	327	PHE	8.3
1	D	327	PHE	8.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	402	1/1	0.97	0.23	1.04	89,89,89,89	0
2	ZN	A	401	1/1	0.97	0.18	0.48	67,67,67,67	0
2	ZN	B	401	1/1	0.94	0.24	0.06	108,108,108,108	0
2	ZN	C	401	1/1	0.99	0.16	-0.13	61,61,61,61	0
2	ZN	A	402	1/1	0.99	0.17	-0.55	70,70,70,70	0
2	ZN	D	401	1/1	0.85	0.16	-0.79	117,117,117,117	0
2	ZN	B	402	1/1	0.92	0.05	-2.38	107,107,107,107	0
2	ZN	D	402	1/1	0.86	0.06	-3.10	107,107,107,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.