



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 02:56 pm GMT

PDB ID : 3OZX  
Title : Crystal structure of ABCE1 of Sulfolobus solfataricus (-FeS domain)  
Authors : Barthelme, D.; Tampe, R.  
Deposited on : 2010-09-27  
Resolution : 2.05 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

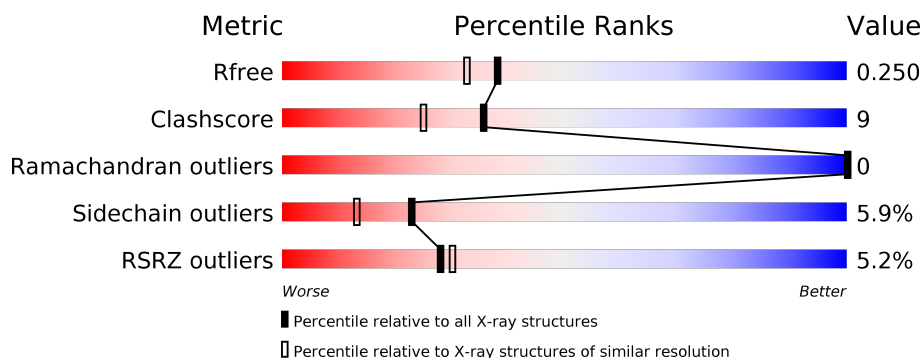
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	538	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	538	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8757 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 RNase L inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4118	2640	703	767	8			
1	B	515	Total	C	N	O	S	0	0	0
			4127	2645	705	769	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	EXPRESSION TAG	UNP Q980K5
A	238	GLN	GLU	ENGINEERED MUTATION	UNP Q980K5
A	485	GLN	GLU	ENGINEERED MUTATION	UNP Q980K5
A	601	GLY	-	EXPRESSION TAG	UNP Q980K5
A	602	SER	-	EXPRESSION TAG	UNP Q980K5
A	603	ILE	-	EXPRESSION TAG	UNP Q980K5
A	604	GLU	-	EXPRESSION TAG	UNP Q980K5
A	605	GLY	-	EXPRESSION TAG	UNP Q980K5
A	606	ARG	-	EXPRESSION TAG	UNP Q980K5
A	607	HIS	-	EXPRESSION TAG	UNP Q980K5
A	608	HIS	-	EXPRESSION TAG	UNP Q980K5
A	609	HIS	-	EXPRESSION TAG	UNP Q980K5
A	610	HIS	-	EXPRESSION TAG	UNP Q980K5
A	611	HIS	-	EXPRESSION TAG	UNP Q980K5
A	612	HIS	-	EXPRESSION TAG	UNP Q980K5
B	75	MET	-	EXPRESSION TAG	UNP Q980K5
B	238	GLN	GLU	ENGINEERED MUTATION	UNP Q980K5
B	485	GLN	GLU	ENGINEERED MUTATION	UNP Q980K5
B	601	GLY	-	EXPRESSION TAG	UNP Q980K5
B	602	SER	-	EXPRESSION TAG	UNP Q980K5
B	603	ILE	-	EXPRESSION TAG	UNP Q980K5
B	604	GLU	-	EXPRESSION TAG	UNP Q980K5
B	605	GLY	-	EXPRESSION TAG	UNP Q980K5
B	606	ARG	-	EXPRESSION TAG	UNP Q980K5
B	607	HIS	-	EXPRESSION TAG	UNP Q980K5

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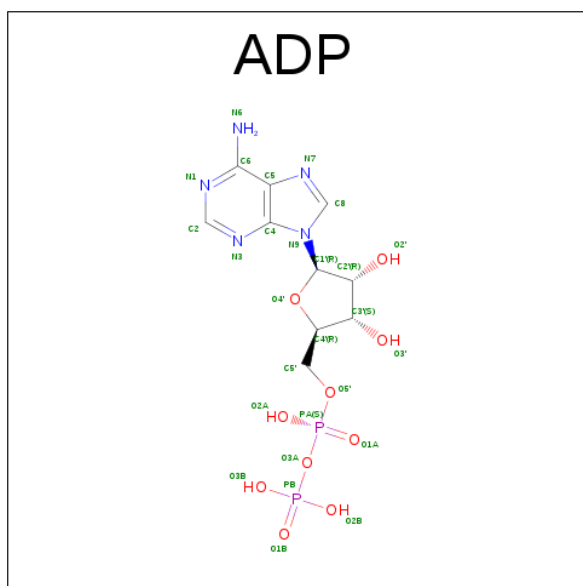
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Chain	Residue	Modelled	Actual	Comment	Reference
B	608	HIS	-	EXPRESSION TAG	UNP Q980K5
B	609	HIS	-	EXPRESSION TAG	UNP Q980K5
B	610	HIS	-	EXPRESSION TAG	UNP Q980K5
B	611	HIS	-	EXPRESSION TAG	UNP Q980K5
B	612	HIS	-	EXPRESSION TAG	UNP Q980K5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	191	Total	O	0	0
			191	191		
5	B	204	Total	O	0	0
			204	204		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.37Å 63.66Å 81.78Å 89.15° 84.47° 69.82°	Depositor
Resolution (Å)	20.00 – 2.05 19.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.3 (20.00-2.05) 90.7 (19.89-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, $R_{free}$	0.186 , 0.245 0.200 , 0.250	Depositor DCC
$R_{free}$ test set	3182 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.97% 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: PO4, MG, ADP

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	0.72	0/4187	0.76	1/5640 (0.0%)
1	B	0.80	0/4196	0.82	3/5652 (0.1%)
All	All	0.76	0/8383	0.79	4/11292 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	LEU	CA-CB-CG	6.28	129.75	115.30
1	B	566	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	116	LEU	CB-CG-CD1	5.57	120.48	111.00
1	B	270	ASP	CB-CG-OD2	5.12	122.91	118.30

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	4118	0	4237	75	0
1	B	4127	0	4245	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	54	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	54	0	24	1	0
4	A	5	0	0	0	0
5	A	191	0	0	7	0
5	B	204	0	0	6	0
All	All	8757	0	8530	155	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 9.

The worst 5 of 155 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:204:ASN:HB2	5:A:3246:HOH:O	1.54	1.08
1:B:76:GLU:HA	1:B:293:ARG:HH22	1.18	1.04
1:B:196:VAL:HG21	1:B:228:LEU:HD21	1.46	0.98
1:B:359:VAL:HB	1:B:542:LEU:HD13	1.45	0.98
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.25	0.97

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	510/538 (95%)	496 (97%)	14 (3%)	0	100	100
1	B	511/538 (95%)	498 (98%)	13 (2%)	0	100	100
All	All	1021/1076 (95%)	994 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	449/471 (95%)	425 (95%)	24 (5%)	26	16
1	B	450/471 (96%)	421 (94%)	29 (6%)	20	11
All	All	899/942 (95%)	846 (94%)	53 (6%)	23	13

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	595	MET
1	B	196	VAL
1	B	565	ARG
1	B	105	LEU
1	B	165	LYS

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	B	201	ASN
1	B	204	ASN
1	B	458	ASN
1	A	485	GLN
1	A	554	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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$
4	PO4	A	1	-	4,4,4	0.91	0	6,6,6	0.68	0
3	ADP	A	615	2	25,29,29	1.02	2 (8%)	24,45,45	2.26	4 (16%)
3	ADP	A	616	2	25,29,29	1.07	3 (12%)	24,45,45	2.21	3 (12%)
3	ADP	B	615	2	25,29,29	0.97	2 (8%)	24,45,45	2.30	5 (20%)
3	ADP	B	616	2	25,29,29	0.85	1 (4%)	24,45,45	2.16	3 (12%)

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
4	PO4	A	1	-	-	0/0/0/0	0/0/0/0
3	ADP	A	615	2	-	0/12/32/32	0/3/3/3
3	ADP	A	616	2	-	0/12/32/32	0/3/3/3
3	ADP	B	615	2	-	0/12/32/32	0/3/3/3
3	ADP	B	616	2	-	0/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	616	ADP	PB-O2B	-2.40	1.45	1.54
3	A	616	ADP	C2-N3	2.13	1.35	1.32
3	B	615	ADP	O4'-C1'	2.21	1.44	1.41
3	A	615	ADP	C2-N3	2.26	1.36	1.32
3	A	615	ADP	O4'-C1'	2.30	1.44	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	615	ADP	N3-C2-N1	-9.26	120.80	128.86
3	B	615	ADP	N3-C2-N1	-9.15	120.89	128.86
3	A	616	ADP	N3-C2-N1	-8.98	121.04	128.86
3	B	616	ADP	N3-C2-N1	-8.84	121.16	128.86
3	A	616	ADP	O3'-C3'-C4'	-3.47	100.94	111.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	615	ADP	1	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 [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	514/538 (95%)	0.25	29 (5%) 25 28	13, 33, 77, 101	0
1	B	515/538 (95%)	0.14	25 (4%) 30 33	11, 31, 65, 105	0
All	All	1029/1076 (95%)	0.19	54 (5%) 28 30	11, 32, 71, 105	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	TYR	8.3
1	B	328	LEU	7.4
1	A	340	LEU	6.8
1	B	599	THR	6.6
1	B	329	LYS	5.8

### 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
3	ADP	B	615	27/27	0.95	0.12	0.19	14,29,47,53	0
4	PO4	A	1	5/5	0.99	0.10	-0.22	33,33,42,46	0
3	ADP	A	616	27/27	0.97	0.09	-0.38	11,25,35,36	0
3	ADP	B	616	27/27	0.98	0.09	-0.61	11,22,29,32	0
2	MG	B	614	1/1	0.94	0.04	-1.42	18,18,18,18	0
3	ADP	A	615	27/27	0.99	0.07	-1.65	11,20,25,27	0
2	MG	B	613	1/1	0.96	0.04	-2.15	15,15,15,15	0
2	MG	A	614	1/1	0.99	0.03	-3.55	16,16,16,16	0
2	MG	A	613	1/1	0.97	0.04	-	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.