



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:08 am GMT

PDB ID : 3TQJ  
Title : Structure of the superoxide dismutase (Fe) (sodB) from Coxiella burnetii  
Authors : Franklin, M.C.; Cheung, J.; Cassidy, M.; Love, J.  
Deposited on : 2011-09-09  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
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

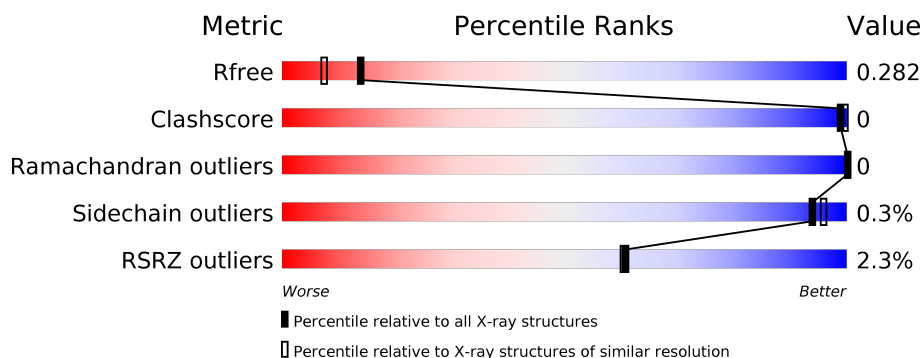
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	210	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
1	B	210	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3518 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 Superoxide dismutase [Fe].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1567	1003	270	288	6			
1	B	192	Total	C	N	O	S	0	0	0
			1567	1003	270	288	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	GLU	-	EXPRESSION TAG	UNP P19685
A	195	ASN	-	EXPRESSION TAG	UNP P19685
A	196	LEU	-	EXPRESSION TAG	UNP P19685
A	197	TYR	-	EXPRESSION TAG	UNP P19685
A	198	PHE	-	EXPRESSION TAG	UNP P19685
A	199	GLN	-	EXPRESSION TAG	UNP P19685
A	200	GLY	-	EXPRESSION TAG	UNP P19685
A	201	HIS	-	EXPRESSION TAG	UNP P19685
A	202	HIS	-	EXPRESSION TAG	UNP P19685
A	203	HIS	-	EXPRESSION TAG	UNP P19685
A	204	HIS	-	EXPRESSION TAG	UNP P19685
A	205	HIS	-	EXPRESSION TAG	UNP P19685
A	206	HIS	-	EXPRESSION TAG	UNP P19685
A	207	HIS	-	EXPRESSION TAG	UNP P19685
A	208	HIS	-	EXPRESSION TAG	UNP P19685
A	209	HIS	-	EXPRESSION TAG	UNP P19685
A	210	HIS	-	EXPRESSION TAG	UNP P19685
B	194	GLU	-	EXPRESSION TAG	UNP P19685
B	195	ASN	-	EXPRESSION TAG	UNP P19685
B	196	LEU	-	EXPRESSION TAG	UNP P19685
B	197	TYR	-	EXPRESSION TAG	UNP P19685
B	198	PHE	-	EXPRESSION TAG	UNP P19685
B	199	GLN	-	EXPRESSION TAG	UNP P19685
B	200	GLY	-	EXPRESSION TAG	UNP P19685
B	201	HIS	-	EXPRESSION TAG	UNP P19685

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Chain	Residue	Modelled	Actual	Comment	Reference
B	202	HIS	-	EXPRESSION TAG	UNP P19685
B	203	HIS	-	EXPRESSION TAG	UNP P19685
B	204	HIS	-	EXPRESSION TAG	UNP P19685
B	205	HIS	-	EXPRESSION TAG	UNP P19685
B	206	HIS	-	EXPRESSION TAG	UNP P19685
B	207	HIS	-	EXPRESSION TAG	UNP P19685
B	208	HIS	-	EXPRESSION TAG	UNP P19685
B	209	HIS	-	EXPRESSION TAG	UNP P19685
B	210	HIS	-	EXPRESSION TAG	UNP P19685

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

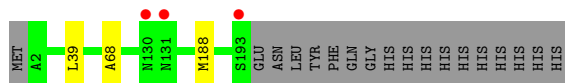
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	200	Total O 200 200	0	0
3	B	182	Total O 182 182	0	0

**i**

- Molecule 1: Superoxide dismutase [Fe]



- [illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.10Å 65.28Å 110.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.15 – 2.00 41.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (56.15-2.00) 91.1 (41.03-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.09 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.233 , 0.271 0.246 , 0.282	Depositor DCC
$R_{free}$ test set	1388 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.79 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0071e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.31	0/1618	0.42	0/2195
1	B	0.31	0/1618	0.43	0/2195
All	All	0.31	0/3236	0.43	0/4390

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

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	1567	0	1479	2	0
1	B	1567	0	1479	1	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	200	0	0	1	0
3	B	182	0	0	0	0
All	All	3518	0	2958	3	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 0.

All (3) 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:188:MET:HE2	3:A:333:HOH:O	2.07	0.55
1:B:8:LEU:HD13	1:B:28:HIS:CD2	2.53	0.44
1:A:39:LEU:HD22	1:A:68:ALA:HA	2.03	0.40

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	190/210 (90%)	186 (98%)	4 (2%)	0	100	100
1	B	190/210 (90%)	186 (98%)	4 (2%)	0	100	100
All	All	380/420 (90%)	372 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	167/184 (91%)	167 (100%)	0	100	100
1	B	167/184 (91%)	166 (99%)	1 (1%)	89	92
All	All	334/368 (91%)	333 (100%)	1 (0%)	94	96



All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	HIS
1	B	79	HIS
1	B	118	HIS

### 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 2 ligands modelled in this entry, 2 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 ⓘ

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	192/210 (91%)	0.24	3 (1%) 72 71	14, 24, 41, 47	0
1	B	192/210 (91%)	0.22	6 (3%) 49 49	14, 25, 46, 57	0
All	All	384/420 (91%)	0.23	9 (2%) 61 60	14, 25, 43, 57	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ASN	6.0
1	B	131	ASN	4.9
1	A	193	SER	3.8
1	A	130	ASN	3.7
1	B	193	SER	3.5
1	B	48	PHE	2.7
1	A	131	ASN	2.6
1	B	2	ALA	2.2
1	B	50	LYS	2.1

### 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	FE2	B	1001	1/1	1.00	0.06	-6.34	16,16,16,16	0
2	FE2	A	1001	1/1	1.00	0.05	-6.79	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.