



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:31 PM GMT

PDB ID : 2D2A  
Title : Crystal Structure of Escherichia coli SufA Involved in Biosynthesis of Iron-sulfur Clusters  
Authors : Wada, K.; Hasegawa, Y.; Gong, Z.; Minami, Y.; Fukuyama, K.; Takahashi, Y.  
Deposited on : 2005-09-05  
Resolution : 2.70 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>

---

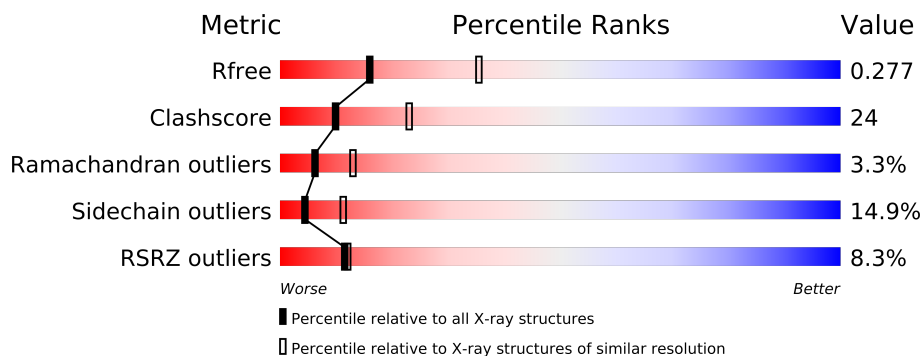
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	145	
1	B	145	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1677 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 SufA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			854	546	143	160	5			
1	B	102	Total	C	N	O	S	0	0	0
			786	510	131	143	2			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP P77667
A	-21	GLY	-	EXPRESSION TAG	UNP P77667
A	-20	HIS	-	EXPRESSION TAG	UNP P77667
A	-19	HIS	-	EXPRESSION TAG	UNP P77667
A	-18	HIS	-	EXPRESSION TAG	UNP P77667
A	-17	HIS	-	EXPRESSION TAG	UNP P77667
A	-16	HIS	-	EXPRESSION TAG	UNP P77667
A	-15	HIS	-	EXPRESSION TAG	UNP P77667
A	-14	HIS	-	EXPRESSION TAG	UNP P77667
A	-13	HIS	-	EXPRESSION TAG	UNP P77667
A	-12	HIS	-	EXPRESSION TAG	UNP P77667
A	-11	HIS	-	EXPRESSION TAG	UNP P77667
A	-10	SER	-	EXPRESSION TAG	UNP P77667
A	-9	SER	-	EXPRESSION TAG	UNP P77667
A	-8	GLY	-	EXPRESSION TAG	UNP P77667
A	-7	HIS	-	EXPRESSION TAG	UNP P77667
A	-6	ILE	-	EXPRESSION TAG	UNP P77667
A	-5	ASP	-	EXPRESSION TAG	UNP P77667
A	-4	ASP	-	EXPRESSION TAG	UNP P77667
A	-3	ASP	-	EXPRESSION TAG	UNP P77667
A	-2	ASP	-	EXPRESSION TAG	UNP P77667
A	-1	LEU	-	EXPRESSION TAG	UNP P77667
A	0	HIS	-	EXPRESSION TAG	UNP P77667
B	-22	MET	-	EXPRESSION TAG	UNP P77667
B	-21	GLY	-	EXPRESSION TAG	UNP P77667

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	EXPRESSION TAG	UNP P77667
B	-19	HIS	-	EXPRESSION TAG	UNP P77667
B	-18	HIS	-	EXPRESSION TAG	UNP P77667
B	-17	HIS	-	EXPRESSION TAG	UNP P77667
B	-16	HIS	-	EXPRESSION TAG	UNP P77667
B	-15	HIS	-	EXPRESSION TAG	UNP P77667
B	-14	HIS	-	EXPRESSION TAG	UNP P77667
B	-13	HIS	-	EXPRESSION TAG	UNP P77667
B	-12	HIS	-	EXPRESSION TAG	UNP P77667
B	-11	HIS	-	EXPRESSION TAG	UNP P77667
B	-10	SER	-	EXPRESSION TAG	UNP P77667
B	-9	SER	-	EXPRESSION TAG	UNP P77667
B	-8	GLY	-	EXPRESSION TAG	UNP P77667
B	-7	HIS	-	EXPRESSION TAG	UNP P77667
B	-6	ILE	-	EXPRESSION TAG	UNP P77667
B	-5	ASP	-	EXPRESSION TAG	UNP P77667
B	-4	ASP	-	EXPRESSION TAG	UNP P77667
B	-3	ASP	-	EXPRESSION TAG	UNP P77667
B	-2	ASP	-	EXPRESSION TAG	UNP P77667
B	-1	LEU	-	EXPRESSION TAG	UNP P77667
B	0	HIS	-	EXPRESSION TAG	UNP P77667

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	19	Total	O	0	0
			19	19		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	25.16Å 88.50Å 122.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.60 – 2.70 41.60 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.60-2.70) 95.0 (41.60-2.69)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.272 0.236 , 0.277	Depositor DCC
$R_{free}$ test set	816 reflections (10.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 31.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 8095 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	1677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality i

### 5.1 Standard geometry i

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	2.96	80/875 (9.1%)	2.45	50/1187 (4.2%)
1	B	0.88	4/806 (0.5%)	0.85	0/1093
All	All	2.22	84/1681 (5.0%)	1.87	50/2280 (2.2%)

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	0	2

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ASP	CB-CG	15.10	1.83	1.51
1	A	66	ASP	CB-CG	13.85	1.80	1.51
1	A	47	GLN	CG-CD	13.52	1.82	1.51
1	A	62	GLU	CD-OE2	11.95	1.38	1.25
1	A	11	GLN	CG-CD	11.35	1.77	1.51

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ARG	NE-CZ-NH1	-20.90	109.85	120.30
1	A	29	ARG	NE-CZ-NH2	18.18	129.39	120.30
1	A	66	ASP	CB-CG-OD2	15.62	132.36	118.30
1	A	93	ASP	CB-CG-OD1	14.28	131.16	118.30
1	A	73	ASP	CB-CG-OD1	13.88	130.79	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	VAL	Peptide
1	A	49	GLY	Peptide

## 5.2 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 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	854	0	808	51	0
1	B	786	0	759	29	0
2	A	18	0	0	4	0
2	B	19	0	0	0	0
All	All	1677	0	1567	77	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 24.

The worst 5 of 77 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:GLN:CB	1:A:11:GLN:CG	1.79	1.59
1:B:104:LYS:CE	1:B:104:LYS:NZ	1.68	1.54
1:A:36:PRO:CB	1:A:36:PRO:CG	1.78	1.52
1:A:11:GLN:CD	1:A:11:GLN:CG	1.77	1.50
1:A:66:ASP:CB	1:A:66:ASP:CG	1.80	1.48

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	112/145 (77%)	93 (83%)	13 (12%)	6 (5%)	3	5
1	B	98/145 (68%)	93 (95%)	4 (4%)	1 (1%)	22	51
All	All	210/290 (72%)	186 (89%)	17 (8%)	7 (3%)	6	13

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	111	GLN
1	B	6	GLY
1	A	14	ALA
1	A	11	GLN

### 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	87/120 (72%)	69 (79%)	18 (21%)	2	4
1	B	81/120 (68%)	74 (91%)	7 (9%)	15	33
All	All	168/240 (70%)	143 (85%)	25 (15%)	4	11

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	A	99	LEU
1	B	96	ARG
1	A	97	GLU
1	A	100	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	HIS
1	B	101	GLN
1	B	35	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	9	ASN
1	B	100	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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

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	114/145 (78%)	0.15	12 (10%) <b>7</b> <b>7</b>	15, 29, 87, 96	0
1	B	102/145 (70%)	-0.05	6 (5%) <b>22</b> <b>23</b>	12, 28, 58, 74	0
All	All	216/290 (74%)	0.06	18 (8%) <b>11</b> <b>12</b>	12, 29, 74, 96	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	CYS	7.8
1	A	115	GLY	6.7
1	A	111	GLN	5.3
1	A	51	ALA	4.9
1	A	49	GLY	4.6

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.