



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 07:10 AM BST

PDB ID : 6GSB  
Title : Sphingobacterium sp. T2 manganese superoxide dismutase catalyses the oxidative demethylation of polymeric lignin via generation of hydroxyl radical  
Authors : Rashid, G.M.; Zhang, X.; Wilkinson, R.C.; Fulop, V.; Cottyn, B.; Baumberger, S.; Bugg, D.H.  
Deposited on : 2018-06-13  
Resolution : 1.45 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

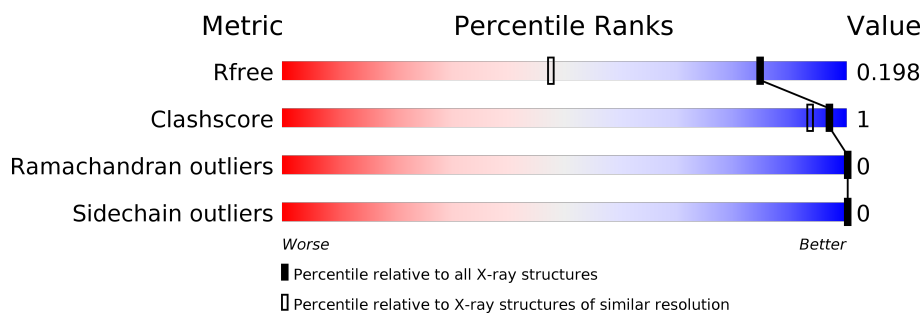
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

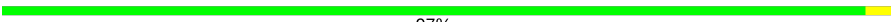

The reported resolution of this entry is 1.45 Å.

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))
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)

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 respectively. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	206	 97%
1	B	206	 98%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3872 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1622	1034	276	310	2			
1	B	206	Total	C	N	O	S	0	0	0
			1622	1034	276	310	2			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ASP	-	expression tag	UNP A0A0M3KL50
A	-2	PRO	-	expression tag	UNP A0A0M3KL50
A	-1	PHE	-	expression tag	UNP A0A0M3KL50
A	0	THR	-	expression tag	UNP A0A0M3KL50
A	1	GLN	-	expression tag	UNP A0A0M3KL50
A	2	PHE	-	expression tag	UNP A0A0M3KL50
A	3	LYS	-	expression tag	UNP A0A0M3KL50
A	4	GLN	-	expression tag	UNP A0A0M3KL50
A	5	THR	-	expression tag	UNP A0A0M3KL50
A	6	PRO	-	expression tag	UNP A0A0M3KL50
A	7	LEU	-	expression tag	UNP A0A0M3KL50
A	8	PRO	-	expression tag	UNP A0A0M3KL50
A	9	TYR	-	expression tag	UNP A0A0M3KL50
A	10	ALA	-	expression tag	UNP A0A0M3KL50
A	11	TYR	-	expression tag	UNP A0A0M3KL50
A	12	ASP	-	expression tag	UNP A0A0M3KL50
A	13	ALA	-	expression tag	UNP A0A0M3KL50
A	14	LEU	-	expression tag	UNP A0A0M3KL50
A	15	GLU	-	expression tag	UNP A0A0M3KL50
A	16	GLY	-	expression tag	UNP A0A0M3KL50
A	17	ALA	-	expression tag	UNP A0A0M3KL50
A	18	ILE	-	expression tag	UNP A0A0M3KL50
A	19	ASP	-	expression tag	UNP A0A0M3KL50
A	20	ALA	-	expression tag	UNP A0A0M3KL50
A	21	LYS	-	expression tag	UNP A0A0M3KL50

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	THR	-	expression tag	UNP A0A0M3KL50
A	27	HIS	TYR	engineered mutation	UNP A0A0M3KL50
B	-3	ASP	-	expression tag	UNP A0A0M3KL50
B	-2	PRO	-	expression tag	UNP A0A0M3KL50
B	-1	PHE	-	expression tag	UNP A0A0M3KL50
B	0	THR	-	expression tag	UNP A0A0M3KL50
B	1	GLN	-	expression tag	UNP A0A0M3KL50
B	2	PHE	-	expression tag	UNP A0A0M3KL50
B	3	LYS	-	expression tag	UNP A0A0M3KL50
B	4	GLN	-	expression tag	UNP A0A0M3KL50
B	5	THR	-	expression tag	UNP A0A0M3KL50
B	6	PRO	-	expression tag	UNP A0A0M3KL50
B	7	LEU	-	expression tag	UNP A0A0M3KL50
B	8	PRO	-	expression tag	UNP A0A0M3KL50
B	9	TYR	-	expression tag	UNP A0A0M3KL50
B	10	ALA	-	expression tag	UNP A0A0M3KL50
B	11	TYR	-	expression tag	UNP A0A0M3KL50
B	12	ASP	-	expression tag	UNP A0A0M3KL50
B	13	ALA	-	expression tag	UNP A0A0M3KL50
B	14	LEU	-	expression tag	UNP A0A0M3KL50
B	15	GLU	-	expression tag	UNP A0A0M3KL50
B	16	GLY	-	expression tag	UNP A0A0M3KL50
B	17	ALA	-	expression tag	UNP A0A0M3KL50
B	18	ILE	-	expression tag	UNP A0A0M3KL50
B	19	ASP	-	expression tag	UNP A0A0M3KL50
B	20	ALA	-	expression tag	UNP A0A0M3KL50
B	21	LYS	-	expression tag	UNP A0A0M3KL50
B	22	THR	-	expression tag	UNP A0A0M3KL50
B	27	HIS	TYR	engineered mutation	UNP A0A0M3KL50

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	338	Total 338	O 338	0	0
3	B	288	Total 288	O 288	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

- Molecule 1: Superoxide dismutase

Chain A:  97%



- Molecule 1: Superoxide dismutase

Chain B:  98%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.68Å 59.09Å 75.21Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	36.66 – 1.45 36.63 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.3 (36.66-1.45) 98.3 (36.63-1.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.149 , 0.169 0.185 , 0.198	Depositor DCC
$R_{free}$ test set	2816 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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: MN

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	0.79	0/1664	0.88	4/2262 (0.2%)
1	B	0.70	0/1664	0.80	1/2262 (0.0%)
All	All	0.75	0/3328	0.84	5/4524 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	172	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	B	120	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	163	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	163	ASP	CB-CG-OD1	5.20	122.98	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	1622	0	1577	3	0
1	B	1622	0	1577	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	338	0	0	2	0
3	B	288	0	0	1	0
All	All	3872	0	3154	6	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 1.

The worst 5 of 6 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:87:LYS:HE2	3:A:617:HOH:O	2.01	0.60
1:B:112:LYS:HE2	3:B:617:HOH:O	2.03	0.57
1:B:57:ALA:O	1:B:150:ASP:HB3	2.11	0.50
1:B:151:PHE:CD1	1:B:151:PHE:C	2.89	0.46
1:A:57:ALA:O	1:A:150:ASP:HB3	2.18	0.42

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	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
1	B	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
All	All	408/412 (99%)	397 (97%)	11 (3%)	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	166/166 (100%)	166 (100%)	0	100	100
1	B	166/166 (100%)	166 (100%)	0	100	100
All	All	332/332 (100%)	332 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 monosaccharides 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.