

# Full wwPDB X-ray Structure Validation Report (i)

#### Jun 20, 2023 – 12:00 PM EDT

PDB ID	:	1BS3
Title	:	P.SHERMANII SOD(FE+3) FLUORIDE
Authors	:	Schmidt, M.
Deposited on		
Resolution	:	1.55  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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

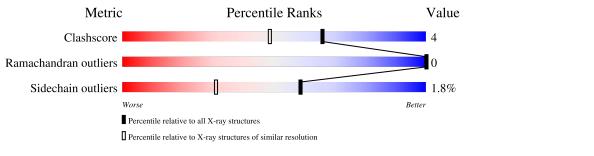
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.55 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	Similar resolution
Methe	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	А	201	89%	10%
1	В	201	90%	9%



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3690 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	Λ	201	Total	С	Ν	Ο	S	0	0	0
		201	1604	1032	270	298	4	0		0
1	В	201	Total	С	Ν	Ο	S	0	0	0
1	Б	B 201	1604	1032	270	298	4	0		

• Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Fe 1 1	0	0
2	В	1	Total Fe 1 1	0	0

• Molecule 3 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total F 1 1	0	0
3	В	1	Total F 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	232	Total         O           232         232	0	0
4	В	246	Total         O           246         246	0	0

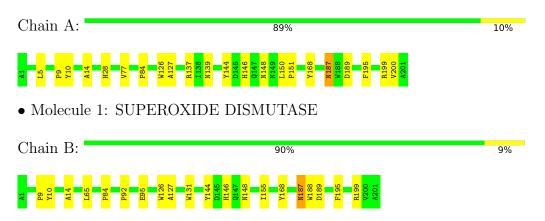


# 3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: SUPEROXIDE DISMUTASE





## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	C 2 2 21	Depositor	
Cell constants	79.42Å 85.28Å 108.40Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	9.00 - 1.55	Depositor	
% Data completeness	78.2 (9.00-1.55)	Depositor	
(in resolution range)	10.2 (0.00-1.00)	Depositor	
$R_{merge}$	(Not available)	Depositor	
R <sub>sym</sub>	0.03	Depositor	
Refinement program	X-PLOR 3.851	Depositor	
$R, R_{free}$	0.174 , $0.206$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3690	wwPDB-VP	
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP	



# 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: FE, F

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.32	0/1653	0.57	1/2249~(0.0%)	
1	В	0.32	0/1653	0.56	1/2249~(0.0%)	
All	All	0.32	0/3306	0.56	2/4498~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	127	ALA	N-CA-C	-5.19	96.99	111.00
1	В	127	ALA	N-CA-C	-5.06	97.34	111.00

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	А	1604	0	1523	14	0
1	В	1604	0	1523	11	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
4	А	232	0	0	1	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	246	0	0	0	2
All	All	3690	0	3046	25	4

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 4.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + am 1	A 4 a ma 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:126:TRP:HE1	1:A:146:HIS:HD2	1.28	0.81
1:B:126:TRP:HE1	1:B:146:HIS:HD2	1.37	0.73
1:A:77:VAL:HG11	4:A:422:HOH:O	1.93	0.67
1:A:5:LEU:HD11	1:A:28:HIS:CE1	2.33	0.64
1:B:144:TYR:HB2	1:B:148:ASN:HB2	1.86	0.57
1:A:187:ASN:HD21	1:A:189:ASP:HB2	1.70	0.56
1:A:126:TRP:HE1	1:A:146:HIS:CD2	2.17	0.55
1:A:144:TYR:HB2	1:A:148:ASN:HB2	1.89	0.54
1:A:14:ALA:HB1	1:A:84:PRO:HG3	1.89	0.53
1:B:187:ASN:HD21	1:B:189:ASP:HB2	1.75	0.51
1:B:195:PHE:CZ	1:B:199:ARG:NH1	2.80	0.49
1:A:137:ARG:HD3	1:A:139:ASN:OD1	2.15	0.47
1:A:126:TRP:NE1	1:A:146:HIS:HD2	2.07	0.47
1:A:200:VAL:HG12	1:A:200:VAL:O	2.15	0.46
1:B:131:TRP:HB3	1:B:155:ILE:HB	1.97	0.46
1:A:9:PRO:HG2	1:A:10:TYR:CD2	2.51	0.45
1:B:126:TRP:HE1	1:B:146:HIS:CD2	2.25	0.44
1:B:92:PRO:HG3	1:B:188:TRP:CE3	2.52	0.44
1:B:14:ALA:HB1	1:B:84:PRO:HG3	1.99	0.44
1:A:9:PRO:HG2	1:A:10:TYR:CE2	2.53	0.44
1:B:9:PRO:HG2	1:B:10:TYR:CE2	2.52	0.44
1:A:195:PHE:O	1:A:199:ARG:HG2	2.18	0.43
1:A:150:LEU:HA	1:A:151:PRO:HD3	1.89	0.42
1:B:195:PHE:HZ	1:B:199:ARG:NH1	2.18	0.41
1:B:92:PRO:HG3	1:B:188:TRP:CD2	2.56	0.40

All (4) 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)
4:B:433:HOH:O	4:B:433:HOH:O[3_655]	0.66	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:334:HOH:O	4:A:334:HOH:O[3_655]	1.13	1.07
4:B:347:HOH:O	4:B:347:HOH:O[3_555]	1.33	0.87
4:A:343:HOH:O	4:A:343:HOH:O[4_566]	1.97	0.23

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#### 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	Perce	ntiles
1	А	199/201~(99%)	190 (96%)	9~(4%)	0	100	100
1	В	199/201~(99%)	192 (96%)	7 (4%)	0	100	100
All	All	398/402~(99%)	382~(96%)	16 (4%)	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	А	163/163~(100%)	161~(99%)	2(1%)	71 49	
1	В	163/163~(100%)	159 (98%)	4 (2%)	47 18	
All	All	326/326~(100%)	320~(98%)	6 (2%)	59 31	

All (6) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	168	TYR
1	А	187	ASN
1	В	65	LEU
1	В	95	GLU
1	В	168	TYR
1	В	187	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	А	146	HIS
1	А	187	ASN
1	В	146	HIS
1	В	187	ASN

#### 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 4 ligands modelled in this entry, 4 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

#### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

#### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

