



Full wwPDB Geometry-Only Validation Report ⓘ

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PDB ID : 9BW2 / pdb_00009bw2
Title : Neutron Structure of Reduced Tyr34Phe MnSOD
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Deposited on : 2024-05-20
Resolution : 2.50 Å(reported)

This is a Full wwPDB Geometry-Only 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

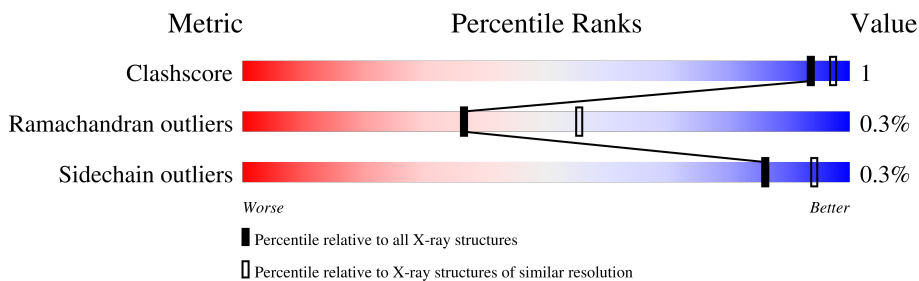
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	199	 98%
1	B	199	 95% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6731 atoms, of which 9 are hydrogens and 3382 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 [Mn], mitochondrial.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	199	Total	C	D	H	N	O	S	0	0	0
			3116	1013	1533	3	276	286	5			
1	B	199	Total	C	D	H	N	O	S	0	0	0
			3117	1013	1531	6	276	286	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P04179
A	34	PHE	TYR	engineered mutation	UNP P04179
B	0	MET	-	initiating methionine	UNP P04179
B	34	PHE	TYR	engineered mutation	UNP P04179

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	98	Total	D	O	0	0
			264	166	98		
3	B	80	Total	D	O	0	0
			232	152	80		

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 [Mn], mitochondrial

Chain A:  98%



- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain B:  95% 5%



4 Model quality

4.1 Standard geometry

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	0.34	0/1626	0.29	0/2205
1	B	0.33	0/1626	0.29	0/2205
All	All	0.33	0/3252	0.29	0/4410

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	3113	3	1537	4	0
1	B	3111	6	1537	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	264	0	0	3	0
3	B	232	0	0	2	0
All	All	6722	9	3074	9	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.

All (9) 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:B:95:GLU:OE2	3:B:301:HOH:O	2.06	0.73
1:A:28:SER:O	3:A:301:HOH:O	2.10	0.68
1:B:21:GLN:OE1	3:B:302:HOH:O	2.15	0.63
1:A:163:HIS:O	3:A:302:HOH:O	2.19	0.61
1:A:44:LYS:NZ	3:A:304:HOH:O	2.31	0.60
1:B:123:TRP:NE1	1:B:143:GLN:OE1	2.41	0.51
1:B:26:HIS:CE1	1:B:159:ASP:OD2	2.65	0.48
1:A:19:ASN:OD1	1:A:19:ASN:C	2.63	0.42
1:B:19:ASN:C	1:B:19:ASN:OD1	2.63	0.42

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
1	B	197/199 (99%)	190 (96%)	6 (3%)	1 (0%)	24	43
All	All	394/398 (99%)	381 (97%)	12 (3%)	1 (0%)	36	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1	LYS

4.3.2 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	163/163 (100%)	163 (100%)	0	100	100
1	B	163/163 (100%)	162 (99%)	1 (1%)	78	91
All	All	326/326 (100%)	325 (100%)	1 (0%)	86	94

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

Mol	Chain	Res	Type
1	B	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	142	ASN
1	B	57	GLN
1	B	134	HIS
1	B	182	ASN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

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.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.