



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 3, 2024 – 08:35 PM EST

PDB ID : 1MSD  
Title : COMPARISON OF THE CRYSTAL STRUCTURES OF GENETICALLY ENGINEERED HUMAN MANGANESE SUPEROXIDE DISMUTASE AND MANGANESE SUPEROXIDE DISMUTASE FROM THERMUS THERMOPHILUS. DIFFERENCES IN DIMER-DIMER INTERACTIONS.  
Authors : Sussman, J.; Wagner, U.G.; Pattridge, K.A.; Ludwig, M.L.  
Deposited on : 1992-11-10  
Resolution : 3.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtrriage (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) : 2.36

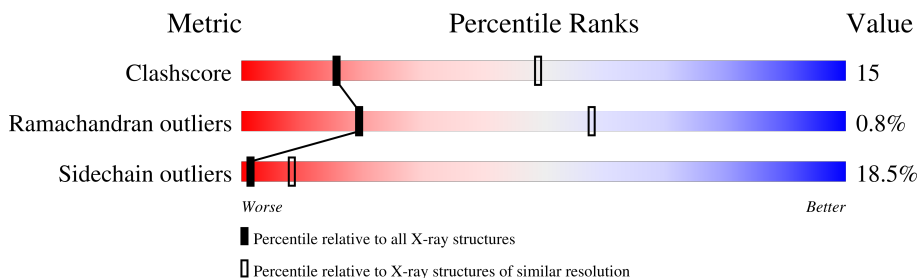
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	198	
1	B	198	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3246 atoms, of which 98 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 MANGANESE SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	198	1622	1008	49	275	286	4	0	0	0
1	B	198	1622	1008	49	275	286	4	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: 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		

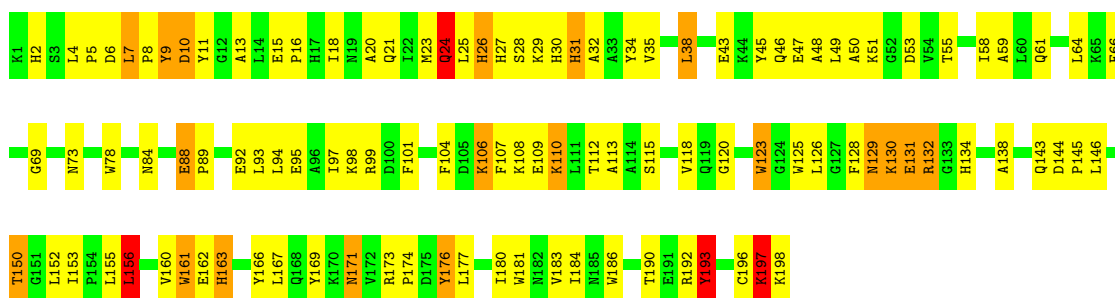
### 3 Residue-property plots

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.

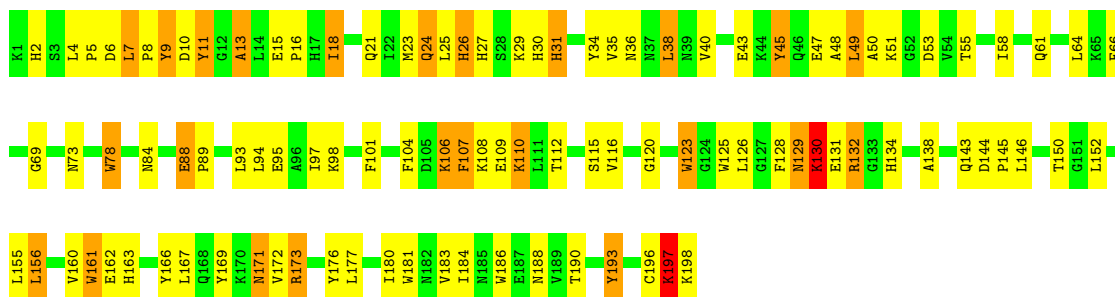
- Molecule 1: MANGANESE SUPEROXIDE DISMUTASE

Chain A: 



- Molecule 1: MANGANESE SUPEROXIDE DISMUTASE

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.80Å 74.10Å 68.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	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: 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	1.12	4/1619 (0.2%)	1.93	48/2197 (2.2%)
1	B	1.13	3/1619 (0.2%)	1.96	48/2197 (2.2%)
All	All	1.12	7/3238 (0.2%)	1.94	96/4394 (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	1
1	B	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	GLU	CD-OE2	8.17	1.34	1.25
1	A	131	GLU	CD-OE2	7.76	1.34	1.25
1	B	88	GLU	CD-OE1	7.27	1.33	1.25
1	B	109	GLU	CD-OE2	5.98	1.32	1.25
1	A	186	TRP	CD1-NE1	-5.73	1.28	1.38

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	TYR	CB-CG-CD2	-12.41	113.55	121.00
1	A	34	TYR	CB-CG-CD2	-10.31	114.82	121.00
1	A	123	TRP	CD1-CG-CD2	9.72	114.08	106.30
1	B	123	TRP	CD1-CG-CD2	9.62	114.00	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	TRP	CD1-CG-CD2	8.90	113.42	106.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	TYR	Sidechain
1	B	107	PHE	Sidechain

## 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	1573	49	1528	49	0
1	B	1573	49	1528	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	3148	98	3056	91	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 15.

The worst 5 of 91 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:167:LEU:HD23	1:B:167:LEU:HD23	1.72	0.72
1:A:161:TRP:CH2	1:B:120:GLY:HA2	2.28	0.69
1:B:9:TYR:HB2	1:B:13:ALA:HB3	1.75	0.68
1:A:9:TYR:HB2	1:A:13:ALA:HB3	1.77	0.66
1:B:94:LEU:HG	1:B:98:LYS:HD2	1.81	0.62

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	196/198 (99%)	176 (90%)	19 (10%)	1 (0%)	29	67
1	B	196/198 (99%)	174 (89%)	20 (10%)	2 (1%)	15	54
All	All	392/396 (99%)	350 (89%)	39 (10%)	3 (1%)	19	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	B	197	LYS
1	B	13	ALA

### 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	162/162 (100%)	131 (81%)	31 (19%)	1	8
1	B	162/162 (100%)	133 (82%)	29 (18%)	2	9
All	All	324/324 (100%)	264 (82%)	60 (18%)	1	8

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	VAL
1	B	177	LEU
1	B	24	GLN

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Mol	Chain	Res	Type
1	B	171	ASN
1	B	198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	ASN
1	B	134	HIS
1	B	185	ASN
1	B	143	GLN
1	A	143	GLN

### 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.