



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:07 pm BST

PDB ID : 1Y67
Title : Crystal Structure of Manganese Superoxide Dismutase from *Deinococcus radiodurans*
Authors : Chan, S.; Tanaka, S.; Sawaya, M.R.; Perry, L.J.
Deposited on : 2004-12-03
Resolution : 1.85 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	2.11
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)	:	2.11

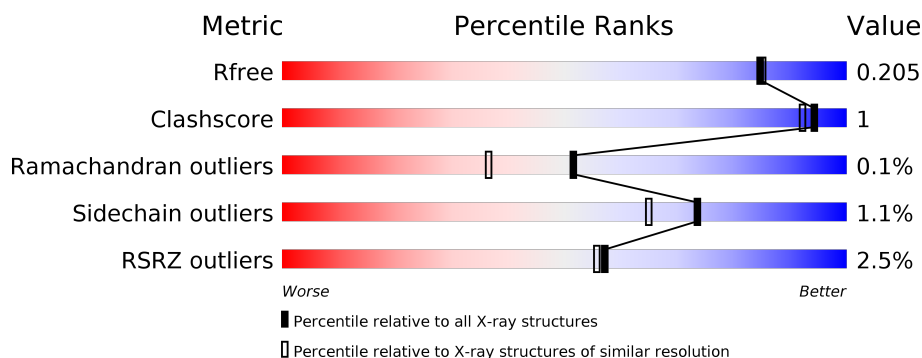
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	229	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
1	B	229	<div> <div></div> <div>86%</div> <div>•</div> <div>11%</div> </div>
1	C	229	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	229	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>• •</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6965 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 Manganese Superoxide dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1651	1048	289	310	4			
1	B	204	Total	C	N	O	S	0	0	0
			1614	1025	282	303	4			
1	C	204	Total	C	N	O	S	0	0	0
			1615	1028	281	302	4			
1	D	214	Total	C	N	O	S	0	0	0
			1685	1067	298	316	4			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q9RUV2
A	1	ALA	-	EXPRESSION TAG	UNP Q9RUV2
A	212	LEU	-	EXPRESSION TAG	UNP Q9RUV2
A	213	VAL	-	EXPRESSION TAG	UNP Q9RUV2
A	214	PRO	-	EXPRESSION TAG	UNP Q9RUV2
A	215	ARG	-	EXPRESSION TAG	UNP Q9RUV2
A	216	GLY	-	EXPRESSION TAG	UNP Q9RUV2
A	217	SER	-	EXPRESSION TAG	UNP Q9RUV2
A	218	ALA	-	EXPRESSION TAG	UNP Q9RUV2
A	219	ALA	-	EXPRESSION TAG	UNP Q9RUV2
A	220	ALA	-	EXPRESSION TAG	UNP Q9RUV2
A	221	LEU	-	EXPRESSION TAG	UNP Q9RUV2
A	222	GLU	-	EXPRESSION TAG	UNP Q9RUV2
A	223	HIS	-	EXPRESSION TAG	UNP Q9RUV2
A	224	HIS	-	EXPRESSION TAG	UNP Q9RUV2
A	225	HIS	-	EXPRESSION TAG	UNP Q9RUV2
A	226	HIS	-	EXPRESSION TAG	UNP Q9RUV2
A	227	HIS	-	EXPRESSION TAG	UNP Q9RUV2
A	228	HIS	-	EXPRESSION TAG	UNP Q9RUV2
B	0	MET	-	EXPRESSION TAG	UNP Q9RUV2
B	1	ALA	-	EXPRESSION TAG	UNP Q9RUV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	212	LEU	-	EXPRESSION TAG	UNP Q9RUV2
B	213	VAL	-	EXPRESSION TAG	UNP Q9RUV2
B	214	PRO	-	EXPRESSION TAG	UNP Q9RUV2
B	215	ARG	-	EXPRESSION TAG	UNP Q9RUV2
B	216	GLY	-	EXPRESSION TAG	UNP Q9RUV2
B	217	SER	-	EXPRESSION TAG	UNP Q9RUV2
B	218	ALA	-	EXPRESSION TAG	UNP Q9RUV2
B	219	ALA	-	EXPRESSION TAG	UNP Q9RUV2
B	220	ALA	-	EXPRESSION TAG	UNP Q9RUV2
B	221	LEU	-	EXPRESSION TAG	UNP Q9RUV2
B	222	GLU	-	EXPRESSION TAG	UNP Q9RUV2
B	223	HIS	-	EXPRESSION TAG	UNP Q9RUV2
B	224	HIS	-	EXPRESSION TAG	UNP Q9RUV2
B	225	HIS	-	EXPRESSION TAG	UNP Q9RUV2
B	226	HIS	-	EXPRESSION TAG	UNP Q9RUV2
B	227	HIS	-	EXPRESSION TAG	UNP Q9RUV2
B	228	HIS	-	EXPRESSION TAG	UNP Q9RUV2
C	0	MET	-	EXPRESSION TAG	UNP Q9RUV2
C	1	ALA	-	EXPRESSION TAG	UNP Q9RUV2
C	212	LEU	-	EXPRESSION TAG	UNP Q9RUV2
C	213	VAL	-	EXPRESSION TAG	UNP Q9RUV2
C	214	PRO	-	EXPRESSION TAG	UNP Q9RUV2
C	215	ARG	-	EXPRESSION TAG	UNP Q9RUV2
C	216	GLY	-	EXPRESSION TAG	UNP Q9RUV2
C	217	SER	-	EXPRESSION TAG	UNP Q9RUV2
C	218	ALA	-	EXPRESSION TAG	UNP Q9RUV2
C	219	ALA	-	EXPRESSION TAG	UNP Q9RUV2
C	220	ALA	-	EXPRESSION TAG	UNP Q9RUV2
C	221	LEU	-	EXPRESSION TAG	UNP Q9RUV2
C	222	GLU	-	EXPRESSION TAG	UNP Q9RUV2
C	223	HIS	-	EXPRESSION TAG	UNP Q9RUV2
C	224	HIS	-	EXPRESSION TAG	UNP Q9RUV2
C	225	HIS	-	EXPRESSION TAG	UNP Q9RUV2
C	226	HIS	-	EXPRESSION TAG	UNP Q9RUV2
C	227	HIS	-	EXPRESSION TAG	UNP Q9RUV2
C	228	HIS	-	EXPRESSION TAG	UNP Q9RUV2
D	0	MET	-	EXPRESSION TAG	UNP Q9RUV2
D	1	ALA	-	EXPRESSION TAG	UNP Q9RUV2
D	212	LEU	-	EXPRESSION TAG	UNP Q9RUV2
D	213	VAL	-	EXPRESSION TAG	UNP Q9RUV2
D	214	PRO	-	EXPRESSION TAG	UNP Q9RUV2
D	215	ARG	-	EXPRESSION TAG	UNP Q9RUV2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	216	GLY	-	EXPRESSION TAG	UNP Q9RUV2
D	217	SER	-	EXPRESSION TAG	UNP Q9RUV2
D	218	ALA	-	EXPRESSION TAG	UNP Q9RUV2
D	219	ALA	-	EXPRESSION TAG	UNP Q9RUV2
D	220	ALA	-	EXPRESSION TAG	UNP Q9RUV2
D	221	LEU	-	EXPRESSION TAG	UNP Q9RUV2
D	222	GLU	-	EXPRESSION TAG	UNP Q9RUV2
D	223	HIS	-	EXPRESSION TAG	UNP Q9RUV2
D	224	HIS	-	EXPRESSION TAG	UNP Q9RUV2
D	225	HIS	-	EXPRESSION TAG	UNP Q9RUV2
D	226	HIS	-	EXPRESSION TAG	UNP Q9RUV2
D	227	HIS	-	EXPRESSION TAG	UNP Q9RUV2
D	228	HIS	-	EXPRESSION TAG	UNP Q9RUV2

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

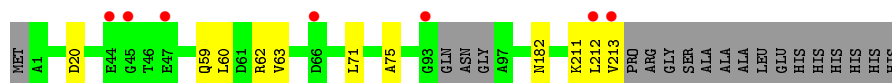
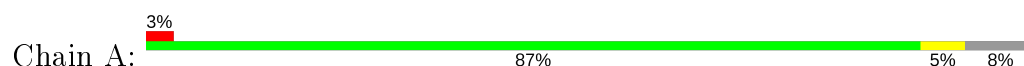
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	116	Total O 116 116	0	0
3	B	89	Total O 89 89	1	0
3	C	94	Total O 94 94	0	0
3	D	97	Total O 97 97	1	0

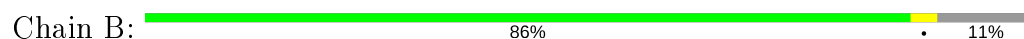
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

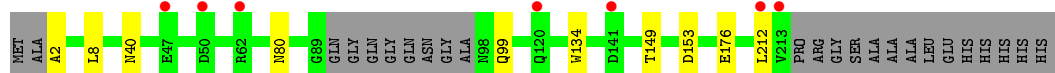
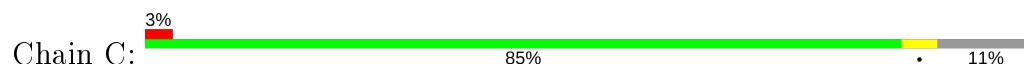
- Molecule 1: Manganese Superoxide dismutase



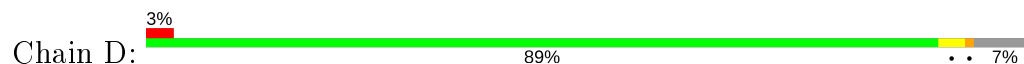
- Molecule 1: Manganese Superoxide dismutase



- Molecule 1: Manganese Superoxide dismutase



- Molecule 1: Manganese Superoxide dismutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.80Å 87.92Å 116.20Å 90.00° 91.14° 90.00°	Depositor
Resolution (Å)	119.52 – 1.85 70.11 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (119.52-1.85) 99.6 (70.11-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.86Å)	Xtriage
Refinement program	REFMAC refmac _5.2.0005	Depositor
R, R_{free}	0.184 , 0.205 0.182 , 0.205	Depositor DCC
R_{free} test set	3697 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6965	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.48	0/1695	0.53	0/2305
1	B	0.43	0/1658	0.51	0/2255
1	C	0.43	0/1659	0.52	0/2257
1	D	0.52	3/1731 (0.2%)	0.54	0/2355
All	All	0.47	3/6743 (0.0%)	0.53	0/9172

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	GLU	C-O	5.91	1.34	1.23
1	D	44	GLU	CB-CG	5.55	1.62	1.52
1	D	44	GLU	C-N	5.47	1.42	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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	1651	0	1571	5	0
1	B	1614	0	1532	4	0
1	C	1615	0	1536	5	0
1	D	1685	0	1601	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	116	0	0	0	0
3	B	89	0	0	0	0
3	C	94	0	0	0	0
3	D	97	0	0	0	0
All	All	6965	0	6240	17	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 17 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:D:214:PRO:O	1:D:215:ARG:HB2	1.92	0.69
1:A:59:GLN:OE1	1:A:62:ARG:NH1	2.33	0.58
1:D:50:ASP:N	1:D:50:ASP:OD1	2.37	0.56
1:A:71:LEU:O	1:A:75:ALA:HB3	2.10	0.51
1:B:209:ALA:HB1	1:C:212:LEU:HD13	1.92	0.51

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	206/229 (90%)	202 (98%)	4 (2%)	0	100	100
1	B	200/229 (87%)	195 (98%)	5 (2%)	0	100	100
1	C	200/229 (87%)	197 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	212/229 (93%)	206 (97%)	5 (2%)	1 (0%)	29	15
All	All	818/916 (89%)	800 (98%)	17 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	95	ASN

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	166/180 (92%)	165 (99%)	1 (1%)	86	83
1	B	163/180 (91%)	161 (99%)	2 (1%)	71	62
1	C	164/180 (91%)	162 (99%)	2 (1%)	71	62
1	D	170/180 (94%)	168 (99%)	2 (1%)	71	62
All	All	663/720 (92%)	656 (99%)	7 (1%)	73	65

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	LEU
1	D	95	ASN
1	C	99	GLN
1	B	124	ASP
1	D	50	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	99	GLN
1	D	95	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 carbohydrates 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](#)

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, 95th 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 ²)	Q<0.9
1	A	210/229 (91%)	0.34	7 (3%) 46 44	21, 28, 39, 46	0
1	B	204/229 (89%)	0.29	1 (0%) 91 91	25, 31, 37, 44	0
1	C	204/229 (89%)	0.27	7 (3%) 45 42	25, 31, 38, 49	0
1	D	214/229 (93%)	0.38	6 (2%) 53 52	25, 31, 42, 50	0
All	All	832/916 (90%)	0.32	21 (2%) 57 56	21, 31, 39, 50	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	213	VAL	5.4
1	A	213	VAL	4.9
1	A	212	LEU	4.1
1	A	45	GLY	3.7
1	C	212	LEU	3.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	D	229	1/1	0.99	0.09	23,23,23,23	1
2	FE	A	229	1/1	0.99	0.09	18,18,18,18	1
2	FE	C	229	1/1	0.99	0.11	20,20,20,20	1
2	FE	B	229	1/1	0.99	0.10	20,20,20,20	1

6.5 Other polymers [i](#)

There are no such residues in this entry.