WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:03 am GMT

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PDB ID	:	1SXN
Title	:	REDUCED BOVINE SUPEROXIDE DISMUTASE AT PH 5.0
Authors	:	Ferraroni, M.; Rypniewski, W.R.; Bruni, B.; Orioli, P.; Wilson, K.S.; Mangani, S.
Deposited on	:	1997-09-17
Resolution	:	1.90 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		0.9%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
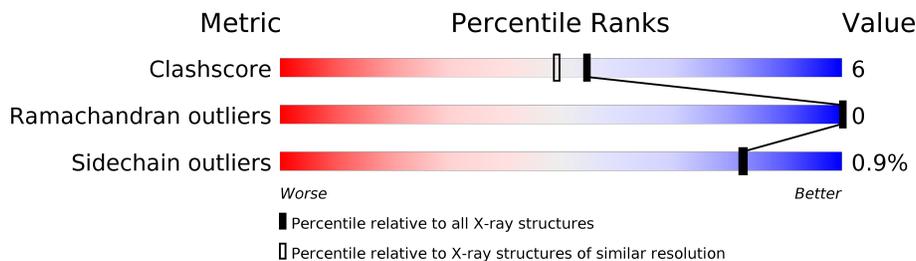
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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. 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% 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	151	79% 20% •
1	B	151	83% 15% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 2508 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 CU, ZN SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total 1076	C 661	N 191	O 220	S 4	0	1	0
1	B	151	Total 1058	C 651	N 188	O 215	S 4	0	0	0

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	248	Total O 248 248	0	0
5	B	120	Total O 120 120	0	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.

Note EDS was not executed.

• Molecule 1: CU, ZN SUPEROXIDE DISMUTASE

Chain A:

• Molecule 1: CU, ZN SUPEROXIDE DISMUTASE

Chain B:
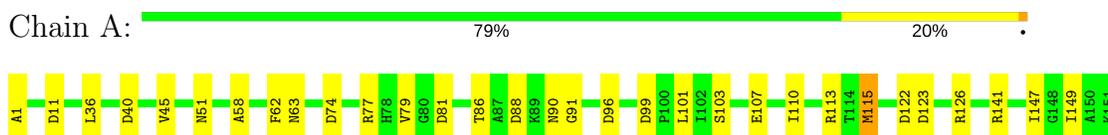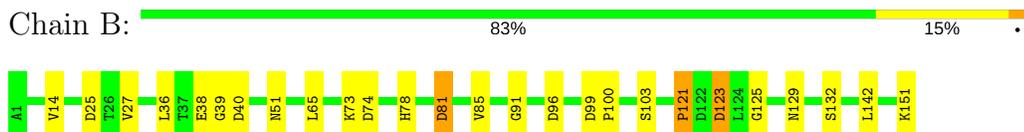
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.69Å 197.80Å 50.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	98.0 (10.00-1.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.95	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2508	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, CU

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	1.04	2/1099 (0.2%)	2.01	25/1489 (1.7%)
1	B	0.76	0/1076	1.75	11/1459 (0.8%)
All	All	0.91	2/2175 (0.1%)	1.88	36/2948 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103[A]	SER	CB-OG	-5.21	1.35	1.42
1	A	103[B]	SER	CB-OG	-5.21	1.35	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	CB-CG-OD1	18.57	135.01	118.30
1	A	126	ARG	NE-CZ-NH2	-13.89	113.35	120.30
1	A	126	ARG	NE-CZ-NH1	13.75	127.17	120.30
1	B	81	ASP	CB-CG-OD1	13.36	130.32	118.30
1	A	99	ASP	CB-CG-OD2	11.96	129.06	118.30
1	A	141	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	88	ASP	CB-CG-OD1	9.71	127.04	118.30
1	B	96	ASP	N-CA-CB	8.54	125.97	110.60
1	B	81	ASP	CB-CG-OD2	-8.25	110.87	118.30
1	A	115	MET	CA-CB-CG	8.09	127.06	113.30
1	A	81	ASP	OD1-CG-OD2	-8.08	107.94	123.30
1	B	103	SER	N-CA-CB	-7.58	99.13	110.50
1	B	129	ASN	N-CA-CB	7.41	123.94	110.60
1	B	96	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	11	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	74	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	123	ASP	CB-CG-OD1	6.44	124.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	PRO	N-CA-CB	6.24	110.79	103.30
1	A	107	GLU	OE1-CD-OE2	-6.24	115.82	123.30
1	A	122	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	58	ALA	O-C-N	-6.16	112.73	123.20
1	A	79	VAL	O-C-N	-6.07	112.89	123.20
1	A	149	ILE	CA-CB-CG1	-5.95	99.70	111.00
1	A	74	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	27	VAL	N-CA-C	-5.58	95.93	111.00
1	A	77	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	113	ARG	CD-NE-CZ	5.42	131.19	123.60
1	B	85	VAL	CG1-CB-CG2	5.42	119.57	110.90
1	A	110	ILE	CA-CB-CG2	-5.38	100.15	110.90
1	A	99	ASP	OD1-CG-OD2	-5.26	113.30	123.30
1	A	62	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	A	40	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	101	LEU	O-C-N	5.18	130.99	122.70
1	A	63	ASN	N-CA-CB	-5.17	101.30	110.60
1	A	86	THR	CA-CB-CG2	-5.10	105.26	112.40
1	B	123	ASP	O-C-N	-5.09	114.56	122.70

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	1076	0	1017	12	0
1	B	1058	0	994	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	248	0	0	5	0
5	B	120	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2508	0	2011	25	1

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 6.

All (25) 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:51:ASN:HB2	5:A:471:HOH:O	1.82	0.79
1:B:151:LYS:NZ	5:B:184:HOH:O	2.20	0.74
1:A:115:MET:HE3	1:A:147:ILE:HD11	1.70	0.71
1:A:45:VAL:HG22	1:A:115:MET:CE	2.20	0.70
1:B:14:VAL:HG21	1:B:142:LEU:HB3	1.74	0.70
1:A:96:ASP:OD1	5:A:515:HOH:O	2.11	0.69
1:A:115:MET:CE	1:A:147:ILE:HD11	2.23	0.68
1:B:51:ASN:HB2	5:B:163:HOH:O	1.93	0.67
1:A:45:VAL:HG22	1:A:115:MET:HE1	1.77	0.66
1:A:1:ALA:N	5:A:586:HOH:O	2.21	0.65
1:B:65:LEU:HD12	5:B:219:HOH:O	2.00	0.62
1:B:36:LEU:O	1:B:91:GLY:HA2	2.00	0.61
1:A:90:ASN:HB3	5:A:502:HOH:O	2.12	0.49
1:B:36:LEU:O	1:B:91:GLY:CA	2.61	0.49
1:B:78:HIS:HB2	1:B:81:ASP:CG	2.33	0.49
1:B:99:ASP:HA	1:B:100:PRO:HD3	1.69	0.47
1:A:96:ASP:CG	5:A:515:HOH:O	2.50	0.47
1:A:115:MET:HA	1:A:115:MET:HE2	1.98	0.45
1:B:123:ASP:OD1	1:B:132:SER:OG	2.33	0.44
1:B:14:VAL:HG21	1:B:142:LEU:HD13	1.99	0.44
1:B:40:ASP:CB	1:B:121:PRO:HB3	2.49	0.43
1:A:36:LEU:O	1:A:91:GLY:HA2	2.19	0.42
1:A:45:VAL:HG22	1:A:115:MET:HE2	1.98	0.41
1:B:125:GLY:HA2	1:B:132:SER:O	2.21	0.41
1:B:38:GLU:HG2	1:B:39:GLY:N	2.35	0.41

All (1) 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)
5:B:203:HOH:O	5:B:203:HOH:O[4_556]	2.07	0.13

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	150/151 (99%)	148 (99%)	2 (1%)	0	100	100
1	B	149/151 (99%)	142 (95%)	7 (5%)	0	100	100
All	All	299/302 (99%)	290 (97%)	9 (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	111/117 (95%)	111 (100%)	0	100	100
1	B	107/117 (92%)	105 (98%)	2 (2%)	62	57
All	All	218/234 (93%)	216 (99%)	2 (1%)	82	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	ASP
1	B	73	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	53	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.