wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:14 PM GMT

PDB ID	:	1SRD
Title	:	Three-dimensional structure of CU,ZN-superoxide dismutase from spinach at 2.0 Angstroms resolution
Authors	:	Kitagawa, Y.; Katsube, Y.
Deposited on	:	1993-04-15
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

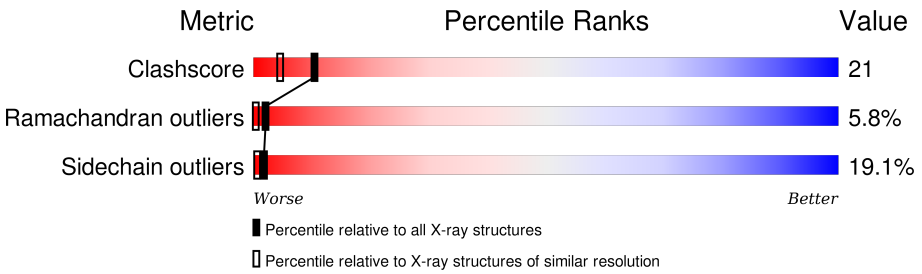
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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	154	46% 29% 19% 6%
1	B	154	49% 29% 19% .
1	C	154	40% 34% 17% 8%
1	D	154	47% 25% 19% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4524 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 COPPER,ZINC SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	154	1103	675	200	225	3	0	0	0
1	B	154	1103	675	200	225	3	0	0	0
1	C	154	1103	675	200	225	3	0	0	0
1	D	154	1103	675	200	225	3	0	0	0

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

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	26	26	26	0	0
			Total	O		
4	B	26	26	26	0	0
			Total	O		
4	C	26	26	26	0	0
			Total	O		
4	D	26	26	26	0	0

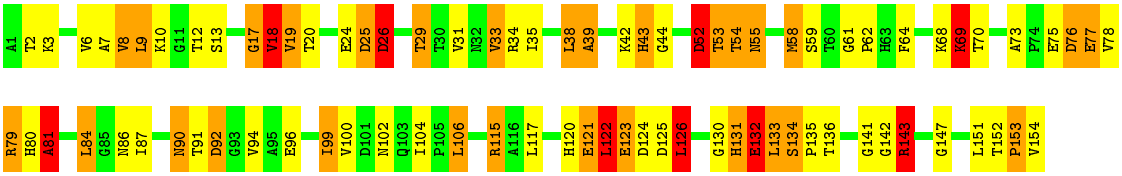
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

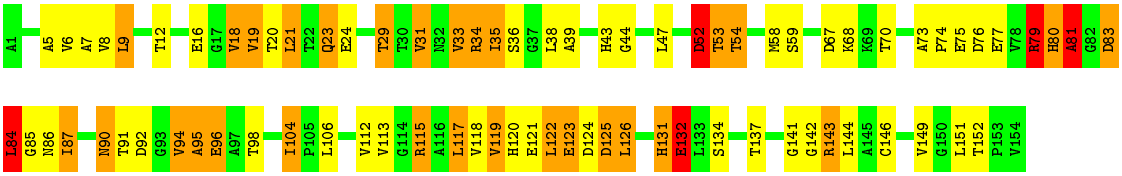
- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain A: 46% 29% 19% 6%



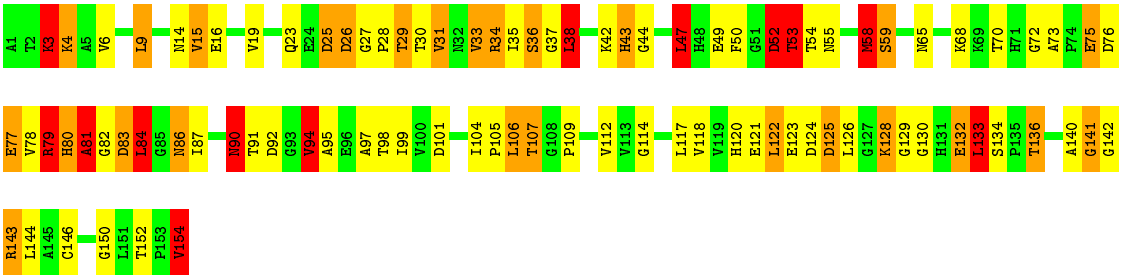
- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain B: 49% 29% 19% •



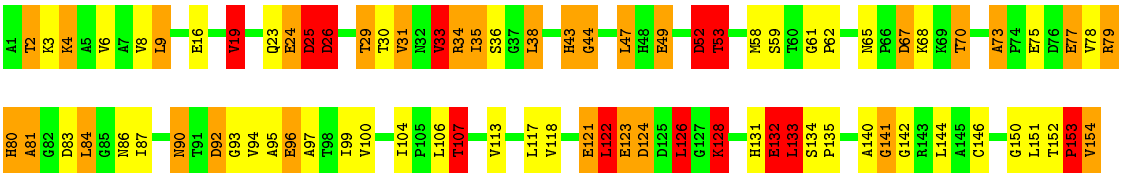
- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain C: 40% 34% 17% 8%



- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain D: 47% 25% 19% 8%


A1 T2 K3 K4 A5 V6 A7 V8 L9 E16 V19 Q23 E24 D25 D26 T29 T30 V31 N32 V33 R34 I35 S36 G37 L38 H43 G44 L47 H48 E49 D52 T53 M58 S59 T60 G61 P62 N65 P66 D67 K68 K69 T70 A73 F74 E75 D76 E77 V78 R79
H80 A81 G82 D83 L84 G85 N86 I87 N90 T91 D92 G93 V94 A95 E96 A97 T98 I99 V100 I104 P105 L106 T107 V113 L117 V118 E121 L122 E123 D124 D125 L126 G127 K128 H131 E132 L133 S134 P135 A140 G141 G142 R143 L144 A145 C146 G150 L151 T152 P153 V154

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.27Å 45.97Å 85.68Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	5.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.249 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4524	wwPDB-VP
Average B, all atoms ($Å^2$)	9.0	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: ZN, 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	1.46	4/1122 (0.4%)	2.56	60/1528 (3.9%)
1	B	1.39	3/1122 (0.3%)	2.14	51/1528 (3.3%)
1	C	1.41	5/1122 (0.4%)	2.18	63/1528 (4.1%)
1	D	1.46	3/1122 (0.3%)	2.32	62/1528 (4.1%)
All	All	1.43	15/4488 (0.3%)	2.31	236/6112 (3.9%)

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	D	0	1
All	All	0	2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	GLY	N-CA	6.77	1.56	1.46
1	A	115	ARG	NE-CZ	-6.76	1.24	1.33
1	D	132	GLU	CD-OE1	-6.19	1.18	1.25
1	C	141	GLY	N-CA	-6.05	1.36	1.46
1	D	141	GLY	N-CA	-5.72	1.37	1.46

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	ARG	CD-NE-CZ	31.36	167.51	123.60
1	A	133	LEU	CA-CB-CG	20.27	161.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	ARG	NE-CZ-NH2	-17.94	111.33	120.30
1	B	143	ARG	CD-NE-CZ	17.30	147.82	123.60
1	A	99	ILE	CB-CG1-CD1	17.25	162.19	113.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ARG	Sidechain
1	D	133	LEU	Mainchain

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	1103	0	1072	38	5
1	B	1103	0	1074	48	1
1	C	1103	0	1073	64	5
1	D	1103	0	1074	56	4
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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	26	0	0	7	0
4	B	26	0	0	13	0
4	C	26	0	0	15	4
4	D	26	0	0	7	1
All	All	4524	0	4293	187	10

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 21.

The worst 5 of 187 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:C:150:GLY:HA3	4:C:180:HOH:O	1.16	1.26
1:C:50:PHE:CE2	1:D:153:PRO:HG3	1.84	1.12
1:B:118:VAL:HG12	4:B:178:HOH:O	1.51	1.08
1:C:150:GLY:CA	4:C:180:HOH:O	1.86	0.91
1:B:54:THR:HG23	4:B:174:HOH:O	1.74	0.87

The worst 5 of 10 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)
1:D:97:ALA:O	4:C:172:HOH:O[4_547]	1.00	1.20
1:D:97:ALA:C	4:C:172:HOH:O[4_547]	1.14	1.06
1:A:24:GLU:OE1	1:C:130:GLY:CA[4_547]	1.65	0.55
1:D:97:ALA:CA	4:C:172:HOH:O[4_547]	1.68	0.52
1:A:39:ALA:CB	1:C:132:GLU:OE2[4_557]	1.83	0.37

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	152/154 (99%)	128 (84%)	15 (10%)	9 (6%)	2	0
1	B	152/154 (99%)	124 (82%)	21 (14%)	7 (5%)	3	1
1	C	152/154 (99%)	125 (82%)	17 (11%)	10 (7%)	1	0
1	D	152/154 (99%)	126 (83%)	17 (11%)	9 (6%)	2	0
All	All	608/616 (99%)	503 (83%)	70 (12%)	35 (6%)	2	0

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	80	HIS

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Mol	Chain	Res	Type
1	A	153	PRO
1	B	52	ASP
1	B	132	GLU

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	119/119 (100%)	92 (77%)	27 (23%)	1 0
1	B	119/119 (100%)	101 (85%)	18 (15%)	3 1
1	C	119/119 (100%)	97 (82%)	22 (18%)	2 1
1	D	119/119 (100%)	95 (80%)	24 (20%)	1 0
All	All	476/476 (100%)	385 (81%)	91 (19%)	2 0

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	ILE
1	C	47	LEU
1	D	99	ILE
1	B	123	GLU
1	C	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	32	ASN
1	C	86	ASN
1	C	120	HIS
1	B	103	GLN
1	D	55	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 8 ligands modelled in this entry, 8 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.