Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2023 – 12:23 am GMT

PDB ID	:	2C9U
Title	:	1.24 Angstroms resolution structure of as-isolated Cu-Zn Human Superoxide dismutase
Authors	:	Strange, R.W.; Antonyuk, S.V.; Hough, M.A.; Doucette, P.A.; Valentine S, J.S.; Hasnain, S.
Deposited on	:	2005-12-14
Resolution	:	1.24 Å(reported)

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

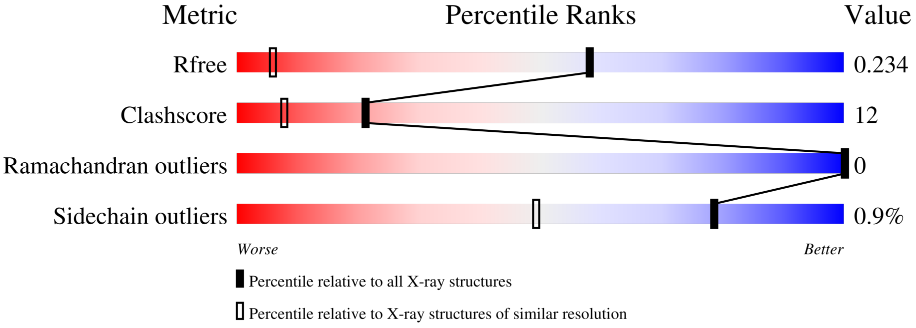
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 1.24 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	2024 (1.28-1.20)
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	153	
1	F	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	F	1154	-	-	X	-
5	ACT	F	1159	-	-	X	-

2 Entry composition ⓘ

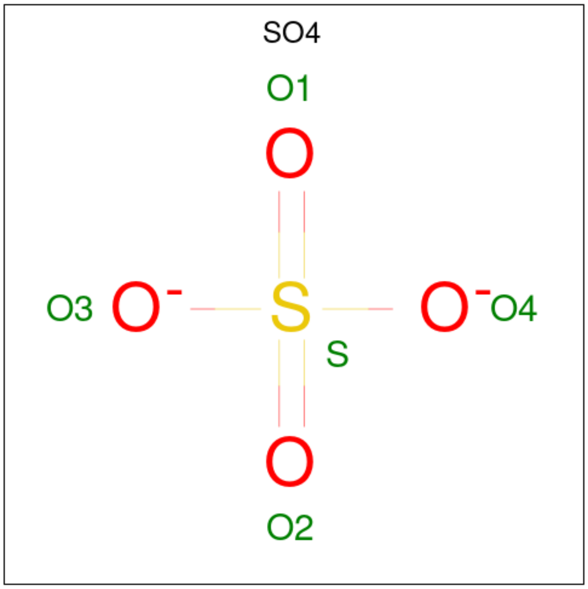
There are 6 unique types of molecules in this entry. The entry contains 2691 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUPEROXIDE DISMUTASE [CU-ZN].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1129	690	208	227	4	0	8	0
1	F	153	1144	699	207	232	6	0	12	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	F	1	5	4	1	0	0

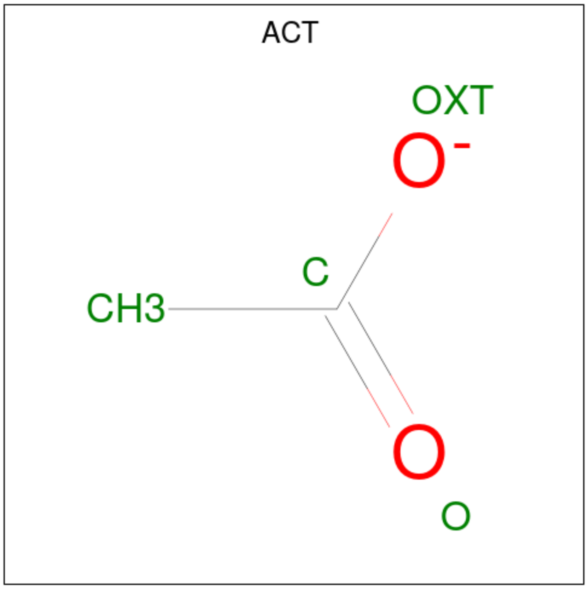
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0
3	F	1	Total Cu 1 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	F	2	Total Zn 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	197	Total O 197 197	0	0

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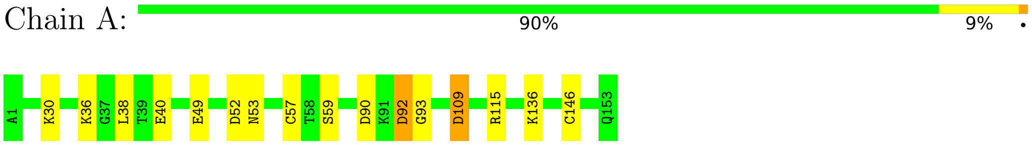
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	192	Total O 192 192	0	0

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.

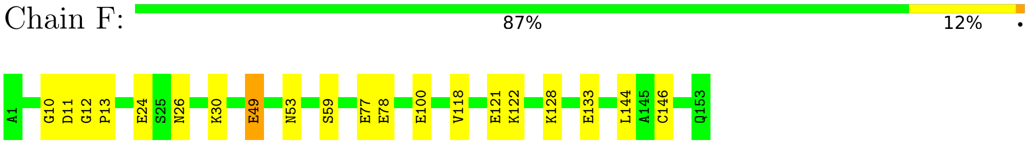
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain A:



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain F:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.64Å 67.55Å 52.32Å 90.00° 106.48° 90.00°	Depositor
Resolution (Å)	50.19 – 1.24 19.67 – 1.24	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.19-1.24) 93.9 (19.67-1.24)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.139 , 0.176 0.251 , 0.234	Depositor DCC
R_{free} test set	3457 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2691	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CU, ACT, SO4, ZN

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	0.93	2/1189 (0.2%)	0.90	2/1602 (0.1%)
1	F	1.03	6/1208 (0.5%)	0.92	0/1630
All	All	0.98	8/2397 (0.3%)	0.91	2/3232 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	49	GLU	CG-CD	-7.05	1.41	1.51
1	F	59[A]	SER	CA-CB	6.97	1.63	1.52
1	F	59[B]	SER	CA-CB	6.97	1.63	1.52
1	F	78	GLU	CD-OE1	6.79	1.33	1.25
1	A	59[A]	SER	CA-CB	6.61	1.62	1.52
1	A	59[B]	SER	CA-CB	6.61	1.62	1.52
1	F	78	GLU	CD-OE2	5.63	1.31	1.25
1	F	78	GLU	CG-CD	5.21	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	115	ARG	NE-CZ-NH2	-5.58	117.51	120.30

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	1129	0	1099	15	0
1	F	1144	0	1116	34	1
2	A	10	0	0	1	0
2	F	5	0	0	2	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
4	A	2	0	0	0	0
4	F	2	0	0	0	0
5	F	8	0	6	11	0
6	A	197	0	0	9	2
6	F	192	0	0	20	3
All	All	2691	0	2221	53	3

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 12.

All (53) 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:53[B]:ASN:OD1	6:A:2069:HOH:O	1.57	1.17
1:F:11:ASP:OD1	5:F:1159:ACT:OXT	1.65	1.13
1:A:40:GLU:OE2	6:A:2049:HOH:O	1.71	1.08
1:A:49[B]:GLU:OE1	6:A:2061:HOH:O	1.67	1.08
1:F:53[B]:ASN:OD1	6:F:2075:HOH:O	1.70	1.07
2:F:1154:SO4:O4	6:F:2186:HOH:O	1.72	1.06
1:F:11:ASP:CG	5:F:1159:ACT:OXT	1.93	1.06
2:A:1154:SO4:O1	6:A:2191:HOH:O	1.75	1.03
1:F:133:GLU:OE1	6:F:2168:HOH:O	1.76	1.01
1:F:13:PRO:HA	6:F:2011:HOH:O	1.59	1.00
1:F:12:GLY:N	6:F:2011:HOH:O	1.95	0.98
1:A:90:ASP:OD1	1:A:92[A]:ASP:OD1	1.80	0.98
1:F:77:GLU:O	6:F:2109:HOH:O	1.80	0.96
2:F:1154:SO4:O1	6:F:2189:HOH:O	1.85	0.93
1:F:10:GLY:O	6:F:2011:HOH:O	1.85	0.92
1:A:57:CYS:HG	1:A:146:CYS:HG	0.89	0.87
1:F:10:GLY:O	6:F:2012:HOH:O	1.96	0.83
1:F:121:GLU:OE1	1:F:122:LYS:NZ	2.14	0.80
1:F:11:ASP:C	6:F:2011:HOH:O	2.18	0.80
1:F:11:ASP:N	5:F:1159:ACT:C	2.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ASP:CA	6:F:2011:HOH:O	2.32	0.76
1:F:10:GLY:HA2	5:F:1159:ACT:O	1.84	0.76
1:F:49:GLU:HG3	6:F:2068:HOH:O	1.84	0.75
1:F:11:ASP:H	5:F:1159:ACT:C	2.00	0.75
1:A:53[B]:ASN:ND2	6:A:2070:HOH:O	2.00	0.71
1:A:52:ASP:OD2	6:A:2064:HOH:O	2.09	0.70
1:A:109:ASP:O	1:A:109:ASP:OD1	2.16	0.64
1:A:136:LYS:NZ	6:A:2176:HOH:O	2.29	0.64
1:F:11:ASP:HA	6:F:2011:HOH:O	1.97	0.62
1:A:36:LYS:HE3	6:A:2012:HOH:O	2.01	0.60
1:A:109:ASP:OD1	1:A:109:ASP:C	2.39	0.60
1:A:90:ASP:CG	1:A:92[A]:ASP:OD1	2.41	0.59
1:F:11:ASP:H	5:F:1159:ACT:CH3	2.19	0.55
1:F:10:GLY:CA	5:F:1159:ACT:O	2.53	0.55
1:F:128:LYS:HD3	6:F:2165:HOH:O	2.07	0.55
1:A:57:CYS:HG	1:A:146:CYS:CB	2.20	0.55
1:F:11:ASP:H	5:F:1159:ACT:H2	1.73	0.54
1:F:30[A]:LYS:HD3	6:F:2040:HOH:O	2.06	0.54
1:F:11:ASP:N	5:F:1159:ACT:O	2.41	0.52
1:F:30[A]:LYS:CD	6:F:2040:HOH:O	2.58	0.52
1:F:121:GLU:CD	1:F:122:LYS:HZ1	2.15	0.50
1:F:30[A]:LYS:HG3	1:F:100:GLU:HG2	1.92	0.50
1:F:118:VAL:HG22	1:F:146[B]:CYS:SG	2.52	0.50
1:F:121:GLU:CD	1:F:122:LYS:NZ	2.66	0.49
1:F:10:GLY:N	6:F:2012:HOH:O	2.27	0.47
1:F:10:GLY:C	5:F:1159:ACT:O	2.53	0.46
1:A:30[A]:LYS:HG2	6:A:2141:HOH:O	2.14	0.46
1:F:30[B]:LYS:HG3	6:F:2135:HOH:O	2.14	0.46
1:F:24:GLU:HG3	1:F:26:ASN:OD1	2.17	0.44
1:F:49:GLU:CG	6:F:2068:HOH:O	2.56	0.44
5:F:1159:ACT:H3	6:F:2175:HOH:O	2.20	0.41
1:A:38:LEU:O	1:A:93:GLY:HA2	2.21	0.41
1:F:10:GLY:HA3	1:F:144:LEU:O	2.21	0.41

All (3) 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)
6:A:2110:HOH:O	6:F:2067:HOH:O[2_746]	1.96	0.24
6:A:2058:HOH:O	6:F:2124:HOH:O[2_645]	2.08	0.12
1:F:26:ASN:ND2	6:F:2012:HOH:O[1_655]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	159/153 (104%)	158 (99%)	1 (1%)	0	100	100
1	F	162/153 (106%)	161 (99%)	1 (1%)	0	100	100
All	All	321/306 (105%)	319 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	124/118 (105%)	121 (98%)	3 (2%)	49	11
1	F	129/118 (109%)	129 (100%)	0	100	100
All	All	253/236 (107%)	250 (99%)	3 (1%)	78	36

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92[A]	ASP
1	A	92[B]	ASP
1	A	109	ASP

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

Mol	Chain	Res	Type
1	A	26	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1154	4	4,4,4	0.60	0	6,6,6	0.30	0
5	ACT	F	1158	-	3,3,3	1.21	0	3,3,3	3.16	2 (66%)
2	SO4	A	1155	-	4,4,4	0.31	0	6,6,6	0.67	0
5	ACT	F	1159	-	3,3,3	0.96	0	3,3,3	1.51	1 (33%)
2	SO4	F	1154	4	4,4,4	0.43	0	6,6,6	0.48	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1158	ACT	OXT-C-CH3	3.86	131.14	115.18
5	F	1158	ACT	OXT-C-O	-3.80	108.03	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1159	ACT	OXT-C-O	-2.08	114.39	122.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1154	SO4	1	0
5	F	1159	ACT	11	0
2	F	1154	SO4	2	0

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.