

Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 09:18 PM EDT

PDB ID : 2GBV

Title : C6A/C111A/C57A/C146A holo CuZn Superoxide dismutase Authors : Hornberg, A.; Logan, D.T.; Marklund, S.L.; Oliveberg, M.

Deposited on : 2006-03-11

Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS: 2.36

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)

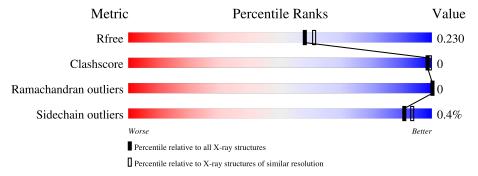
 $Validation\ Pipeline\ (wwPDB-VP) \quad : \quad 2.36$

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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	97%
1	В	153	97%
1	С	153	100%
1	D	153	97%
1	Е	153	98%
1	F	153	98%
1	G	153	99%



 $Continued\ from\ previous\ page...$

		I	
Mol	Chain	n Length	Quality of chain
1	Н	153	97%
1	Ι	153	100%
1	J	153	100%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12578 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		Ato	ms		ZeroOcc	AltConf	Trace
1	Λ	153	Total	С	N	О	0	0	0
1	A	199	1106	679	203	224	U	U	
1	В	153	Total	С	N	О	0	0	0
1	Б	100	1106	679	203	224		0	0
1	С	153	Total	С	N	О	0	0	0
1		100	1106	679	203	224	0	U	U
1	D	153	Total	С	N	О	0	0	0
1	D	100	1106	679	203	224		U	
1	E	153	Total	С	N	O	0	0	0
1	L	100	1106	679	203	224	O	U	U
1	F	153	Total	\mathbf{C}	N	O	0	0	0
1	1	100	1106	679	203	224	0	U	
1	G	153	Total	\mathbf{C}	N	O	0	0	0
1	G G	100	1106	679	203	224	0	Ü	0
1	Н	153	Total	\mathbf{C}	N	О	0	0	0
1	11	100	1106	679	203	224	0	U	U
1	I	153	Total	\mathbf{C}	N	O	0	0	0
1	1	100	1106	679	203	224		U	U
1	J	153	Total	\mathbf{C}	N	О	0	0	0
1	J	100	1106	679	203	224			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	CYS	engineered mutation	UNP P00441
A	57	ALA	CYS	engineered mutation	UNP P00441
A	111	ALA	CYS	engineered mutation	UNP P00441
A	146	ALA	CYS	engineered mutation	UNP P00441
В	6	ALA	CYS	engineered mutation	UNP P00441
В	57	ALA	CYS	engineered mutation	UNP P00441
В	111	ALA	CYS	engineered mutation	UNP P00441
В	146	ALA	CYS	engineered mutation	UNP P00441
С	6	ALA	CYS	engineered mutation	UNP P00441



Continued from previous page...

Chain	Residue	Modelled Modelled	Actual	Comment	Reference
С	57	ALA	CYS	engineered mutation	UNP P00441
С	111	ALA	CYS	engineered mutation	UNP P00441
С	146	ALA	CYS	engineered mutation	UNP P00441
D	6	ALA	CYS	engineered mutation	UNP P00441
D	57	ALA	CYS	engineered mutation	UNP P00441
D	111	ALA	CYS	engineered mutation	UNP P00441
D	146	ALA	CYS	engineered mutation	UNP P00441
Е	6	ALA	CYS	engineered mutation	UNP P00441
E	57	ALA	CYS	engineered mutation	UNP P00441
Е	111	ALA	CYS	engineered mutation	UNP P00441
Е	146	ALA	CYS	engineered mutation	UNP P00441
F	6	ALA	CYS	engineered mutation	UNP P00441
F	57	ALA	CYS	engineered mutation	UNP P00441
F	111	ALA	CYS	engineered mutation	UNP P00441
F	146	ALA	CYS	engineered mutation	UNP P00441
G	6	ALA	CYS	engineered mutation	UNP P00441
G	57	ALA	CYS	engineered mutation	UNP P00441
G	111	ALA	CYS	engineered mutation	UNP P00441
G	146	ALA	CYS	engineered mutation	UNP P00441
Н	6	ALA	CYS	engineered mutation	UNP P00441
Н	57	ALA	CYS	engineered mutation	UNP P00441
Н	111	ALA	CYS	engineered mutation	UNP P00441
Н	146	ALA	CYS	engineered mutation	UNP P00441
I	6	ALA	CYS	engineered mutation	UNP P00441
I	57	ALA	CYS	engineered mutation	UNP P00441
I	111	ALA	CYS	engineered mutation	UNP P00441
I	146	ALA	CYS	engineered mutation	UNP P00441
J	6	ALA	CYS	engineered mutation	UNP P00441
J	57	ALA	CYS	engineered mutation	UNP P00441
J	111	ALA	CYS	engineered mutation	UNP P00441
J	146	ALA	CYS	engineered mutation	UNP P00441

 \bullet Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
2	В	1	Total Cu 1 1	0	0
2	С	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0



 $Continued\ from\ previous\ page...$

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0
2	G	1	Total Cu 1 1	0	0
2	Н	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	J	1	Total Cu 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	Е	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0
3	Н	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	179	Total O 179 179	0	0



 $Continued\ from\ previous\ page...$

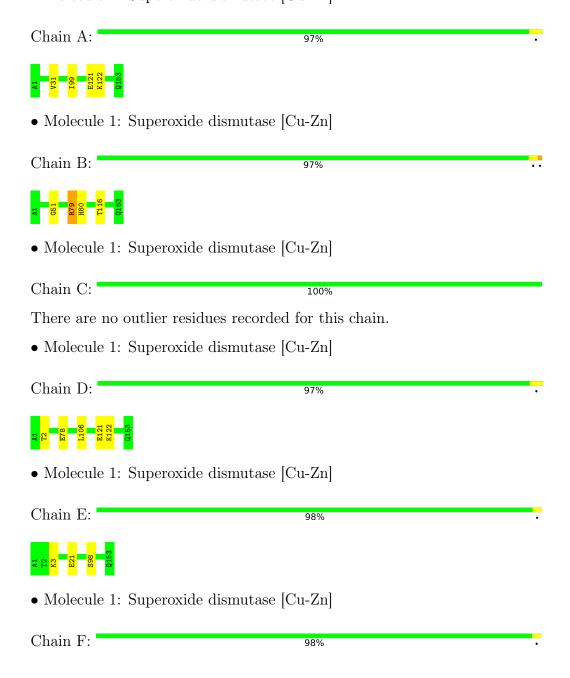
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	89	Total O 89 89	0	0
4	С	179	Total O 179 179	0	0
4	D	146	Total O 146 146	0	0
4	Е	98	Total O 98 98	0	0
4	F	169	Total O 169 169	0	0
4	G	190	Total O 190 190	0	0
4	Н	160	Total O 160 160	0	0
4	I	153	Total O 153 153	0	0
4	J	135	Total O 135 135	0	0



3 Residue-property plots (i)

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]





11	121	1131	153
_	щ	_	٥

• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain G: 99%



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain H: 97%



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain I:

There are no outlier residues recorded for this chain.

• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain J:

There are no outlier residues recorded for this chain.



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	166.80Å 202.37Å 143.64Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 - 2.00	Depositor
Resolution (A)	19.88 - 2.00	EDS
% Data completeness	100.0 (19.88-2.00)	Depositor
(in resolution range)	100.0 (19.88-2.00)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	7.01 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
D D	0.183 , 0.207	Depositor
R, R_{free}	0.212 , 0.230	DCC
R_{free} test set	8162 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 44.3	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12578	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 5.45% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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, CU1

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).

Mal	Mol Chain		Bond lengths		angles
IVIOI			# Z > 5	RMSZ	# Z > 5
1	A	0.33	0/1124	0.53	0/1516
1	В	0.32	0/1124	0.54	0/1516
1	С	0.36	0/1124	0.56	0/1516
1	D	0.33	0/1124	0.51	0/1516
1	Е	0.31	0/1124	0.51	0/1516
1	F	0.35	0/1124	0.54	0/1516
1	G	0.36	0/1124	0.57	0/1516
1	Н	0.37	0/1124	0.59	0/1516
1	I	0.35	0/1124	0.56	0/1516
1	J	0.32	0/1124	0.53	0/1516
All	All	0.34	0/11240	0.55	0/15160

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1106	0	1079	3	0
1	В	1106	0	1079	2	0
1	С	1106	0	1079	0	0



Continued from previous page...

Mol	Chain	Non-H		H(added)	Clashes	Symm-Clashes
1	D	1106	0	1079	2	0
1	Ε	1106	0	1079	2	0
1	F	1106	0	1079	2	0
1	G	1106	0	1079	0	0
1	Н	1106	0	1079	2	0
1	I	1106	0	1079	0	0
1	J	1106	0	1079	0	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Ε	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Ε	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	Η	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	179	0	0	0	0
4	В	89	0	0	0	0
4	С	179	0	0	0	0
4	D	146	0	0	0	0
4	Е	98	0	0	0	0
4	F	169	0	0	0	0
4	G	190	0	0	0	0
4	Н	160	0	0	0	0
4	I	153	0	0	0	0
4	J	135	0	0	0	0
All	All	12578	0	10790	11	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 0.

All (11) 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:121:GLU:HG3	1:D:122:LYS:HG3	1.79	0.64
1:E:98:SER:OG	1:F:21:GLU:OE1	2.21	0.52
1:A:121:GLU:HG3	1:A:122:LYS:HG3	1.94	0.49
1:A:121:GLU:CG	1:A:122:LYS:HG3	2.43	0.48
1:H:53:ASN:ND2	1:H:56:GLY:C	2.67	0.48
1:E:3:LYS:NZ	1:E:21:GLU:OE1	2.46	0.48
1:B:79:ARG:HD3	1:B:80:HIS:O	2.16	0.45
1:F:131:ASN:HB3	1:H:96:ASP:O	2.17	0.45
1:A:31:VAL:HB	1:A:99:ILE:HB	2.00	0.43
1:B:51:GLY:HA2	1:B:116:THR:OG1	2.19	0.42
1:D:2:THR:HG23	1:D:106:LEU:HD12	2.03	0.40

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	Perce	ntiles
1	A	151/153~(99%)	151 (100%)	0	0	100	100
1	В	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	С	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	D	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	Е	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	F	151/153 (99%)	151 (100%)	0	0	100	100
1	G	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	Н	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	I	151/153 (99%)	151 (100%)	0	0	100	100
1	J	151/153 (99%)	151 (100%)	0	0	100	100
All	All	1510/1530 (99%)	1504 (100%)	6 (0%)	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	$114/114\ (100\%)$	114 (100%)	0	100 100
1	В	$114/114\ (100\%)$	113 (99%)	1 (1%)	78 83
1	C	$114/114\ (100\%)$	114 (100%)	0	100 100
1	D	$114/114\ (100\%)$	113 (99%)	1 (1%)	78 83
1	E	$114/114\ (100\%)$	114 (100%)	0	100 100
1	F	$114/114\ (100\%)$	113 (99%)	1 (1%)	78 83
1	G	$114/114\ (100\%)$	113 (99%)	1 (1%)	78 83
1	Н	$114/114\ (100\%)$	113 (99%)	1 (1%)	78 83
1	I	$114/114\ (100\%)$	114 (100%)	0	100 100
1	J	$114/114\ (100\%)$	114 (100%)	0	100 100
All	All	1140/1140 (100%)	1135 (100%)	5 (0%)	91 93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	79	ARG
1	D	78	GLU
1	F	153	GLN
1	G	24	GLU
1	Н	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	53	ASN
1	F	153	GLN
1	G	53	ASN
1	Н	53	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 20 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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

