

wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 02:46 AM EDT

PDB ID	:	1LUW
Title	:	CATALYTIC AND STRUCTURAL EFFECTS OF AMINO-ACID SUBSTI-
		TUTION AT HIS 30 IN HUMAN MANGANESE SUPEROXIDE DISMU-
		TASE: INSERTION OF VAL CGAMMA INTO THE SUBSTRATE ACCESS
		CHANNEL
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Deposited on	:	2002-05-23
Resolution	:	2.30 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 (i) symbol.

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

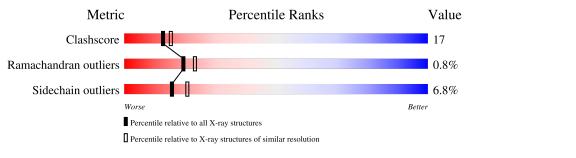
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 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)	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	А	198	73%	25%	•		
1	В	198	62%	33%	5%		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3351 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 [Mn].

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	198	Total	С	Ν	Ο	S	0	0	0
	Л	198	1572	1007	274	287	4			
1	В	198	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	190	1572	1007	274	287	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

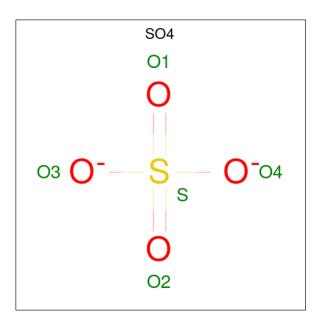
Chair	1 Residue	Modelled	Actual	Comment	Reference
A	30	GLN	HIS	engineered mutation	UNP P04179
В	30	GLN	HIS	engineered mutation	UNP P04179

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Mn 1 1	0	0
2	В	1	Total Mn 1 1	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.

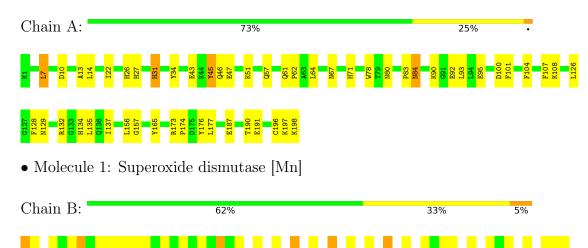
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	118	Total O 118 118	0	0
4	В	77	Total O 77 77	0	0



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.

Note EDS was not executed.



• Molecule 1: Superoxide dismutase [Mn]



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	79.36Å 79.36Å 242.58Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.81 - 2.30	Depositor
% Data completeness	93.5 (16.81-2.30)	Depositor
(in resolution range)	35.5 (10.01-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3351	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	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: SO4, MN

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		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.36	0/1617	0.59	0/2194	
1	В	0.36	0/1617	0.59	0/2194	
All	All	0.36	0/3234	0.59	0/4388	

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	А	1572	0	1529	37	0
1	В	1572	0	1529	68	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	5	0	0	0	0
3	В	5	0	0	0	0
4	А	118	0	0	0	0
4	В	77	0	0	3	1
All	All	3351	0	3058	103	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 17.



Atom-1	Atom-1 Atom-2		Clash overlap (Å)
1:B:146:LEU:HD21	1:B:152:LEU:HB2	1.47	0.94
1:B:31:HIS:HD2	1:B:78:TRP:HE1	1.09	0.91
1:A:31:HIS:HD2	1:A:78:TRP:HE1	1.18	0.89
1:A:84:ASN:HD22	1:A:84:ASN:H	1.20	0.89
1:B:193:TYR:CE1	1:B:197:LYS:HD2	2.08	0.89

The worst 5 of 103 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	tom-1 Atom-2 Interatomic distance (Å)		Clash overlap (Å)	
4:B:208:HOH:O	4:B:208:HOH:O[11_555]	1.95	0.25	

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	Percent	tiles
1	А	196/198~(99%)	187 (95%)	8 (4%)	1 (0%)	29	35
1	В	196/198~(99%)	178 (91%)	16 (8%)	2(1%)	15	17
All	All	392/396~(99%)	365(93%)	24~(6%)	3~(1%)	19	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	131	GLU
1	В	165	TYR
1	А	165	TYR



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	А	162/162~(100%)	153~(94%)	9~(6%)	21 29	
1	В	162/162~(100%)	149 (92%)	13 (8%)	12 15	
All	All	324/324~(100%)	302~(93%)	22 (7%)	16 21	

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	45	TYR
1	В	105	ASP
1	В	81	LEU
1	В	107	PHE
1	А	95	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such side chains are listed below:

Mol	Chain	Res	Type
1	В	27	HIS
1	В	67	ASN
1	В	168	GLN
1	В	119	GLN
1	А	84	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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 Cha	e Chain Res Linl	Link	Bond lengths		Bond angles					
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	SO4	В	899	-	4,4,4	0.24	0	$6,\!6,\!6$	0.05	0
3	SO4	А	898	-	4,4,4	0.20	0	$6,\!6,\!6$	0.07	0

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

