wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 03:22 pm GMT

PDB ID	:	7B4O
Title	:	A Bacteroidetes bacterium CuZn-superoxide dismutase with ZnZn metalation
Authors	:	Wright, G.S.A.
Deposited on	:	2020-12-02
Resolution	:	1.41 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

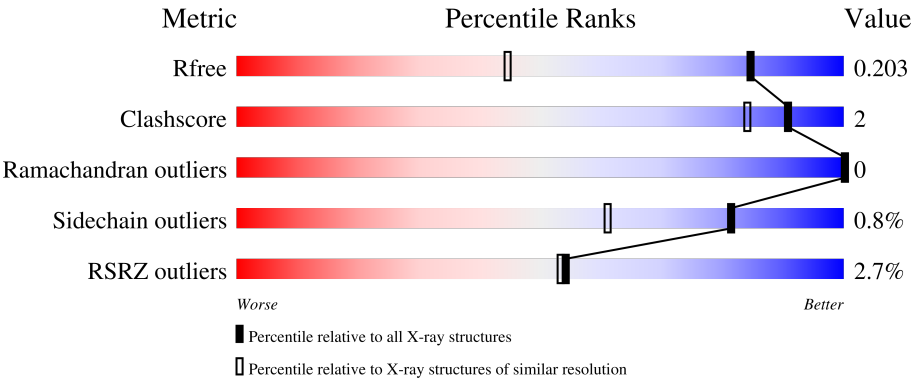
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 1.41 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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% 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.

Mol	Chain	Length	Quality of chain
1	AAA	153	2% 93% 5%
1	BBB	153	3% 94%
1	CCC	153	3% 92% 6%
1	DDD	153	3% 95%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9579 atoms, of which 4441 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
1	AAA	150	Total	C	H	N	O	S	42	2	0
			2216	690	1095	199	223	9			
1	BBB	150	Total	C	H	N	O	S	44	7	0
			2285	713	1125	205	233	9			
1	CCC	150	Total	C	H	N	O	S	44	6	0
			2270	708	1119	204	230	9			
1	DDD	150	Total	C	H	N	O	S	42	3	0
			2229	695	1102	199	225	8			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	4	Total	Zn	0	0
			4	4		
2	BBB	4	Total	Zn	0	0
			4	4		
2	CCC	4	Total	Zn	0	0
			4	4		
2	DDD	3	Total	Zn	0	0
			3	3		

- Molecule 3 is water.

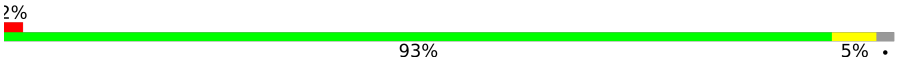
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	175	Total	O	0	0
			175	175		
3	BBB	107	Total	O	0	0
			107	107		
3	CCC	106	Total	O	0	0
			106	106		
3	DDD	176	Total	O	0	1
			176	176		

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 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.

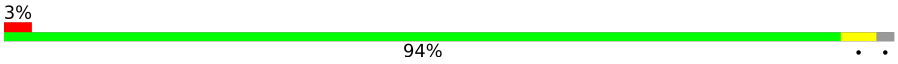
• Molecule 1: Superoxide dismutase [Cu-Zn]

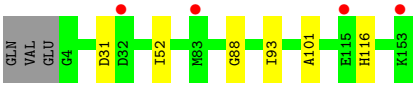
Chain AAA:



• Molecule 1: Superoxide dismutase [Cu-Zn]

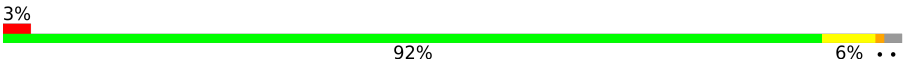
Chain BBB:

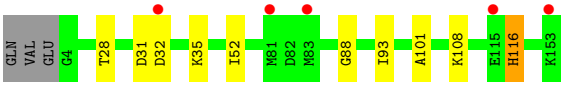




• Molecule 1: Superoxide dismutase [Cu-Zn]

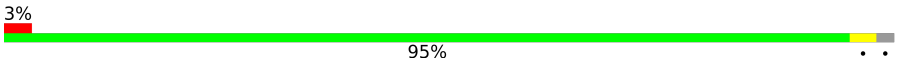
Chain CCC:

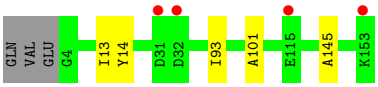




• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain DDD:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	96.47Å 96.64Å 136.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.27 – 1.41 68.27 – 1.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.27-1.41) 100.0 (68.27-1.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 1.41Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.159 , 0.192 0.168 , 0.203	Depositor DCC
R_{free} test set	6227 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	11.1	Xtriage
Anisotropy	1.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.477 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 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	AAA	0.63	0/1144	0.74	0/1538
1	BBB	0.62	0/1190	0.73	0/1601
1	CCC	0.62	0/1181	0.72	0/1589
1	DDD	0.64	0/1153	0.73	0/1551
All	All	0.63	0/4668	0.73	0/6279

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

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	AAA	1121	1095	1085	4	0
1	BBB	1160	1125	1112	2	0
1	CCC	1151	1119	1107	6	0
1	DDD	1127	1102	1093	3	0
2	AAA	4	0	0	0	0
2	BBB	4	0	0	0	0
2	CCC	4	0	0	0	0
2	DDD	3	0	0	0	0
3	AAA	175	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	107	0	0	0	0
3	CCC	106	0	0	2	0
3	DDD	176	0	0	1	0
All	All	5138	4441	4397	15	0

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 2.

The worst 5 of 15 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:AAA:14:TYR:OH	3:AAA:301:HOH:O	1.90	0.90
1:DDD:14:TYR:OH	3:DDD:301:HOH:O	1.99	0.80
1:CCC:116:HIS:O	3:CCC:301:HOH:O	2.17	0.58
1:AAA:73:GLU:OE2	1:AAA:116:HIS:NE2	2.35	0.54
1:DDD:13[A]:ILE:HG23	1:DDD:145:ALA:HB1	1.92	0.52

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	Percentiles	
1	AAA	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	BBB	155/153 (101%)	153 (99%)	2 (1%)	0	100	100
1	CCC	154/153 (101%)	152 (99%)	2 (1%)	0	100	100
1	DDD	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
All	All	610/612 (100%)	604 (99%)	6 (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	AAA	121/122 (99%)	121 (100%)	0	100	100
1	BBB	126/122 (103%)	124 (98%)	2 (2%)	62	32
1	CCC	125/122 (102%)	123 (98%)	2 (2%)	62	32
1	DDD	122/122 (100%)	122 (100%)	0	100	100
All	All	494/488 (101%)	490 (99%)	4 (1%)	81	61

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	31	ASP
1	BBB	116	HIS
1	CCC	31	ASP
1	CCC	116	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 15 ligands modelled in this entry, 15 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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	150/153 (98%)	-0.09	3 (2%)	65	65	11, 15, 34, 54	0
1	BBB	150/153 (98%)	-0.08	4 (2%)	54	53	11, 18, 44, 57	0
1	CCC	150/153 (98%)	-0.12	5 (3%)	46	46	11, 18, 41, 55	0
1	DDD	150/153 (98%)	-0.07	4 (2%)	54	53	11, 15, 35, 122	2 (1%)
All	All	600/612 (98%)	-0.09	16 (2%)	54	53	11, 17, 42, 122	2 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	32	ASP	3.8
1	BBB	32	ASP	3.4
1	CCC	32	ASP	3.2
1	CCC	83	MET	3.0
1	AAA	32	ASP	2.7

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	AAA	204	1/1	0.96	0.06	37,37,37,37	1
2	ZN	BBB	204	1/1	0.96	0.06	31,31,31,31	1
2	ZN	DDD	203	1/1	0.96	0.08	39,39,39,39	1
2	ZN	CCC	204	1/1	0.97	0.04	35,35,35,35	1
2	ZN	CCC	203	1/1	0.98	0.10	24,24,24,24	1
2	ZN	BBB	203	1/1	0.99	0.10	24,24,24,24	1
2	ZN	AAA	202	1/1	1.00	0.09	13,13,13,13	0
2	ZN	AAA	203	1/1	1.00	0.10	24,24,24,24	1
2	ZN	CCC	201	1/1	1.00	0.09	16,16,16,16	0
2	ZN	CCC	202	1/1	1.00	0.09	17,17,17,17	0
2	ZN	AAA	201	1/1	1.00	0.09	17,17,17,17	0
2	ZN	BBB	201	1/1	1.00	0.09	15,15,15,15	0
2	ZN	DDD	201	1/1	1.00	0.08	16,16,16,16	0
2	ZN	DDD	202	1/1	1.00	0.10	13,13,13,13	0
2	ZN	BBB	202	1/1	1.00	0.09	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.