Full wwPDB X-ray Structure Validation Report (i)

May 27, 2024 – 06:05 PM EDT

PDB ID	:	4YIP
Title	:	X-ray structure of the iron/manganese cambialistic superoxide dismutase from Streptococcus mutans
Authors	:	Russo Krauss, I.; Merlino, A.; Pica, A.; Sica, F.
Deposited on	:	2015-03-02
Resolution	:	2.15 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 (i)) were used in the production of this report:

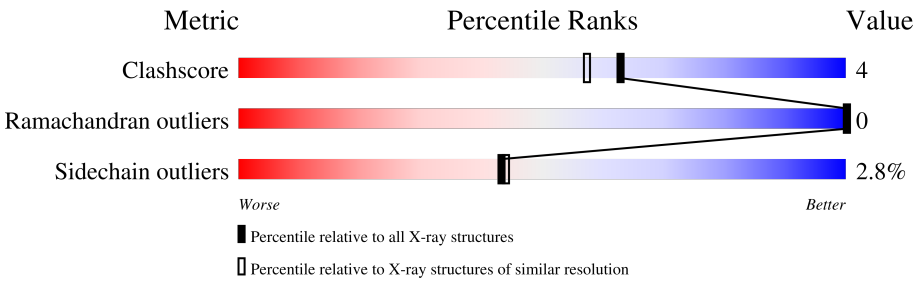
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.15 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	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	210	83% 12% • •
1	B	210	89% 8% •
1	C	210	86% 10% •
1	D	210	86% 10% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6699 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/Fe].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	203	1615	1042	266	306	1	0	2	0
1	B	203	1607	1036	265	305	1	0	1	0
1	C	201	1586	1022	263	300	1	0	0	0
1	D	203	1609	1037	265	306	1	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	LEU	-	expression tag	UNP P09738
A	203	GLU	-	expression tag	UNP P09738
A	204	HIS	-	expression tag	UNP P09738
A	205	HIS	-	expression tag	UNP P09738
A	206	HIS	-	expression tag	UNP P09738
A	207	HIS	-	expression tag	UNP P09738
A	208	HIS	-	expression tag	UNP P09738
A	209	HIS	-	expression tag	UNP P09738
B	202	LEU	-	expression tag	UNP P09738
B	203	GLU	-	expression tag	UNP P09738
B	204	HIS	-	expression tag	UNP P09738
B	205	HIS	-	expression tag	UNP P09738
B	206	HIS	-	expression tag	UNP P09738
B	207	HIS	-	expression tag	UNP P09738
B	208	HIS	-	expression tag	UNP P09738
B	209	HIS	-	expression tag	UNP P09738
C	202	LEU	-	expression tag	UNP P09738
C	203	GLU	-	expression tag	UNP P09738
C	204	HIS	-	expression tag	UNP P09738
C	205	HIS	-	expression tag	UNP P09738
C	206	HIS	-	expression tag	UNP P09738

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Chain	Residue	Modelled	Actual	Comment	Reference
C	207	HIS	-	expression tag	UNP P09738
C	208	HIS	-	expression tag	UNP P09738
C	209	HIS	-	expression tag	UNP P09738
D	202	LEU	-	expression tag	UNP P09738
D	203	GLU	-	expression tag	UNP P09738
D	204	HIS	-	expression tag	UNP P09738
D	205	HIS	-	expression tag	UNP P09738
D	206	HIS	-	expression tag	UNP P09738
D	207	HIS	-	expression tag	UNP P09738
D	208	HIS	-	expression tag	UNP P09738
D	209	HIS	-	expression tag	UNP P09738

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	71	72	72	0	1
			Total	O		
3	B	70	70	70	0	0
			Total	O		
3	C	65	65	65	0	0
			Total	O		
3	D	71	71	71	0	0

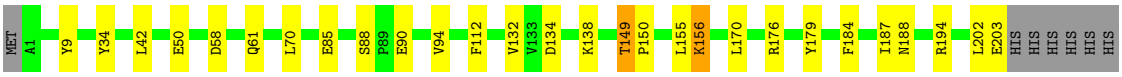
3 Residue-property plots (i)

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 failed to run properly.

- Molecule 1: Superoxide dismutase [Mn/Fe]

Chain A:

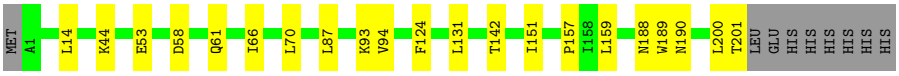


- Molecule 1: Superoxide dismutase [Mn/Fe]

Chain B:

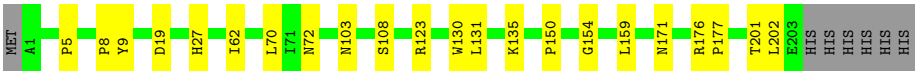
- Molecule 1: Superoxide dismutase [Mn/Fe]

Chain C:



- Molecule 1: Superoxide dismutase [Mn/Fe]

Chain D:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.96Å 82.88Å 72.78Å 90.00° 94.25° 90.00°	Depositor
Resolution (Å)	31.39 – 2.15	Depositor
% Data completeness (in resolution range)	99.0 (31.39-2.15)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.259	Depositor
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.304	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6699	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.75	0/1664	0.83	0/2275
1	B	0.78	0/1653	0.88	1/2262 (0.0%)
1	C	0.76	0/1629	0.81	0/2229
1	D	0.78	0/1655	0.83	1/2264 (0.0%)
All	All	0.77	0/6601	0.84	2/9030 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	ASP	CB-CG-OD1	7.56	125.10	118.30
1	D	123	ARG	NE-CZ-NH1	5.29	122.95	120.30

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	1615	0	1570	15	0
1	B	1607	0	1558	9	0
1	C	1586	0	1534	20	0
1	D	1609	0	1557	11	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	72	0	0	2	0
3	B	70	0	0	3	0
3	C	65	0	0	4	0
3	D	71	0	0	0	0
All	All	6699	0	6219	54	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 4.

All (54) 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:200:LEU:O	1:C:201:THR:HB	1.79	0.80
1:C:142:THR:HG22	3:C:426:HOH:O	1.90	0.71
1:B:88:SER:HB2	1:B:188:ASN:HB2	1.71	0.71
1:A:88:SER:HB2	1:A:188:ASN:HB2	1.73	0.70
1:A:134:ASP:HB2	1:A:138:LYS:H	1.58	0.67
1:B:154:GLY:HA2	3:B:421:HOH:O	1.96	0.65
1:C:53:GLU:HG3	3:C:427:HOH:O	1.96	0.64
1:C:93:LYS:HG3	1:C:94:VAL:O	1.97	0.64
1:A:94:VAL:HG23	3:A:423:HOH:O	1.97	0.64
1:C:93:LYS:HE2	1:C:94:VAL:H	1.63	0.64
1:B:134:ASP:HB3	1:B:136:GLU:H	1.66	0.60
1:C:58:ASP:OD2	1:C:61:GLN:HG2	2.02	0.60
1:A:58:ASP:O	1:A:61:GLN:HG2	2.02	0.59
1:A:85[A]:GLU:OE1	1:A:194:ARG:NH2	2.37	0.58
1:C:66:ILE:HD12	1:C:70:LEU:HD22	1.85	0.58
1:A:34:TYR:HE2	3:A:470:HOH:O	1.89	0.56
1:C:93:LYS:HB2	3:C:448:HOH:O	2.06	0.56
1:B:82:LEU:HD11	1:B:195:LEU:HD11	1.86	0.56
1:D:62:ILE:HD13	1:D:70:LEU:HD23	1.86	0.56
1:C:93:LYS:HE2	1:C:94:VAL:N	2.20	0.55
1:D:135:LYS:HE2	1:D:154:GLY:O	2.07	0.54
1:D:201:THR:O	1:D:202:LEU:HB2	2.08	0.54
1:C:188:ASN:OD1	1:C:190:ASN:HB2	2.08	0.53
1:B:156:LYS:NZ	3:B:438:HOH:O	2.38	0.53
1:D:176:ARG:N	1:D:177:PRO:CD	2.72	0.52
1:D:8:PRO:HD2	1:D:9:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:N	1:A:156:LYS:HD2	2.25	0.52
1:D:131:LEU:HB3	1:D:159:LEU:HB3	1.92	0.51
1:C:151:ILE:HD12	1:C:157:PRO:CD	2.41	0.51
1:C:14:LEU:HD11	1:C:87:LEU:HB3	1.93	0.51
1:D:103:ASN:OD1	1:D:108:SER:HA	2.10	0.51
1:A:202:LEU:O	1:A:203:GLU:HG2	2.10	0.50
1:C:200:LEU:O	1:C:201:THR:CB	2.55	0.49
1:C:44:LYS:HD3	3:C:440:HOH:O	2.13	0.48
1:A:132:VAL:HG21	1:A:155:LEU:HD13	1.97	0.46
1:C:70:LEU:HD12	1:C:70:LEU:HA	1.79	0.46
1:C:151:ILE:HD12	1:C:157:PRO:HD2	1.98	0.46
1:C:151:ILE:CD1	1:C:157:PRO:HD2	2.46	0.45
1:A:184:PHE:HA	1:A:187:ILE:HD12	1.98	0.44
1:D:19:ASP:OD1	1:D:171:ASN:HB2	2.18	0.44
1:A:149:THR:HA	1:A:150:PRO:HD3	1.88	0.43
1:C:94:VAL:HG22	1:C:189:TRP:CD2	2.54	0.43
1:B:131:LEU:HB3	1:B:159:LEU:HB3	2.00	0.42
1:D:5:PRO:O	1:D:27:HIS:NE2	2.52	0.41
1:C:131:LEU:HB3	1:C:159:LEU:HB3	2.01	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD12	1.36	0.41
1:A:42:LEU:HD13	1:A:50:GLU:HG2	2.03	0.41
1:D:130:TRP:CE2	1:D:150:PRO:HD3	2.56	0.41
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.82	0.41
1:B:97:GLU:HG2	1:B:98:VAL:N	2.36	0.41
1:B:130:TRP:CZ2	1:B:150:PRO:HD3	2.56	0.40
1:C:124:PHE:CZ	1:D:72:ASN:HB3	2.57	0.40
1:A:176:ARG:O	1:A:179:TYR:HB3	2.21	0.40
1:B:94:VAL:HG23	3:B:408:HOH:O	2.21	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	Percentiles	
1	A	203/210 (97%)	190 (94%)	13 (6%)	0	100	100
1	B	202/210 (96%)	194 (96%)	8 (4%)	0	100	100
1	C	167/210 (80%)	162 (97%)	5 (3%)	0	100	100
All	All	572/630 (91%)	546 (96%)	26 (4%)	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	166/171 (97%)	161 (97%)	5 (3%)	41	40
1	B	51/171 (30%)	50 (98%)	1 (2%)	55	59
All	All	217/342 (64%)	211 (97%)	6 (3%)	43	44

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	90	GLU
1	A	112	PHE
1	A	149	THR
1	A	156	LYS
1	B	48	ILE

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

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, 4 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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.