



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:46 PM UTC

PDB ID : 1O9I / pdb_00001o9i
Title : Crystal structure of the Y42F mutant of manganese catalase from *Lactobacillus plantarum* at 1.33Å resolution
Authors : Barynin, V.V.; Whittaker, M.M.; Whittaker, J.W.
Deposited on : 2002-12-13
Resolution : 1.33 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

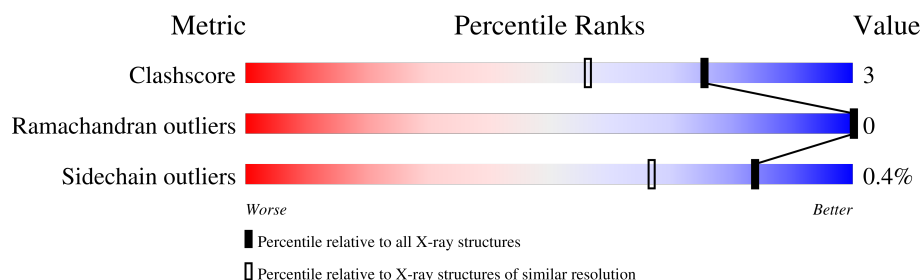
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 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	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	266	
1	B	266	
1	C	266	
1	D	266	
1	E	266	
1	F	266	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14325 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 Manganese catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	9	0
			2123	1322	364	419	18			
1	B	266	Total	C	N	O	S	0	6	0
			2107	1310	363	416	18			
1	C	266	Total	C	N	O	S	0	13	0
			2140	1329	367	426	18			
1	D	266	Total	C	N	O	S	0	14	0
			2146	1334	370	424	18			
1	E	266	Total	C	N	O	S	0	14	0
			2144	1334	372	420	18			
1	F	266	Total	C	N	O	S	0	8	0
			2120	1318	365	419	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	PHE	TYR	conflict	UNP P60355
B	42	PHE	TYR	conflict	UNP P60355
C	42	PHE	TYR	conflict	UNP P60355
D	42	PHE	TYR	conflict	UNP P60355
E	42	PHE	TYR	conflict	UNP P60355
F	42	PHE	TYR	conflict	UNP P60355

- Molecule 2 is MANGANESE (III) ION (CCD ID: MN3) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0

- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0
4	C	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0
4	E	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	232	Total	O	0	0
			232	232		
7	B	242	Total	O	0	0
			242	242		
7	C	242	Total	O	0	0
			242	242		

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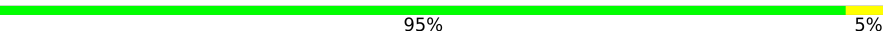
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	243	Total 243	O 243	0	0
7	E	248	Total 248	O 248	0	0
7	F	252	Total 252	O 252	0	0

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.

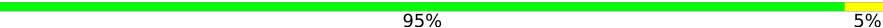
Note EDS was not executed.

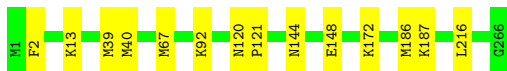
- Molecule 1: Manganese catalase

Chain A: 

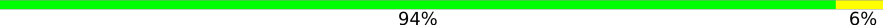


- Molecule 1: Manganese catalase

Chain B: 

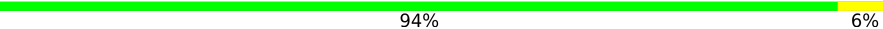


- Molecule 1: Manganese catalase

Chain C: 



- Molecule 1: Manganese catalase

Chain D: 



- Molecule 1: Manganese catalase

Chain E: 



- Molecule 1: Manganese catalase

Chain F:

93%

7%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.49Å 95.27Å 105.00Å 90.00° 106.55° 90.00°	Depositor
Resolution (Å)	50.00 – 1.33	Depositor
% Data completeness (in resolution range)	89.1 (50.00-1.33)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.115 , 0.145	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14325	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: CA, MES, NA, MN3, O

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	0.76	0/2204	0.86	0/2964
1	B	0.76	1/2175 (0.0%)	0.87	0/2926
1	C	0.79	1/2236 (0.0%)	0.87	1/3007 (0.0%)
1	D	0.78	0/2248	0.86	0/3020
1	E	0.77	0/2249	0.87	1/3022 (0.0%)
1	F	0.79	0/2196	0.83	0/2953
All	All	0.77	2/13308 (0.0%)	0.86	2/17892 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	MET	SD-CE	-5.92	1.64	1.79
1	C	186	MET	SD-CE	-5.48	1.65	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	VAL	N-CA-C	-5.38	105.47	110.53
1	E	138	VAL	N-CA-C	-5.35	105.50	110.53

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	2123	0	2035	11	0
1	B	2107	0	2016	10	0
1	C	2140	0	2036	16	0
1	D	2146	0	2057	14	0
1	E	2144	0	2053	18	0
1	F	2120	0	2027	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	12	0	13	0	0
5	E	24	0	25	2	0
5	F	24	0	26	0	0
6	A	2	0	0	0	0
7	A	232	0	0	2	0
7	B	242	0	0	4	0
7	C	242	0	0	4	0
7	D	243	0	0	3	0
7	E	248	0	0	7	0
7	F	252	0	0	9	0
All	All	14325	0	12288	76	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 3.

The worst 5 of 76 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:260[B]:ARG:NH2	1:E:89:GLU:OE1	1.76	1.17
1:C:23[B]:ARG:NH2	7:C:2025:HOH:O	1.92	1.03
1:D:260[B]:ARG:CZ	1:E:89:GLU:OE1	2.15	0.93
1:F:89[B]:GLU:OE2	7:F:2090:HOH:O	1.92	0.86
1:B:13:LYS:NZ	7:B:2007:HOH:O	2.10	0.84

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	273/266 (103%)	267 (98%)	6 (2%)	0	100	100
1	B	270/266 (102%)	265 (98%)	5 (2%)	0	100	100
1	C	277/266 (104%)	270 (98%)	7 (2%)	0	100	100
1	D	278/266 (104%)	274 (99%)	4 (1%)	0	100	100
1	E	278/266 (104%)	273 (98%)	5 (2%)	0	100	100
1	F	272/266 (102%)	266 (98%)	6 (2%)	0	100	100
All	All	1648/1596 (103%)	1615 (98%)	33 (2%)	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	231/222 (104%)	231 (100%)	0	100	100
1	B	228/222 (103%)	227 (100%)	1 (0%)	84	67
1	C	235/222 (106%)	235 (100%)	0	100	100
1	D	236/222 (106%)	232 (98%)	4 (2%)	53	18
1	E	236/222 (106%)	235 (100%)	1 (0%)	84	67
1	F	230/222 (104%)	230 (100%)	0	100	100
All	All	1396/1332 (105%)	1390 (100%)	6 (0%)	84	67

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	194[B]	GLU
1	D	246	GLU
1	E	15	ASP
1	D	147	ARG
1	B	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	189	GLN
1	E	242	GLN
1	F	242	GLN
1	F	189	GLN
1	C	242	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 26 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
5	MES	A	273	-	12,12,12	0.97	1 (8%)	15,16,16	1.55	3 (20%)
5	MES	E	273	-	12,12,12	0.88	1 (8%)	15,16,16	1.30	2 (13%)
5	MES	E	274	-	12,12,12	0.72	0	15,16,16	1.64	4 (26%)
5	MES	F	274	-	12,12,12	1.15	1 (8%)	15,16,16	1.11	1 (6%)
5	MES	F	273	-	12,12,12	1.57	1 (8%)	15,16,16	1.63	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	A	273	-	-	2/6/14/14	0/1/1/1
5	MES	E	273	-	-	3/6/14/14	0/1/1/1
5	MES	E	274	-	-	1/6/14/14	0/1/1/1
5	MES	F	274	-	-	4/6/14/14	0/1/1/1
5	MES	F	273	-	-	2/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	273	MES	C8-S	4.97	1.84	1.77
5	F	274	MES	C8-S	3.46	1.82	1.77
5	A	273	MES	C8-S	2.87	1.81	1.77
5	E	273	MES	C8-S	2.56	1.81	1.77

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	273	MES	C6-C5-N4	3.17	114.94	110.12
5	E	274	MES	C7-N4-C3	2.99	119.22	111.24
5	A	273	MES	C6-C5-N4	2.88	114.49	110.12
5	F	273	MES	C7-N4-C3	2.64	118.28	111.24
5	E	273	MES	O3S-S-C8	2.54	110.98	106.00

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	273	MES	C8-C7-N4-C3
5	E	273	MES	C8-C7-N4-C3
5	E	273	MES	N4-C7-C8-S
5	E	274	MES	C8-C7-N4-C3
5	F	273	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	273	MES	2	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.