



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5HST / pdb_00005hst
Title : Crystal structure of the dehydratase domain of MlnB from *Bacillus amyloliquefaciens*
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Deposited on : 2016-01-26
Resolution : 2.10 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 ⓘ 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

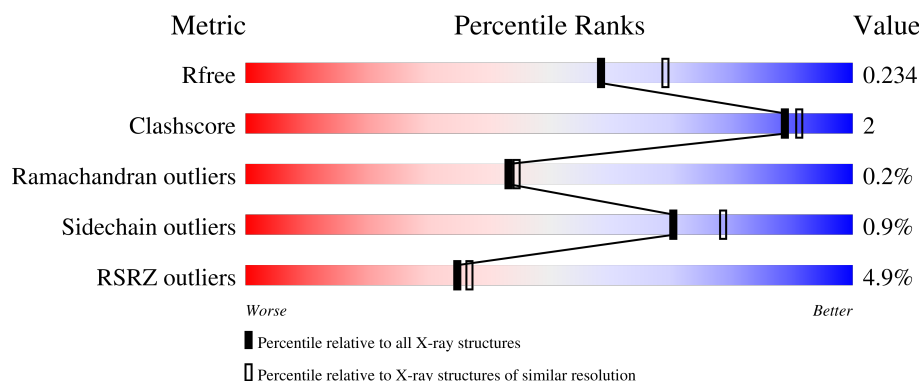
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	A	303	5% 83% 5% 11%
1	B	303	4% 84% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8744 atoms, of which 4159 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 Polyketide synthase type I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	270	Total	C	H	N	O	S	0	1	0
			4217	1348	2096	358	406	9			
1	B	265	Total	C	H	N	O	S	0	1	0
			4149	1328	2063	350	399	9			

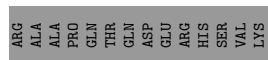
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q1RS66
A	2	MET	-	expression tag	UNP Q1RS66
B	1	SER	-	expression tag	UNP Q1RS66
B	2	MET	-	expression tag	UNP Q1RS66

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	206	Total	O	0	0
			206	206		
2	B	172	Total	O	0	0
			172	172		

- Molecule 1: Polyketide synthase type I



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.66Å 77.44Å 138.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.10 – 2.10 36.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.10-2.10) 99.7 (36.10-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10pre_2131: ???)	Depositor
R, R_{free}	0.186 , 0.228 0.190 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8744	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	0.19	0/2166	0.40	1/2928 (0.0%)
1	B	0.16	0/2131	0.36	0/2880
All	All	0.18	0/4297	0.38	1/5808 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LYS	N-CA-C	-5.09	103.43	110.35

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	2121	2096	2097	11	0
1	B	2086	2063	2064	5	0
2	A	206	0	0	2	0
2	B	172	0	0	0	0
All	All	4585	4159	4161	16	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.

All (16) 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:A:41:TYR:OH	1:A:205:GLU:OE1	2.02	0.78
1:B:41:TYR:OH	1:B:205:GLU:OE1	2.11	0.67
1:A:114:MET:N	1:A:114:MET:SD	2.81	0.53
1:B:77:LYS:HB3	1:B:127:ILE:HB	1.95	0.49
1:A:132:GLN:NE2	2:A:409:HOH:O	2.46	0.48
1:B:130:GLY:H	1:B:133:ASP:CG	2.21	0.48
1:A:198:LYS:HB3	1:A:205:GLU:HG2	1.96	0.47
1:A:192:LEU:HD22	1:A:207[B]:CYS:SG	2.56	0.45
1:A:132:GLN:HG2	1:A:132:GLN:O	2.16	0.44
1:A:159:TYR:CZ	1:A:174:GLN:HA	2.53	0.44
1:A:36:LEU:O	1:A:92:GLU:HA	2.17	0.44
1:A:132:GLN:CD	2:A:409:HOH:O	2.61	0.43
1:A:175:VAL:HG12	1:A:193:PRO:HD3	2.00	0.42
1:B:196:ILE:HD13	1:B:207[A]:CYS:SG	2.59	0.42
1:B:159:TYR:CZ	1:B:174:GLN:HA	2.54	0.41
1:A:98:ASP:O	1:A:108:PHE:HA	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	267/303 (88%)	260 (97%)	6 (2%)	1 (0%)	30	28
1	B	262/303 (86%)	257 (98%)	5 (2%)	0	100	100
All	All	529/606 (87%)	517 (98%)	11 (2%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ILE

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	229/258 (89%)	227 (99%)	2 (1%)	70	78
1	B	227/258 (88%)	225 (99%)	2 (1%)	70	78
All	All	456/516 (88%)	452 (99%)	4 (1%)	70	78

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

Mol	Chain	Res	Type
1	A	114	MET
1	A	198	LYS
1	B	114	MET
1	B	196	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	123	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95th 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	A	270/303 (89%)	-0.02	14 (5%) 33 35	18, 37, 87, 142	1 (0%)
1	B	265/303 (87%)	0.02	12 (4%) 38 40	16, 36, 89, 130	1 (0%)
All	All	535/606 (88%)	-0.00	26 (4%) 35 37	16, 36, 89, 142	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	SER	3.6
1	A	257	GLU	3.5
1	B	256	ASP	3.4
1	A	114	MET	3.2
1	B	198	LYS	3.1
1	B	132	GLN	3.0
1	B	130	GLY	3.0
1	A	198	LYS	3.0
1	B	114	MET	3.0
1	A	135	SER	2.9
1	A	20	ALA	2.9
1	A	292	ALA	2.8
1	B	21	PRO	2.7
1	B	91	LYS	2.7
1	A	256	ASP	2.6
1	B	136	HIS	2.6
1	A	196	ILE	2.6
1	A	199	LYS	2.6
1	B	134	ALA	2.5
1	A	197	HIS	2.5
1	A	261	ASP	2.3
1	A	194	GLU	2.3
1	A	200	SER	2.1
1	B	196	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	HIS	2.1
1	B	131	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.