



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 10:47 PM EDT

PDB ID : 3DHU
Title : Crystal structure of an alpha-amylase from *Lactobacillus plantarum*
Authors : Bonanno, J.B.; Dickey, M.; Bain, K.T.; Iizuka, M.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-06-18
Resolution : 2.00 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 ⓘ 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

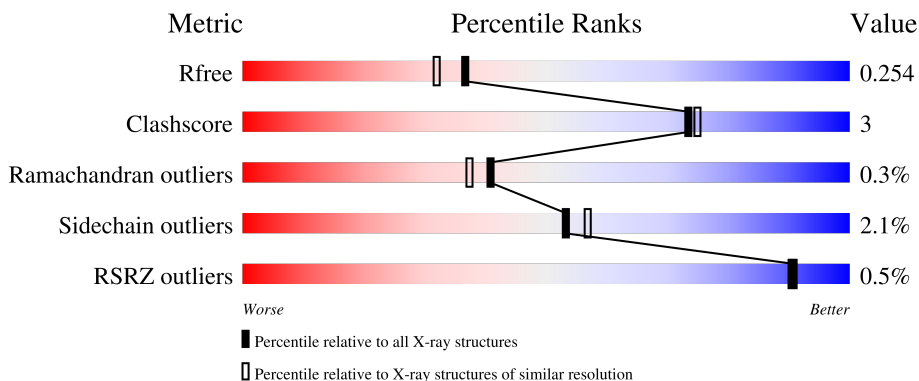
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	449	
1	B	449	
1	C	449	
1	D	449	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14732 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 Alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3361	2155	563	632	11			
1	B	418	Total	C	N	O	S	0	0	0
			3338	2142	558	627	11			
1	C	422	Total	C	N	O	S	0	0	0
			3364	2156	563	634	11			
1	D	418	Total	C	N	O	S	0	0	0
			3338	2142	558	627	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	insertion	UNP Q88ZW5
A	1	SER	-	insertion	UNP Q88ZW5
A	2	LEU	-	insertion	UNP Q88ZW5
A	441	GLU	-	insertion	UNP Q88ZW5
A	442	GLY	-	insertion	UNP Q88ZW5
A	443	HIS	-	insertion	UNP Q88ZW5
A	444	HIS	-	insertion	UNP Q88ZW5
A	445	HIS	-	insertion	UNP Q88ZW5
A	446	HIS	-	insertion	UNP Q88ZW5
A	447	HIS	-	insertion	UNP Q88ZW5
A	448	HIS	-	insertion	UNP Q88ZW5
B	0	MET	-	insertion	UNP Q88ZW5
B	1	SER	-	insertion	UNP Q88ZW5
B	2	LEU	-	insertion	UNP Q88ZW5
B	441	GLU	-	insertion	UNP Q88ZW5
B	442	GLY	-	insertion	UNP Q88ZW5
B	443	HIS	-	insertion	UNP Q88ZW5
B	444	HIS	-	insertion	UNP Q88ZW5
B	445	HIS	-	insertion	UNP Q88ZW5
B	446	HIS	-	insertion	UNP Q88ZW5
B	447	HIS	-	insertion	UNP Q88ZW5

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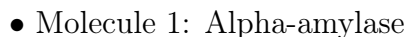
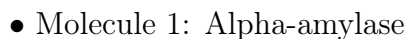
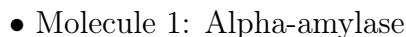
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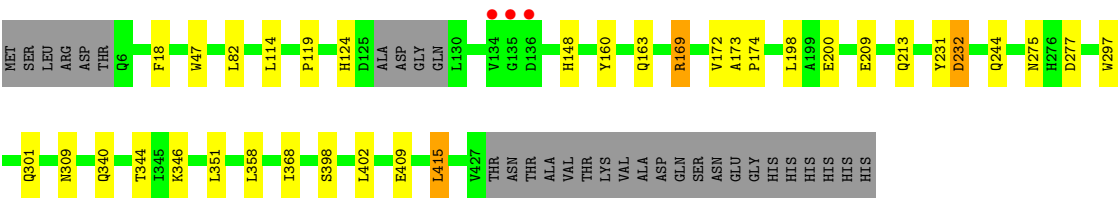
Chain	Residue	Modelled	Actual	Comment	Reference
B	448	HIS	-	insertion	UNP Q88ZW5
C	0	MET	-	insertion	UNP Q88ZW5
C	1	SER	-	insertion	UNP Q88ZW5
C	2	LEU	-	insertion	UNP Q88ZW5
C	441	GLU	-	insertion	UNP Q88ZW5
C	442	GLY	-	insertion	UNP Q88ZW5
C	443	HIS	-	insertion	UNP Q88ZW5
C	444	HIS	-	insertion	UNP Q88ZW5
C	445	HIS	-	insertion	UNP Q88ZW5
C	446	HIS	-	insertion	UNP Q88ZW5
C	447	HIS	-	insertion	UNP Q88ZW5
C	448	HIS	-	insertion	UNP Q88ZW5
D	0	MET	-	insertion	UNP Q88ZW5
D	1	SER	-	insertion	UNP Q88ZW5
D	2	LEU	-	insertion	UNP Q88ZW5
D	441	GLU	-	insertion	UNP Q88ZW5
D	442	GLY	-	insertion	UNP Q88ZW5
D	443	HIS	-	insertion	UNP Q88ZW5
D	444	HIS	-	insertion	UNP Q88ZW5
D	445	HIS	-	insertion	UNP Q88ZW5
D	446	HIS	-	insertion	UNP Q88ZW5
D	447	HIS	-	insertion	UNP Q88ZW5
D	448	HIS	-	insertion	UNP Q88ZW5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	340	Total O 340 340	0	0
2	B	314	Total O 314 314	0	0
2	C	357	Total O 357 357	0	0
2	D	320	Total O 320 320	0	0

- Molecule 1: Alpha-amylase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	202.28Å 63.77Å 155.68Å 90.00° 102.93° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 24.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.00) 98.6 (24.41-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.251 0.205 , 0.254	Depositor DCC
R_{free} test set	6500 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.5	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	0.92	EDS
Total number of atoms	14732	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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

5.1 Standard geometry

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	0.65	0/3446	0.73	4/4695 (0.1%)
1	B	0.66	0/3422	0.71	2/4661 (0.0%)
1	C	0.68	0/3449	0.72	2/4699 (0.0%)
1	D	0.64	0/3422	0.71	1/4661 (0.0%)
All	All	0.66	0/13739	0.72	9/18716 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	LEU	CA-CB-CG	8.58	135.03	115.30
1	A	169	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	D	415	LEU	CA-CB-CG	7.83	133.31	115.30
1	C	415	LEU	CA-CB-CG	7.09	131.60	115.30
1	B	415	LEU	CA-CB-CG	6.65	130.59	115.30

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	A	3361	0	3243	31	0
1	B	3338	0	3224	17	0
1	C	3364	0	3245	21	0
1	D	3338	0	3224	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	340	0	0	4	0
2	B	314	0	0	1	0
2	C	357	0	0	6	0
2	D	320	0	0	2	0
All	All	14732	0	12936	88	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 88 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:244:GLN:NE2	2:D:552:HOH:O	2.04	0.91
1:D:47:TRP:CZ2	1:D:169:ARG:HD3	2.07	0.90
1:B:169:ARG:HG3	1:B:198:LEU:HD23	1.57	0.86
1:A:47:TRP:CZ2	1:A:169:ARG:HD3	2.13	0.83
1:C:112:SER:O	1:C:116:THR:HG23	1.78	0.81

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	420/449 (94%)	407 (97%)	12 (3%)	1 (0%)	47	44
1	B	414/449 (92%)	402 (97%)	10 (2%)	2 (0%)	29	23
1	C	420/449 (94%)	406 (97%)	13 (3%)	1 (0%)	47	44
1	D	414/449 (92%)	401 (97%)	12 (3%)	1 (0%)	47	44
All	All	1668/1796 (93%)	1616 (97%)	47 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	232	ASP
1	D	232	ASP
1	C	232	ASP
1	A	361	VAL
1	B	172	VAL

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	A	352/384 (92%)	343 (97%)	9 (3%)	46	48
1	B	351/384 (91%)	345 (98%)	6 (2%)	60	65
1	C	353/384 (92%)	345 (98%)	8 (2%)	50	53
1	D	351/384 (91%)	344 (98%)	7 (2%)	55	58
All	All	1407/1536 (92%)	1377 (98%)	30 (2%)	53	57

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	402	LEU
1	D	309	ASN
1	C	82	LEU
1	D	415	LEU
1	D	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	132	ASN
1	D	278	ASN
1	C	118	HIS
1	C	124	HIS
1	C	132	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](#)

There are no ligands in this entry.

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](#)

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	422/449 (93%)	-0.38	1 (0%) 95 94	7, 15, 27, 36	0
1	B	418/449 (93%)	-0.37	1 (0%) 95 94	8, 15, 27, 33	0
1	C	422/449 (93%)	-0.36	4 (0%) 84 83	7, 14, 26, 41	0
1	D	418/449 (93%)	-0.30	3 (0%) 87 87	8, 16, 27, 48	0
All	All	1680/1796 (93%)	-0.35	9 (0%) 91 90	7, 15, 27, 48	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	5.1
1	C	134	VAL	4.6
1	D	136	ASP	4.5
1	D	135	GLY	4.3
1	C	136	ASP	3.7

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 monosaccharides 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.