



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 10:11 AM EST

PDB ID : 4QK0
Title : Crystal structure of Ara127N-Se, a GH127 beta-L-arabinofuranosidase from Geobacillus Stearothermophilus T6
Authors : Lansky, S.; Salama, R.; Dann, R.; Shner, I.; Manjasetty, B.; Belrhali, H.; Shoham, Y.; Shoham, G.
Deposited on : 2014-06-05
Resolution : 2.26 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

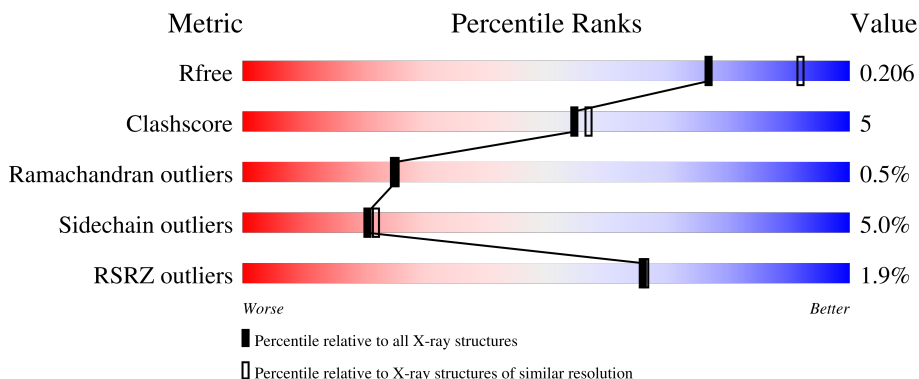
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	648	<div> <div>0%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	648	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	648	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	648	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22177 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 GH127 beta-L-arabinofuranoside.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	Se	0	1	0
			5152	3297	880	949	11	15			
1	B	635	Total	C	N	O	S	Se	0	6	0
			5179	3316	883	952	11	17			
1	C	635	Total	C	N	O	S	Se	0	3	0
			5165	3306	883	949	11	16			
1	D	635	Total	C	N	O	S	Se	0	3	0
			5163	3304	881	952	11	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP B3EYN9
A	-2	HIS	-	expression tag	UNP B3EYN9
A	-1	HIS	-	expression tag	UNP B3EYN9
A	0	HIS	-	expression tag	UNP B3EYN9
A	1	HIS	-	expression tag	UNP B3EYN9
A	2	HIS	-	expression tag	UNP B3EYN9
B	-3	HIS	-	expression tag	UNP B3EYN9
B	-2	HIS	-	expression tag	UNP B3EYN9
B	-1	HIS	-	expression tag	UNP B3EYN9
B	0	HIS	-	expression tag	UNP B3EYN9
B	1	HIS	-	expression tag	UNP B3EYN9
B	2	HIS	-	expression tag	UNP B3EYN9
C	-3	HIS	-	expression tag	UNP B3EYN9
C	-2	HIS	-	expression tag	UNP B3EYN9
C	-1	HIS	-	expression tag	UNP B3EYN9
C	0	HIS	-	expression tag	UNP B3EYN9
C	1	HIS	-	expression tag	UNP B3EYN9
C	2	HIS	-	expression tag	UNP B3EYN9
D	-3	HIS	-	expression tag	UNP B3EYN9
D	-2	HIS	-	expression tag	UNP B3EYN9
D	-1	HIS	-	expression tag	UNP B3EYN9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP B3EYN9
D	1	HIS	-	expression tag	UNP B3EYN9
D	2	HIS	-	expression tag	UNP B3EYN9

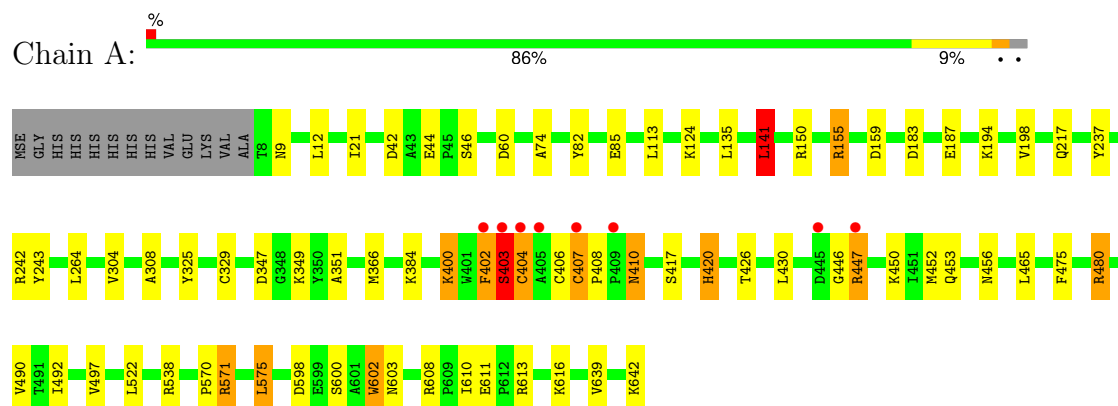
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	343	Total 343	O 343	0	0
2	B	311	Total 311	O 311	0	0
2	C	401	Total 401	O 401	0	0
2	D	463	Total 463	O 463	0	0

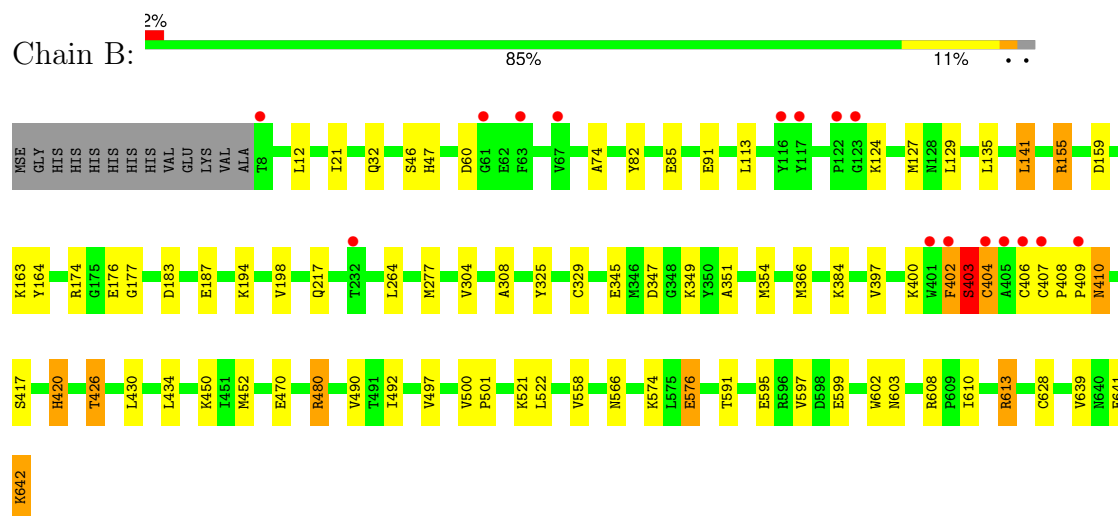
3 Residue-property plots [i](#)

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 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.

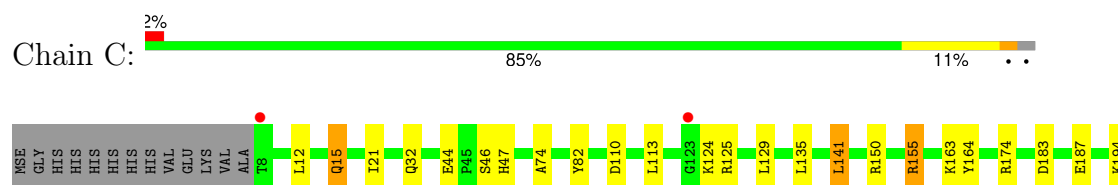
- Molecule 1: GH127 beta-L-arabinofuranoside

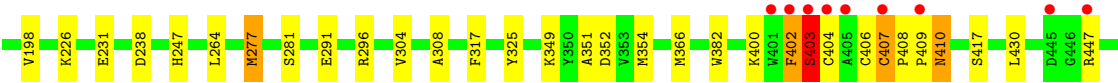


- Molecule 1: GH127 beta-L-arabinofuranoside

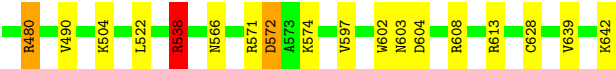
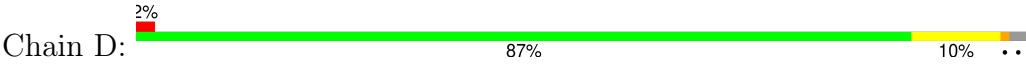


- Molecule 1: GH127 beta-L-arabinofuranoside





● Molecule 1: GH127 beta-L-arabinofuranoside



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.38Å 132.27Å 109.05Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	40.00 – 2.26 40.00 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.26) 99.5 (40.00-2.26)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.157 , 0.200 0.170 , 0.206	Depositor DCC
R_{free} test set	6452 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22177	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.18% 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	0.80	0/5278	0.84	5/7137 (0.1%)
1	B	0.78	0/5320	0.82	3/7192 (0.0%)
1	C	0.85	0/5297	0.85	8/7161 (0.1%)
1	D	0.85	0/5295	0.87	9/7160 (0.1%)
All	All	0.82	0/21190	0.85	25/28650 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	538	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	D	538	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	C	480	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	D	150	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	D	480	ARG	NE-CZ-NH2	-6.45	117.08	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	572[A]	ASP	Mainchain
1	D	572[B]	ASP	Mainchain

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	5152	0	4996	40	0
1	B	5179	0	5036	46	0
1	C	5165	0	5018	59	0
1	D	5163	0	5008	54	0
2	A	343	0	0	14	0
2	B	311	0	0	17	0
2	C	401	0	0	18	0
2	D	463	0	0	11	0
All	All	22177	0	20058	190	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 5.

The worst 5 of 190 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:642:LYS:HE2	1:D:642:LYS:HB3	1.44	0.98
1:A:329:CYS:SG	2:A:1019:HOH:O	2.22	0.97
1:C:642:LYS:HE2	1:D:642:LYS:CB	1.97	0.95
1:B:426:THR:HG21	2:B:895:HOH:O	1.65	0.94
1:B:595:GLU:OE1	1:B:642:LYS:HE3	1.75	0.87

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	634/648 (98%)	612 (96%)	19 (3%)	3 (0%)	25	25
1	B	639/648 (99%)	618 (97%)	18 (3%)	3 (0%)	25	25
1	C	636/648 (98%)	614 (96%)	19 (3%)	3 (0%)	25	25
1	D	636/648 (98%)	614 (96%)	19 (3%)	3 (0%)	25	25
All	All	2545/2592 (98%)	2458 (97%)	75 (3%)	12 (0%)	25	25

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLU
1	B	187	GLU
1	C	187	GLU
1	D	187	GLU
1	A	403	SER

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	535/530 (101%)	507 (95%)	28 (5%)	19	20
1	B	540/530 (102%)	510 (94%)	30 (6%)	17	17
1	C	537/530 (101%)	513 (96%)	24 (4%)	23	26
1	D	537/530 (101%)	512 (95%)	25 (5%)	22	24
All	All	2149/2120 (101%)	2042 (95%)	107 (5%)	20	22

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	642	LYS
1	C	407	CYS
1	D	430	LEU
1	C	46	SER
1	C	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	377	ASN
1	C	566	ASN
1	D	566	ASN
1	C	515	GLN
1	D	217	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 [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	621/648 (95%)	-0.32	8 (1%) 74 76	18, 32, 63, 108	0
1	B	621/648 (95%)	-0.05	16 (2%) 57 58	15, 37, 84, 118	3 (0%)
1	C	621/648 (95%)	-0.47	11 (1%) 67 68	12, 27, 64, 101	1 (0%)
1	D	621/648 (95%)	-0.56	11 (1%) 67 68	15, 25, 56, 99	2 (0%)
All	All	2484/2592 (95%)	-0.35	46 (1%) 66 66	12, 30, 70, 118	6 (0%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	PRO	6.3
1	B	409	PRO	5.9
1	D	409	PRO	5.4
1	C	409	PRO	4.9
1	B	123	GLY	4.2

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.