



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5KBP / pdb_00005kbp
Title : The crystal structure of an alpha-mannosidase from Enterococcus faecalis V583
Authors : Tan, K.; Chhor, G.; Jedrzejczak, R.; Anderson, W.F.; Joachimiak, A.; Center
for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2016-06-03
Resolution : 2.40 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)	:	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

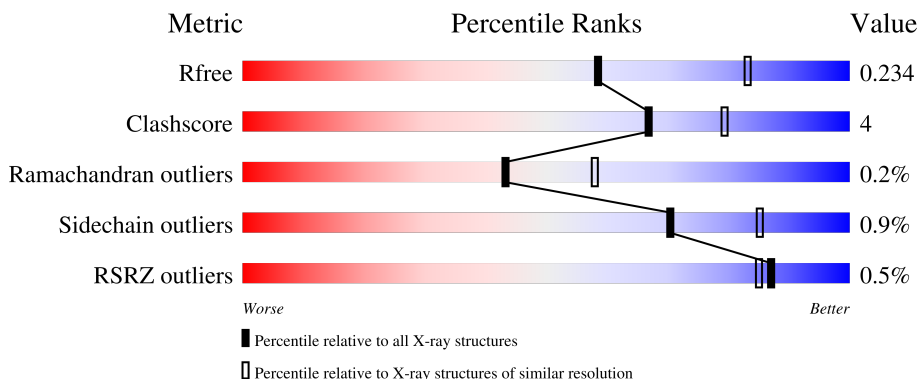
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	899	 87% 11% .
1	B	899	 89% 9% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14490 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 Glycosyl hydrolase, family 38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	886	Total	C	N	O	S	0	0	0
			7065	4501	1184	1356	24			
1	B	884	Total	C	N	O	S	0	0	0
			7040	4484	1180	1352	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q834E8
A	-1	ASN	-	expression tag	UNP Q834E8
A	0	ALA	-	expression tag	UNP Q834E8
A	821	HIS	THR	conflict	UNP Q834E8
B	-2	SER	-	expression tag	UNP Q834E8
B	-1	ASN	-	expression tag	UNP Q834E8
B	0	ALA	-	expression tag	UNP Q834E8
B	821	HIS	THR	conflict	UNP Q834E8

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

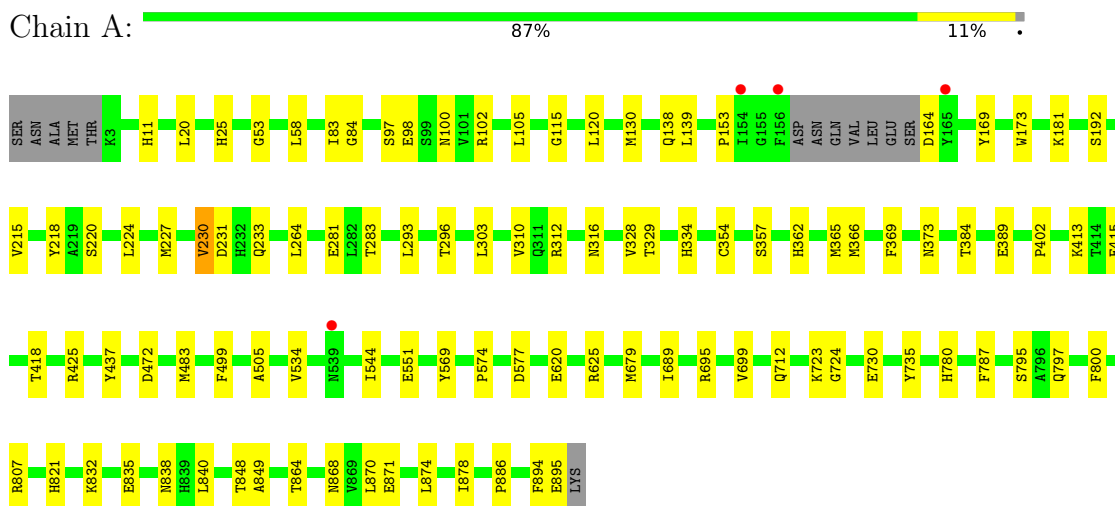
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		
3	B	139	Total	O	0	0
			139	139		

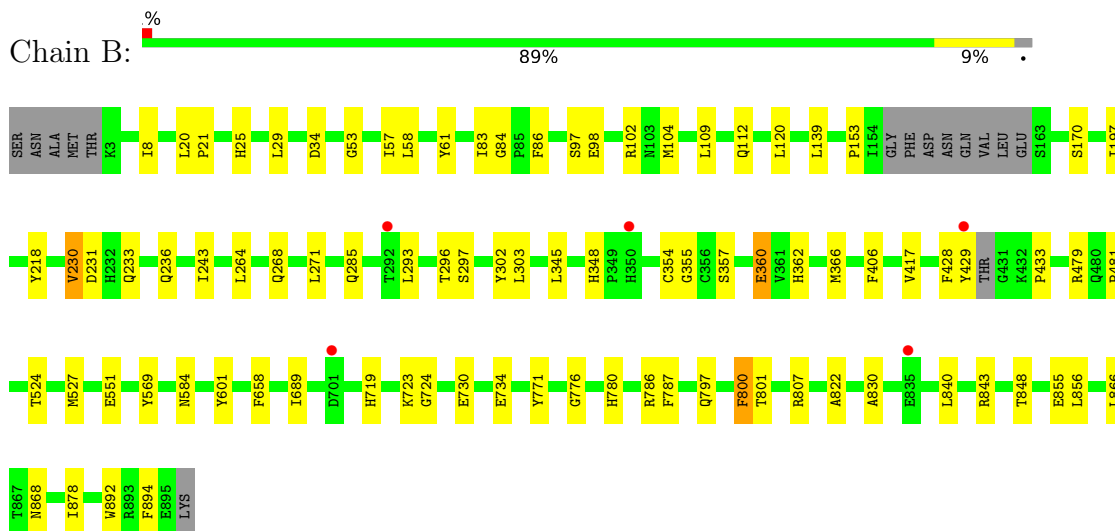
3 Residue-property plots [i](#)

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: Glycosyl hydrolase, family 38



- Molecule 1: Glycosyl hydrolase, family 38



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.83Å 127.83Å 223.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.40) 99.5 (50.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX dev_2386	Depositor
R, R_{free}	0.187 , 0.232 0.190 , 0.234	Depositor DCC
R_{free} test set	4145 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14490	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.09	0/7243	0.28	0/9856
1	B	0.10	0/7217	0.28	0/9822
All	All	0.10	0/14460	0.28	0/19678

There are no bond length outliers.

There are no bond angle outliers.

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	7065	0	6763	54	0
1	B	7040	0	6715	48	0
2	A	50	0	0	1	0
2	B	70	0	0	2	0
3	A	126	0	0	0	0
3	B	139	0	0	0	0
All	All	14490	0	13478	102	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.

The worst 5 of 102 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:B:21:PRO:HG3	1:B:360:GLU:HG3	1.71	0.72
1:A:230:VAL:HG22	1:A:231:ASP:H	1.61	0.66
1:B:840:LEU:HB3	1:B:894:PHE:HB2	1.77	0.66
1:A:303:LEU:HD23	1:A:366:MET:HE3	1.81	0.63
1:B:230:VAL:HG12	1:B:233:GLN:HB2	1.80	0.62

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	882/899 (98%)	849 (96%)	31 (4%)	2 (0%)	43	58
1	B	878/899 (98%)	848 (97%)	29 (3%)	1 (0%)	48	64
All	All	1760/1798 (98%)	1697 (96%)	60 (3%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	VAL
1	B	230	VAL
1	A	115	GLY

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	751/785 (96%)	744 (99%)	7 (1%)	70	85
1	B	746/785 (95%)	740 (99%)	6 (1%)	73	86
All	All	1497/1570 (95%)	1484 (99%)	13 (1%)	70	85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	285	GLN
1	B	360	GLU
1	B	800	PHE
1	B	479	ARG
1	B	524	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	655	GLN
1	B	792	GLN
1	B	710	GLN
1	B	119	GLN
1	B	602	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 ⓘ

24 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	A	910	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	907	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	902	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	905	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	901	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	901	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	902	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	906	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	909	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	905	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	903	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	908	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	903	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	B	908	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	B	913	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	911	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	B	912	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	909	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	904	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	914	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	B	910	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	904	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	906	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	907	-	4,4,4	0.23	0	6,6,6	0.08	0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	SO4	1	0
2	B	906	SO4	1	0
2	B	914	SO4	1	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 [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	886/899 (98%)	-0.18	4 (0%) 87 85	37, 57, 81, 125	0
1	B	884/899 (98%)	-0.21	5 (0%) 85 83	33, 51, 91, 133	0
All	All	1770/1798 (98%)	-0.20	9 (0%) 87 85	33, 54, 86, 133	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	PHE	3.6
1	B	429	TYR	3.5
1	A	165	TYR	3.0
1	B	701	ASP	2.8
1	A	154	ILE	2.8

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	909	5/5	0.59	0.08	133,133,135,136	5
2	SO4	B	911	5/5	0.59	0.09	102,102,105,106	5
2	SO4	A	906	5/5	0.69	0.10	98,99,102,103	5
2	SO4	A	903	5/5	0.71	0.08	134,134,136,136	0
2	SO4	B	910	5/5	0.74	0.09	92,96,96,96	5
2	SO4	B	906	5/5	0.76	0.10	73,73,76,78	5
2	SO4	B	909	5/5	0.76	0.09	95,100,102,106	5
2	SO4	A	907	5/5	0.76	0.10	93,98,103,103	5
2	SO4	B	905	5/5	0.76	0.10	99,104,108,111	0
2	SO4	B	914	5/5	0.76	0.12	106,106,112,115	5
2	SO4	B	904	5/5	0.77	0.07	92,93,96,96	5
2	SO4	B	912	5/5	0.78	0.13	80,91,94,95	5
2	SO4	A	910	5/5	0.80	0.07	119,121,124,124	5
2	SO4	B	913	5/5	0.81	0.11	106,108,109,110	5
2	SO4	A	908	5/5	0.81	0.09	107,109,110,111	5
2	SO4	A	901	5/5	0.82	0.08	89,99,101,102	0
2	SO4	B	903	5/5	0.83	0.07	99,102,104,109	0
2	SO4	B	902	5/5	0.84	0.09	69,77,79,86	0
2	SO4	B	907	5/5	0.84	0.08	111,112,116,118	5
2	SO4	B	901	5/5	0.86	0.08	75,81,84,87	5
2	SO4	B	908	5/5	0.86	0.07	76,81,84,86	5
2	SO4	A	904	5/5	0.87	0.08	84,88,89,95	5
2	SO4	A	905	5/5	0.91	0.08	89,91,95,101	5
2	SO4	A	902	5/5	0.91	0.07	67,68,71,75	5

6.5 Other polymers [i](#)

There are no such residues in this entry.