



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 06:25 am BST

PDB ID : 5C70
Title : The structure of Aspergillus oryzae beta-glucuronidase
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Deposited on : 2015-06-24
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

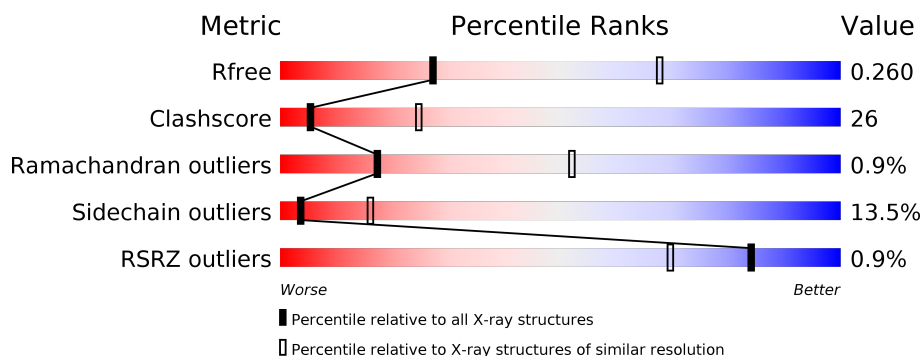
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	612	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>34%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	612	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>5%</div> <div>5%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9320 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 Glucuronidase.

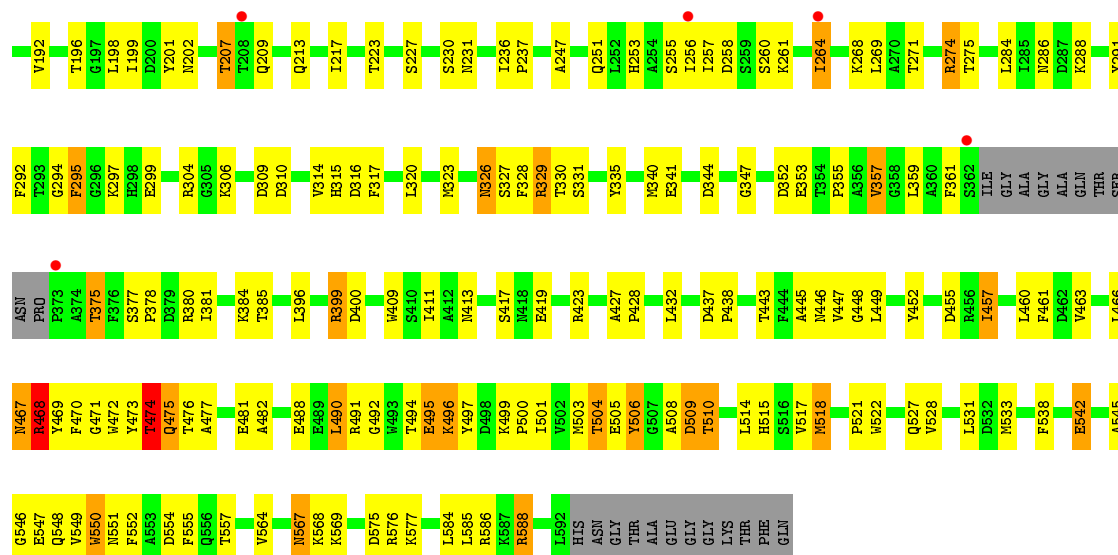
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4670	2965	806	886	13			
1	B	584	Total	C	N	O	S	0	0	0
			4650	2950	801	886	13			

These plots are drawn for all protein, RNA and DNA 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.

[illegible]

Chain B:

Amino Acid	Category
ALA	Special
ALA	Special
GLN	Polar
GLY	Polar
SER	Polar
ALA	Special
G-1	Polar
S0	Polar
M1	Polar
L2	Polar
K3	Polar
T7	Polar
D11	Polar
L18	Polar
W19	Aromatic
R20	Aromatic
F21	Aromatic
A22	Polar
L23	Polar
A24	Polar
W33	Aromatic
T34	Polar
T39	Aromatic
S40	Polar
L41	Polar
E42	Polar
C43	Special
P44	Polar
V45	Polar
P46	Polar
A47	Polar
S48	Polar
Y49	Aromatic
N50	Polar
D51	Polar
I52	Polar
W64	Aromatic
V65	Polar
Y66	Aromatic
R69	Aromatic
I72	Polar
V73	Polar
F74	Aromatic
W77	Aromatic
S78	Polar
E79	Polar
E80	Polar
R81	Aromatic
Q180	Polar
Y82	Aromatic
L83	Polar
W84	Aromatic
R85	Aromatic
C86	Special
T90	Aromatic
H91	Aromatic
V97	Polar
N100	Polar
L101	Polar
V102	Polar
F112	Aromatic
D115	Polar
I116	Polar
T117	Polar
D118	Polar
L119	Polar
V120	Polar
A121	Polar
E124	Polar
Q125	Polar
L128	Polar
T129	Polar
V132	Polar
D133	Polar
N134	Polar
E135	Polar
L136	Polar
T137	Polar
Y138	Aromatic
I141	Polar
P142	Polar
P143	Polar
G144	Polar
E150	Polar
A151	Polar
V156	Polar
Q157	Polar
Y164	Aromatic
N165	Polar
Y166	Aromatic
A167	Polar
G168	Polar
S177	Polar
V178	Polar
P179	Polar
Q180	Polar
Q181	Polar
V198	Polar



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	110.32Å 110.32Å 480.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 47.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.10) 99.1 (47.84-3.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.45 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.254 0.209 , 0.260	Depositor DCC
R_{free} test set	1655 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9320	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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

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	0.55	0/4790	0.73	5/6521 (0.1%)
1	B	0.54	0/4770	0.70	4/6496 (0.1%)
All	All	0.54	0/9560	0.71	9/13017 (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	A	0	2
1	B	0	4
All	All	0	6

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	B	474	THR	N-CA-C	7.04	130.00	111.00
1	A	162	ASP	CB-CA-C	-6.84	96.72	110.40
1	A	252	LEU	CA-CB-CG	6.63	130.56	115.30
1	B	468	ARG	CB-CA-C	-6.49	97.42	110.40
1	A	269	LEU	CA-CB-CG	5.86	128.77	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ILE	Peptide
1	A	295	PHE	Peptide
1	B	141	ILE	Peptide
1	B	295	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	48	SER	Peptide

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	4670	0	4505	240	0
1	B	4650	0	4477	246	0
All	All	9320	0	8982	479	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 26.

The worst 5 of 479 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:361:PHE:CZ	1:A:380:ARG:HD2	1.71	1.25
1:A:90:THR:CG2	1:A:91:HIS:H	1.50	1.23
1:B:467:ASN:HB3	1:B:505:GLU:CG	1.73	1.18
1:B:21:PHE:O	1:B:39:THR:HG21	1.43	1.16
1:A:90:THR:OG1	1:A:167:ALA:HA	1.47	1.11

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	582/612 (95%)	527 (90%)	46 (8%)	9 (2%)	10	39
1	B	580/612 (95%)	514 (89%)	64 (11%)	2 (0%)	41	73
All	All	1162/1224 (95%)	1041 (90%)	110 (10%)	11 (1%)	17	52

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLY
1	A	471	GLY
1	B	471	GLY
1	A	47	ALA
1	A	359	LEU

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	493/509 (97%)	420 (85%)	73 (15%)	3	13
1	B	493/509 (97%)	433 (88%)	60 (12%)	5	19
All	All	986/1018 (97%)	853 (86%)	133 (14%)	4	16

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	GLU
1	B	7	THR
1	B	504	THR
1	A	496	LYS
1	A	559	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	446	ASN

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Mol	Chain	Res	Type
1	B	50	ASN
1	B	446	ASN
1	A	548	GLN
1	A	139	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 carbohydrates 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	588/612 (96%)	-0.44	5 (0%) 84 69	30, 45, 63, 96	0
1	B	584/612 (95%)	-0.34	5 (0%) 84 69	29, 47, 64, 79	0
All	All	1172/1224 (95%)	-0.39	10 (0%) 84 69	29, 46, 64, 96	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	593	HIS	3.0
1	B	362	SER	2.8
1	A	591	ASN	2.5
1	B	373	PRO	2.4
1	B	264	ILE	2.4

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 carbohydrates 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.