



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:43 am GMT

PDB ID : 5D06
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme
Authors : Zhai, L.; Xiang, S.
Deposited on : 2015-08-02
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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

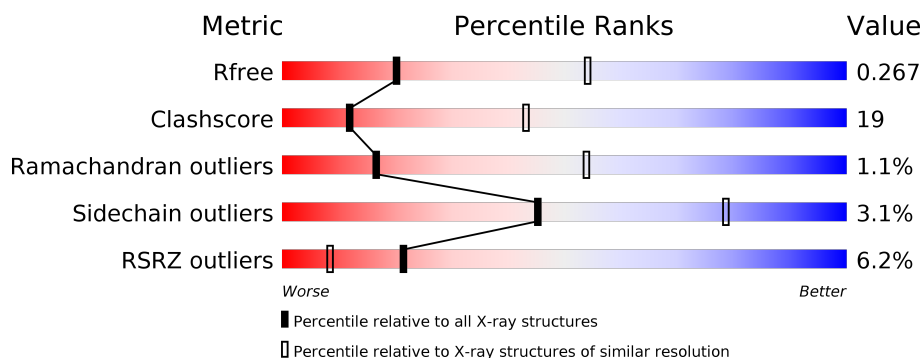
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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. 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	1528	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>.</div> </div> </div>
1	B	1528	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>..</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24403 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.

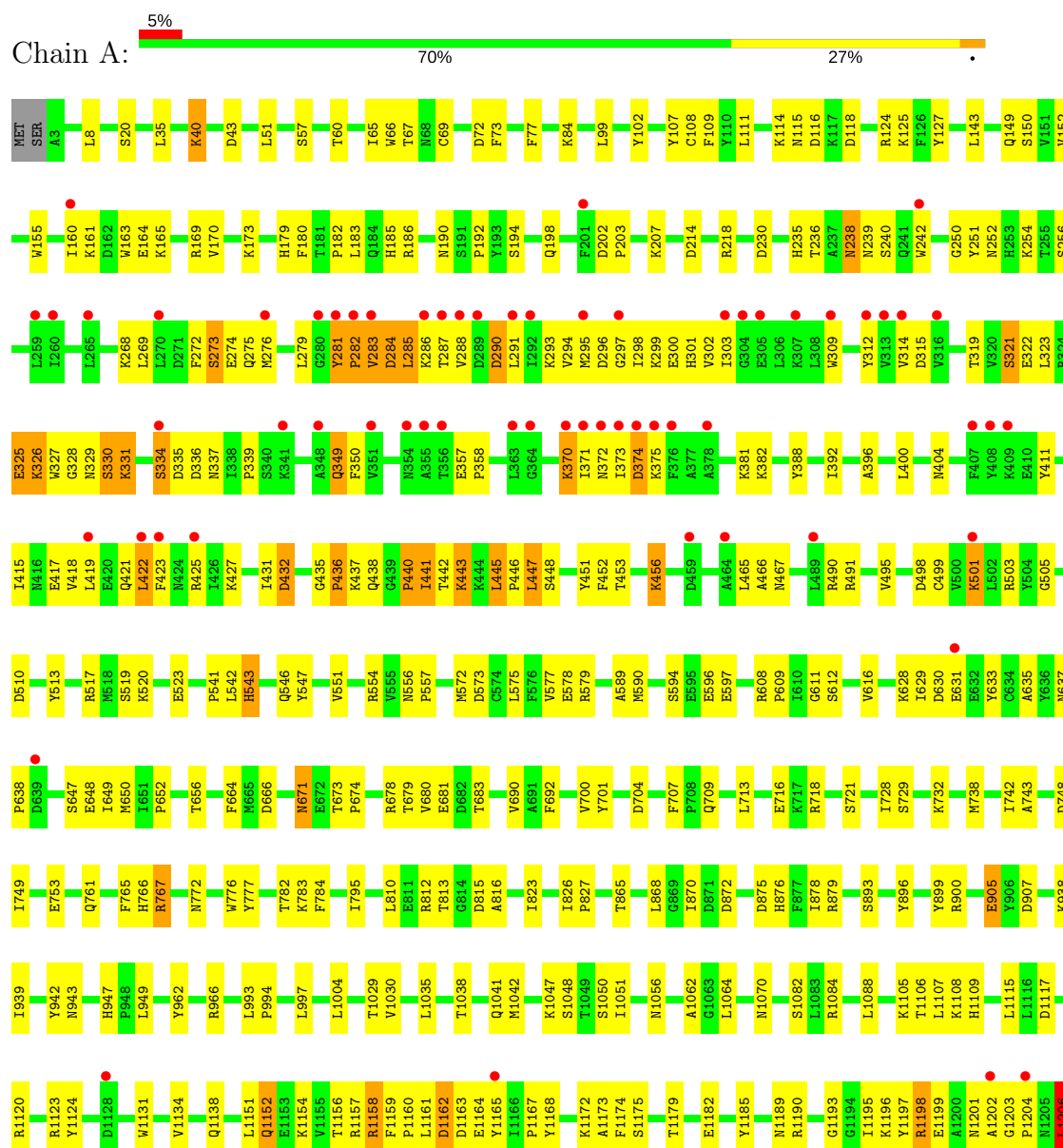
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1526	Total	C	N	O	S	0	0	0
			12278	7830	2065	2331	52			
1	B	1506	Total	C	N	O	S	0	0	0
			12125	7736	2038	2299	52			

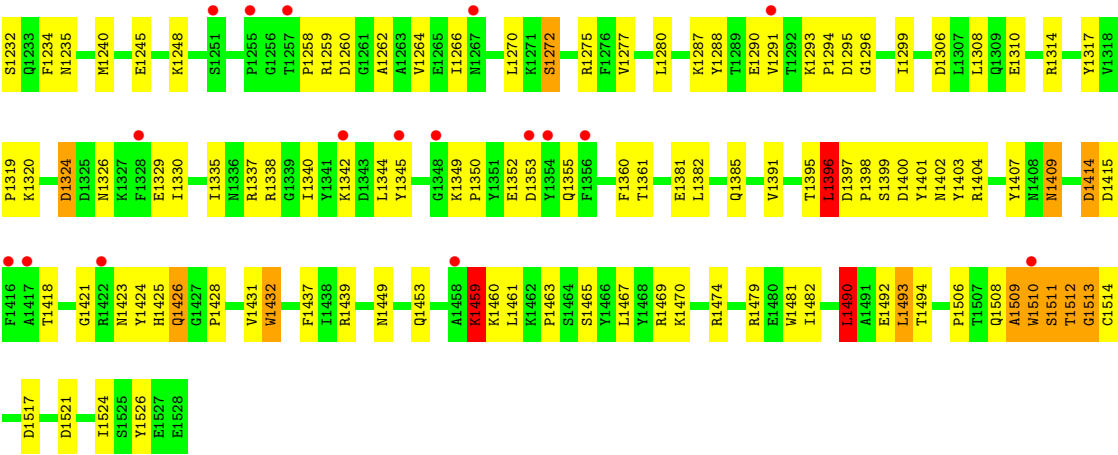
3 Residue-property plots

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.

• Molecule 1: Uncharacterized protein







4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	159.27Å 198.95Å 261.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.75 – 3.10 48.22 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.75-3.10) 97.3 (48.22-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.268 0.235 , 0.267	Depositor DCC
R_{free} test set	2608 reflections (3.56%)	DCC
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24403	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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	0.41	1/12589 (0.0%)	0.77	21/17071 (0.1%)
1	B	0.91	13/12427 (0.1%)	0.90	48/16845 (0.3%)
All	All	0.71	14/25016 (0.1%)	0.84	69/33916 (0.2%)

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	7
1	B	0	8
All	All	0	15

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1174	PHE	CG-CD1	67.60	2.40	1.38
1	B	1174	PHE	CD2-CE2	27.54	1.94	1.39
1	B	1174	PHE	CG-CD2	22.46	1.72	1.38
1	B	1174	PHE	CB-CG	20.87	1.86	1.51
1	B	1174	PHE	CD1-CE1	20.43	1.80	1.39

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1174	PHE	CB-CG-CD1	25.99	138.99	120.80
1	B	1174	PHE	CB-CG-CD2	-16.14	109.50	120.80
1	A	285	LEU	CB-CG-CD2	-10.37	93.38	111.00
1	B	425	ARG	CB-CG-CD	10.31	138.41	111.60
1	B	291	LEU	CA-CB-CG	8.81	135.56	115.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1158	ARG	Peptide
1	A	330	SER	Peptide
1	A	331	LYS	Peptide
1	A	436	PRO	Peptide
1	A	650	MET	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	12278	0	11960	403	0
1	B	12125	0	11812	522	4
All	All	24403	0	23772	925	4

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 19.

The worst 5 of 925 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:1174:PHE:CE1	1:B:1174:PHE:CZ	1.76	1.68
1:B:1174:PHE:CD1	1:B:1174:PHE:CE1	1.80	1.64
1:B:1174:PHE:CG	1:B:1174:PHE:CB	1.86	1.56
1:B:1174:PHE:CD2	1:B:1174:PHE:CE2	1.94	1.55
1:B:1508:GLN:HB3	1:B:1510:TRP:HB3	1.21	1.16

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:PHE:CG	1:B:1174:PHE:CD1[3_656]	1.88	0.32
1:B:1174:PHE:CD1	1:B:1174:PHE:CD1[3_656]	1.88	0.32
1:B:1174:PHE:CG	1:B:1174:PHE:CG[3_656]	1.91	0.29
1:B:116:ASP:O	1:B:390:ASN:ND2[4_567]	2.13	0.07

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	1524/1528 (100%)	1376 (90%)	133 (9%)	15 (1%)	18	57
1	B	1496/1528 (98%)	1337 (89%)	140 (9%)	19 (1%)	14	48
All	All	3020/3056 (99%)	2713 (90%)	273 (9%)	34 (1%)	17	54

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	PRO
1	A	437	LYS
1	A	440	PRO
1	A	1165	TYR
1	A	1167	PRO

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	1344/1346 (100%)	1309 (97%)	35 (3%)	51	82
1	B	1327/1346 (99%)	1279 (96%)	48 (4%)	40	75
All	All	2671/2692 (99%)	2588 (97%)	83 (3%)	45	78

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	ASP

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Mol	Chain	Res	Type
1	B	252	ASN
1	B	1396	LEU
1	B	86	ILE
1	B	164	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	ASN
1	B	661	HIS
1	B	1385	GLN
1	B	421	GLN
1	B	424	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 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	1526/1528 (99%)	0.24	79 (5%) 28 12	52, 93, 140, 187	0
1	B	1506/1528 (98%)	0.34	109 (7%) 16 6	47, 87, 148, 190	0
All	All	3032/3056 (99%)	0.29	188 (6%) 21 8	47, 90, 146, 190	0

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	LEU	6.0
1	B	447	LEU	5.6
1	A	374	ASP	5.5
1	B	1354	TYR	5.0
1	B	289	ASP	4.9

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.