



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2017 – 03:35 PM EDT

PDB ID : 5VVO
Title : Structural Investigations of the Substrate Specificity of Human O-GlcNAcase
Authors : Li, B.; Jiang, J.; Li, H.; Hu, C.-W.
Deposited on : unknown
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : rb-20030345
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) : rb-20030345

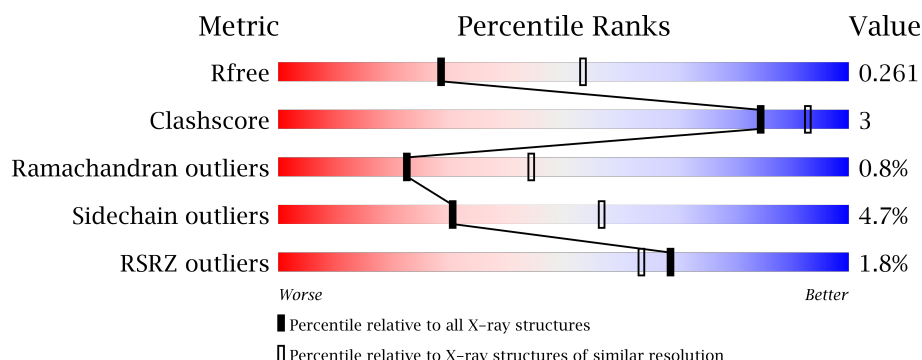
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	504	
1	B	504	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7221 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 Protein O-GlcNAcase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3569	2305	591	650	23			
1	B	429	Total	C	N	O	S	0	0	0
			3520	2280	581	636	23			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	HIS	-	expression tag	UNP O60502
A	175	ASN	ASP	engineered mutation	UNP O60502
A	543	GLY	-	linker	UNP O60502
A	544	GLY	-	linker	UNP O60502
A	545	GLY	-	linker	UNP O60502
A	546	GLY	-	linker	UNP O60502
A	547	SER	-	linker	UNP O60502
A	548	GLY	-	linker	UNP O60502
A	549	GLY	-	linker	UNP O60502
A	550	GLY	-	linker	UNP O60502
A	551	GLY	-	linker	UNP O60502
A	552	SER	-	linker	UNP O60502
B	59	HIS	-	expression tag	UNP O60502
B	175	ASN	ASP	engineered mutation	UNP O60502
B	543	GLY	-	linker	UNP O60502
B	544	GLY	-	linker	UNP O60502
B	545	GLY	-	linker	UNP O60502
B	546	GLY	-	linker	UNP O60502
B	547	SER	-	linker	UNP O60502
B	548	GLY	-	linker	UNP O60502
B	549	GLY	-	linker	UNP O60502
B	550	GLY	-	linker	UNP O60502
B	551	GLY	-	linker	UNP O60502
B	552	SER	-	linker	UNP O60502

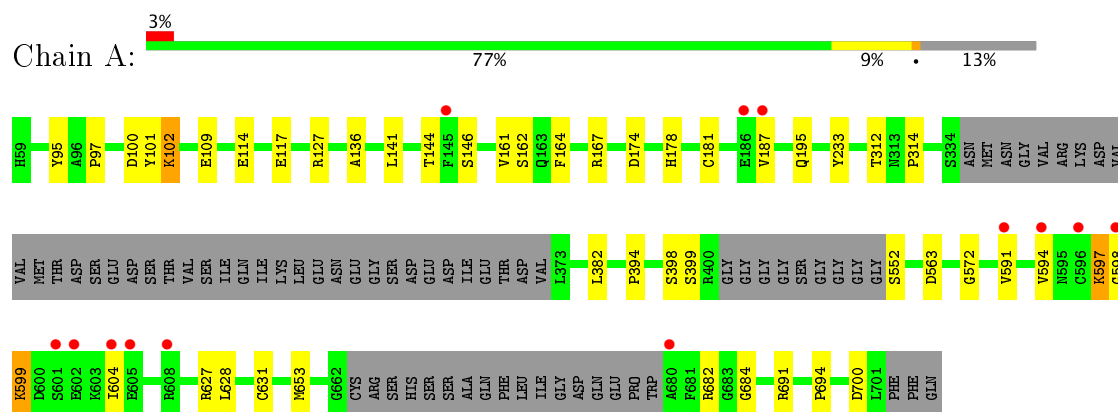
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total 82	O 82	0	0
2	B	50	Total 50	O 50	0	0

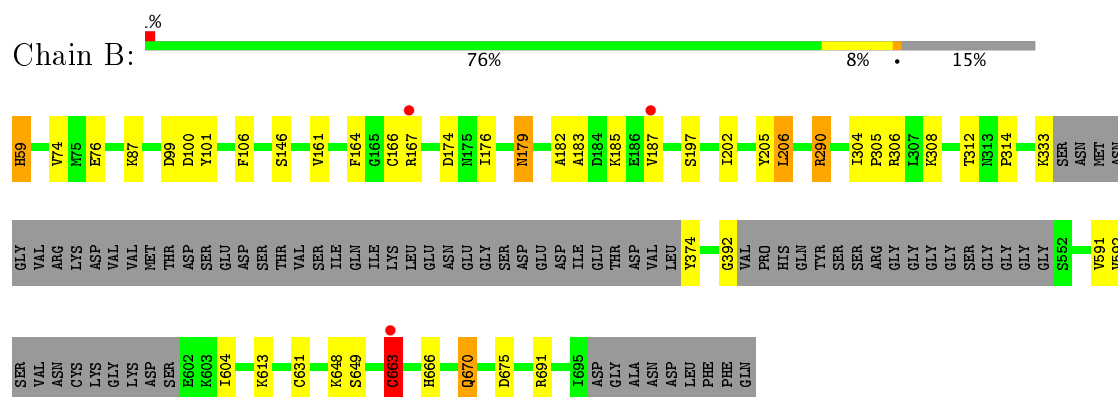
3 Residue-property plots

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: Protein O-GlcNAcase



• Molecule 1: Protein O-GlcNAcase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.40 Å 96.83 Å 89.08 Å 90.00° 115.24° 90.00°	Depositor
Resolution (Å)	80.57 – 2.60 48.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (80.57-2.60) 99.1 (48.41-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.259 0.217 , 0.261	Depositor DCC
R_{free} test set	1878 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7221	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.64	0/3662	0.83	3/4954 (0.1%)
1	B	0.65	2/3615 (0.1%)	0.81	4/4892 (0.1%)
All	All	0.65	2/7277 (0.0%)	0.82	7/9846 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	663	CYS	CB-SG	7.76	1.95	1.82
1	B	663	CYS	CA-CB	5.95	1.67	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	663	CYS	CA-CB-SG	6.86	126.34	114.00
1	B	290	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	663	CYS	CB-CA-C	6.10	122.59	110.40
1	A	628	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	167	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	392	GLY	N-CA-C	5.05	125.73	113.10
1	A	653	MET	CG-SD-CE	5.02	108.23	100.20

There are no chirality outliers.

There are no planarity outliers.

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	3569	0	3501	19	0
1	B	3520	0	3448	22	0
2	A	82	0	0	3	0
2	B	50	0	0	4	0
All	All	7221	0	6949	38	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.

All (38) 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:663:CYS:SG	1:B:666:HIS:NE2	2.05	0.98
1:B:663:CYS:SG	1:B:666:HIS:CE1	2.73	0.81
1:B:663:CYS:HG	1:B:666:HIS:CE1	1.97	0.76
1:A:552:SER:HB3	2:A:801:HOH:O	1.91	0.69
1:B:374:TYR:N	2:B:802:HOH:O	2.26	0.69
1:B:202:ILE:O	1:B:206:LEU:HD12	1.94	0.67
1:B:592:VAL:O	2:B:801:HOH:O	2.15	0.65
1:B:591:VAL:HG21	1:B:604:ILE:HG21	1.81	0.63
1:A:591:VAL:HG23	1:A:604:ILE:HG23	1.81	0.63
1:A:552:SER:CB	2:A:801:HOH:O	2.46	0.61
1:B:663:CYS:HA	1:B:666:HIS:CE1	2.36	0.61
1:B:166:CYS:SG	2:B:832:HOH:O	2.30	0.55
1:A:684:GLY:CA	1:B:290:ARG:HD3	2.38	0.53
1:B:670:GLN:HA	1:B:670:GLN:HE21	1.76	0.51
1:B:604:ILE:O	1:B:604:ILE:HD12	2.11	0.50
1:A:700:ASP:OD1	1:B:691:ARG:NH1	2.44	0.50
1:A:382:LEU:HD22	2:A:869:HOH:O	2.11	0.49
1:A:591:VAL:HG23	1:A:604:ILE:HD12	1.95	0.48
1:B:176:ILE:CG2	1:B:179:ASN:HD21	2.27	0.47
1:A:102:LYS:HD3	1:A:109:GLU:HB2	1.97	0.46
1:B:59:HIS:O	1:B:308:LYS:NZ	2.43	0.46
1:A:394:PRO:HG2	1:B:106:PHE:CE2	2.51	0.45
1:B:146:SER:HB2	1:B:187:VAL:HG21	2.00	0.44
1:B:182:ALA:O	1:B:183:ALA:HB3	2.18	0.44
1:B:161:VAL:HA	1:B:164:PHE:CD2	2.53	0.43
1:A:597:LYS:O	1:A:599:LYS:N	2.51	0.43
1:B:205:TYR:N	2:B:809:HOH:O	2.51	0.43
1:A:146:SER:HB2	1:A:187:VAL:HG21	2.00	0.43
1:A:195:GLN:NE2	1:A:233:TYR:OH	2.44	0.43
1:A:144:THR:HG23	1:A:181:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ILE:HB	1:B:305:PRO:HD3	1.99	0.43
1:B:591:VAL:CG2	1:B:604:ILE:HG21	2.48	0.42
1:A:97:PRO:HG2	1:A:100:ASP:HB2	2.02	0.42
1:A:682:ARG:O	1:A:691:ARG:NH2	2.53	0.42
1:A:552:SER:O	1:A:627:ARG:HD2	2.20	0.41
1:A:161:VAL:HA	1:A:164:PHE:CD2	2.56	0.40
1:A:563:ASP:HA	1:A:572:GLY:HA3	2.03	0.40
1:A:95:TYR:O	1:A:136:ALA:HB3	2.22	0.40

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	429/504 (85%)	406 (95%)	18 (4%)	5 (1%)	15	32
1	B	421/504 (84%)	399 (95%)	20 (5%)	2 (0%)	32	58
All	All	850/1008 (84%)	805 (95%)	38 (4%)	7 (1%)	22	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ASP
1	A	598	GLY
1	B	174	ASP
1	A	314	PRO
1	B	314	PRO
1	A	594	VAL
1	A	694	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	387/442 (88%)	373 (96%)	14 (4%)	40	68
1	B	380/442 (86%)	358 (94%)	22 (6%)	23	46
All	All	767/884 (87%)	731 (95%)	36 (5%)	30	57

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	TYR
1	A	102	LYS
1	A	114	GLU
1	A	117	GLU
1	A	127	ARG
1	A	141	LEU
1	A	162	SER
1	A	178	HIS
1	A	312	THR
1	A	398	SER
1	A	399	SER
1	A	597	LYS
1	A	599	LYS
1	A	631	CYS
1	B	59	HIS
1	B	74	VAL
1	B	76	GLU
1	B	87	LYS
1	B	99	ASP
1	B	100	ASP
1	B	101	TYR
1	B	167	ARG
1	B	179	ASN
1	B	185	LYS
1	B	197	SER
1	B	206	LEU
1	B	306	ARG

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Mol	Chain	Res	Type
1	B	312	THR
1	B	333	LYS
1	B	613	LYS
1	B	631	CYS
1	B	648	LYS
1	B	649	SER
1	B	663	CYS
1	B	670	GLN
1	B	675	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	595	ASN
1	B	179	ASN
1	B	389	GLN
1	B	670	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	437/504 (86%)	-0.06	13 (2%)	51	43	32, 55, 88, 133	0
1	B	429/504 (85%)	-0.11	3 (0%)	87	85	36, 61, 87, 116	0
All	All	866/1008 (85%)	-0.09	16 (1%)	69	63	32, 58, 88, 133	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	PHE	3.8
1	A	596	CYS	3.0
1	A	602	GLU	3.0
1	A	187	VAL	2.9
1	B	167	ARG	2.8
1	A	604	ILE	2.5
1	B	187	VAL	2.5
1	B	663	CYS	2.5
1	A	598	GLY	2.4
1	A	605	GLU	2.4
1	A	594	VAL	2.4
1	A	591	VAL	2.3
1	A	601	SER	2.3
1	A	680	ALA	2.2
1	A	186	GLU	2.1
1	A	608	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.