

Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 05:25 pm BST

PDB ID : 2EPO

> Title : N-acetyl-B-D-glucosaminidase (GCNA) from Streptococcus gordonii

Authors : Langley, D.B. 2007-03-30 Deposited on

1.56 Å(reported) Resolution

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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

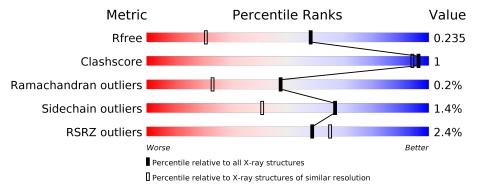
Validation Pipeline (wwPDB-VP) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=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	627	95%	• •
1	В	627	93%	



2 Entry composition (i)

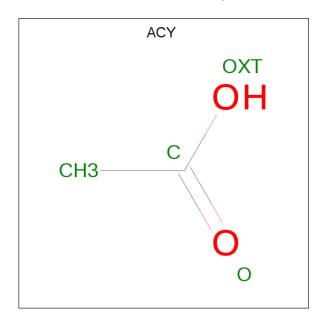
There are 3 unique types of molecules in this entry. The entry contains 10601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-acetyl-beta-D-glucosaminidase.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	A	626	Total 5090	C 3244	11	O 970	S 21	0	1	0
1	В	601	Total 4898	C 3129	N 822	O 926	S 21	0	2	0

• Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



\mathbf{N}	Iol	Chain	Residues	Atoms	ZeroOcc	AltConf
	2	A	1	Total C O 4 2 2	0	0
	2	В	1	Total C O 4 2 2	0	0

• Molecule 3 is water.



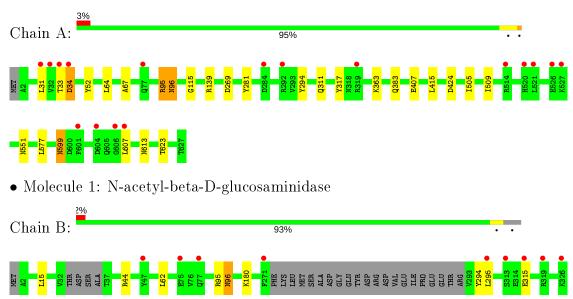
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	325	Total O 325 325	0	0
3	В	280	Total O 280 280	0	0



3 Residue-property plots (i)

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: N-acetyl-beta-D-glucosaminidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	110.04Å 112.49Å 103.99Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.88 - 1.56	Depositor
Resolution (A)	34.87 - 1.56	EDS
% Data completeness	96.8 (34.88-1.56)	Depositor
(in resolution range)	96.8 (34.87-1.56)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.05 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D	0.210 , 0.249	Depositor
R, R_{free}	0.205 , 0.235	DCC
R_{free} test set	8874 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 47.5	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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		
IVIOI	Chain	RMSZ	RMSZ $ \# Z > 5$		# Z > 5	
1	A	0.56	0/5201	0.67	3/7027~(0.0%)	
1	В	0.55	0/5007	0.62	0/6761	
All	All	0.56	0/10208	0.65	3/13788~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	pe Atoms		$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	139	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	95	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	424	ASP	CB-CG-OD1	5.43	123.19	118.30

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	5090	0	4963	13	0
1	В	4898	0	4788	8	0
2	A	4	0	3	0	0
2	В	4	0	3	0	0
3	A	325	0	0	1	0
3	В	280	0	0	0	0

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\mathbf{Mol}	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
All	All	10601	0	9757	19	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 1.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}\;({ m \AA})$	overlap (Å)
1:B:599:ASN:C	1:B:599:ASN:HD22	2.03	0.60
1:A:383:GLN:HE21	1:A:551:ASN:HD21	1.50	0.59
1:A:599:ASN:HD22	1:A:599:ASN:C	2.07	0.57
1:A:67:ALA:HB1	1:A:407:GLU:HG2	1.87	0.55
1:A:31:LEU:HD11	1:A:52:TYR:CE2	2.41	0.55
1:A:96:ASN:HD21	1:B:623:THR:H	1.57	0.53
1:A:623:THR:H	1:B:96:ASN:HD21	1.58	0.50
1:A:509:ILE:HD12	1:A:577:LEU:HD11	1.93	0.49
1:B:562:ARG:HG2	1:B:615:TRP:CE2	2.48	0.48
1:B:515:ASN:OD1	1:B:517:ASP:HB2	2.15	0.46
1:A:269:ASP:HA	1:A:281:TYR:CE2	2.51	0.46
1:A:383:GLN:HE21	1:A:551:ASN:ND2	2.13	0.45
1:A:311:GLN:HB2	1:A:317:TYR:CE1	2.53	0.44
1:B:460:ARG:NH1	1:B:463:LYS:HD3	2.32	0.43
1:B:15:LEU:HD11	1:B:62:LEU:HD13	2.00	0.42
1:A:115:GLY:HA2	3:A:906:HOH:O	2.19	0.42
1:A:505:ILE:O	1:A:509:ILE:HG12	2.20	0.41
1:B:315:GLU:H	1:B:315:GLU:CD	2.23	0.41
1:A:33:THR:O	1:A:34:ASP:C	2.59	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	Percer	ntiles
1	A	$625/627 \; (100\%)$	606 (97%)	17 (3%)	2 (0%)	41	19
1	В	597/627 (95%)	578 (97%)	18 (3%)	1 (0%)	47	23
All	All	1222/1254~(97%)	1184 (97%)	35 (3%)	3 (0%)	47	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	В	96	ASN
1	A	34	ASP

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	${f Analysed}$	Rotameric	Outliers	Percentile	es
1	A	$543/543 \ (100\%)$	535 (98%)	8 (2%)	65 37	
1	В	522/543~(96%)	515 (99%)	7 (1%)	69 44	
All	All	1065/1086~(98%)	1050 (99%)	15 (1%)	67 41	

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	95	ARG
1	A	294	TYR
1	A	363	LYS
1	A	415	LEU
1	A	599	ASN
1	A	607	LEU
1	A	613	ASN
1	В	44	ARG
1	В	95	ARG
1	В	180	LYS
1	В	294	TYR
1	В	295	LEU

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Mol	Chain	Res	Type
1	В	599	ASN
1	В	613	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	148	GLN
1	A	318	ASN
1	A	391	GLN
1	A	492	GLN
1	A	546	GLN
1	A	551	ASN
1	A	599	ASN
1	A	613	ASN
1	В	49	GLN
1	В	54	GLN
1	В	96	ASN
1	В	323	ASN
1	В	391	GLN
1	В	457	GLN
1	В	546	GLN
1	В	599	ASN
1	В	613	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)

2 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	Т	Chain	hain Res I		Res Link		Bond lengths			В	ond ang	gles
MIOI	Mol Type Chain Ro	nes	es Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2			
2	ACY	В	1660	-	1,3,3	3.25	1 (100%)	0,3,3	0.00	-		
2	ACY	A	660	-	1,3,3	5.62	1 (100%)	0,3,3	0.00	-		

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
2	A	660	ACY	СН3-С	5.62	1.55	1.48
2	В	1660	ACY	СН3-С	3.25	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(\AA^2)$	Q < 0.9
1	A	$626/627 \; (99\%)$	-0.06	17 (2%) 5	4 62	12, 18, 34, 45	0
1	В	$601/627 \; (95\%)$	-0.07	13 (2%) 6	2 67	12, 20, 34, 47	0
All	All	1227/1254 (97%)	-0.07	30 (2%) 5	9 65	12, 19, 34, 47	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	604	ASP	6.9
1	В	327	ILE	5.2
1	В	319	ARG	4.4
1	В	326	LYS	4.0
1	В	271	PHE	3.7
1	В	604	ASP	3.4
1	В	607	LEU	3.3
1	A	34	ASP	3.1
1	A	284	ASP	3.0
1	A	520	HIS	2.9
1	A	33	THR	2.9
1	A	514	ARG	2.9
1	A	606	GLY	2.8
1	A	521	LEU	2.8
1	A	292	ARG	2.8
1	A	526	GLU	2.7
1	A	527	LYS	2.6
1	A	319	ARG	2.6
1	A	607	LEU	2.6
1	В	47	TYR	2.4
1	В	605	GLN	2.3
1	A	31	LEU	2.2
1	A	32	VAL	2.2
1	В	75	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	В	77	GLN	2.2
1	В	295	LEU	2.1
1	В	313	SER	2.0
1	A	77	GLN	2.0
1	В	315	GLU	2.0
1	A	601	PHE	2.0

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)

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, 95^{th} 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	${f B-factors}({f \AA}^2)$	Q < 0.9
2	ACY	В	1660	4/4	0.96	0.08	24,27,28,29	0
2	ACY	A	660	4/4	0.98	0.12	16,16,16,18	0

6.5 Other polymers (i)

There are no such residues in this entry.

