

Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 08:48 pm BST

PDB ID	:	1UPS
Title	:	GlcNAc[alpha]1-4Gal releasing endo-[beta]-galactosidase from Clostridium
		perfringens
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		for Structural Genomics (SECSG)
Deposited on	:	2003-10-10
Resolution	:	1.82 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

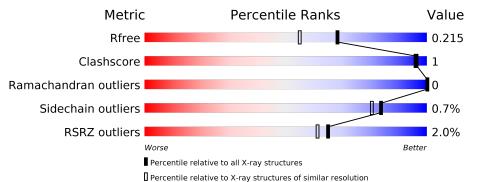
The following versions of software and data (see references (1)) were used in the production of this report:

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 1.82 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	$egin{array}{c} \mathbf{Whole \ archive} \ (\#\mathbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	А	420	^{2%} 90%	6%	·
1	В	420	^{2%} 90%	5%	5%



$1 \mathrm{UPS}$

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6991 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 GLCNAC-ALPHA-1,4-GAL-RELEASING ENDO-BETA-GA LACTOSIDASE.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	402	Total	С	Ν	Ο	S	0	6	0
	402	3318	2124	540	645	9	0	0	0	
1	В	397	Total	С	Ν	Ο	S	0	7	0
	ГВ	091	3293	2106	538	640	9	0	1	U

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Ca 1 1	0	0
2	А	1	Total Ca 1 1	0	0

• Molecule 3 is water.

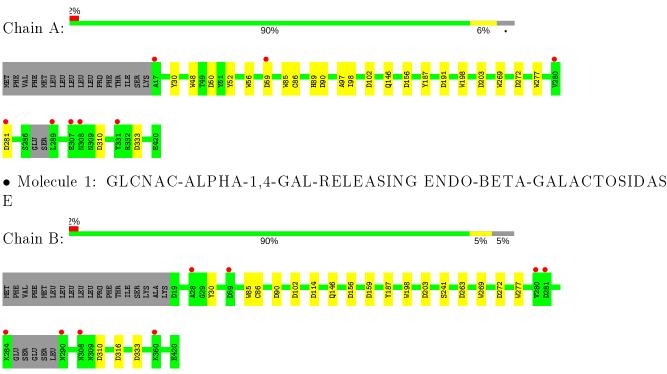
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	192	Total O 192 192	0	0
3	В	186	Total O 186 186	0	0



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.

 \bullet Molecule 1: GLCNAC-ALPHA-1,4-GAL-RELEASING ENDO-BETA-GALACTOSIDAS E





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants	160.43Å 160.43 Å 86.14 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 - 1.82	Depositor
Resolution (A)	36.36 - 1.82	EDS
% Data completeness	95.7 (20.00-1.82)	Depositor
(in resolution range)	95.7 (36.36 - 1.82)	EDS
R _{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.07 (at 1.82 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.1.24$	Depositor
D D .	0.176 , 0.204	Depositor
R, R_{free}	0.193 , 0.215	DCC
R_{free} test set	5398 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	16.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38 , 47.0	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6991	wwPDB-VP
Average B, all atoms $(Å^2)$	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 {\}rm Intensities}$ 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: CA

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.60	0/3460	0.75	11/4722~(0.2%)	
1	В	0.57	0/3440	0.77	13/4692~(0.3%)	
All	All	0.59	0/6900	0.76	24/9414~(0.3%)	

There are no bond length outliers.

All (24) bond angle outliers are listed be	
The fair bond angle buttlets are insteaded	low:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	310[A]	ASP	CB-CG-OD2	7.82	125.34	118.30
1	В	310[B]	ASP	CB-CG-OD2	7.82	125.34	118.30
1	В	156	ASP	CB-CG-OD2	7.60	125.14	118.30
1	А	310	ASP	CB-CG-OD2	6.66	124.29	118.30
1	В	102	ASP	CB-CG-OD2	6.50	124.15	118.30
1	В	159	ASP	CB-CG-OD2	6.46	124.11	118.30
1	В	272	ASP	CB-CG-OD2	6.46	124.11	118.30
1	А	102	ASP	CB-CG-OD2	6.44	124.10	118.30
1	В	203	ASP	CB-CG-OD2	6.44	124.09	118.30
1	А	203	ASP	CB-CG-OD2	6.42	124.08	118.30
1	А	156	ASP	CB-CG-OD2	6.02	123.72	118.30
1	В	263	ASP	CB-CG-OD2	5.91	123.62	118.30
1	А	333	ASP	CB-CG-OD2	5.72	123.45	118.30
1	В	333	ASP	CB-CG-OD2	5.71	123.44	118.30
1	А	50	ASP	CB-CG-OD2	5.71	123.44	118.30
1	А	272	ASP	CB-CG-OD2	5.68	123.41	118.30
1	В	114[A]	ASP	CB-CG-OD2	5.63	123.37	118.30
1	В	114[B]	ASP	CB-CG-OD2	5.63	123.37	118.30
1	В	90	ASP	CB-CG-OD2	5.56	123.30	118.30
1	В	316	ASP	CB-CG-OD2	5.33	123.09	118.30
1	А	59	ASP	CB-CG-OD2	5.32	123.08	118.30
1	А	90	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	191	ASP	CB-CG-OD2	5.18	122.97	118.30
1	А	281	ASP	CB-CG-OD2	5.01	122.81	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	А	3318	0	2972	8	0
1	В	3293	0	2951	4	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	192	0	0	0	0
3	В	186	0	0	0	0
All	All	6991	0	5923	12	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 (12) 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:85:TRP:CE3	1:A:86:CYS:HB2	2.35	0.62
1:A:56:TRP:O	1:A:89:HIS:CD2	2.61	0.54
1:B:85:TRP:CE3	1:B:86:CYS:HB2	2.44	0.52
1:A:56:TRP:O	1:A:89:HIS:HD2	1.95	0.49
1:A:52:TYR:HB2	1:A:97:ALA:HB3	1.98	0.45
1:B:187:TYR:HB2	1:B:198:TRP:CD2	2.52	0.44
1:A:85:TRP:CD2	1:A:86:CYS:HB2	2.53	0.43
1:A:48:TRP:CD2	1:A:98:ILE:HD12	2.53	0.43
1:A:187:TYR:HB2	1:A:198:TRP:CD2	2.54	0.43
1:A:30:TYR:HB3	1:A:277:TRP:HB3	2.00	0.43
1:B:30:TYR:HB3	1:B:277:TRP:HB3	2.01	0.42
1:B:85:TRP:CD2	1:B:86:CYS:HB2	2.55	0.41



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	А	404/420~(96%)	391~(97%)	13 (3%)	0	100	100
1	В	400/420~(95%)	389~(97%)	11 (3%)	0	100	100
All	All	804/840~(96%)	780~(97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	А	346/374~(92%)	344~(99%)	2(1%)	86 83		
1	В	345/374~(92%)	342~(99%)	3 (1%)	78 74		
All	All	691/748~(92%)	686~(99%)	5(1%)	84 80		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	146	GLN
1	А	269	TRP
1	В	146	GLN
1	В	241	SER
1	В	269	TRP



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

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, 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	А	402/420~(95%)	-0.11	8 (1%) 65 61	9, 13, 22, 28	0
1	В	397/420~(94%)	-0.18	8 (2%) 65 61	9, 14, 22, 31	0
All	All	799/840~(95%)	-0.14	16 (2%) 65 61	9, 14, 22, 31	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	289	LEU	4.5
1	А	281	ASP	3.8
1	А	308	ASN	3.3
1	А	17	ALA	3.3
1	В	59	ASP	3.2
1	В	280	VAL	2.9
1	В	28	ALA	2.9
1	В	308	ASN	2.8
1	А	307	GLU	2.5
1	В	290	ASN	2.4
1	В	284	LYS	2.3
1	В	281	ASP	2.3
1	А	280	VAL	2.2
1	А	331	TYR	2.1
1	В	360	LYS	2.1
1	А	59	ASP	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
2	CA	В	501	1/1	0.98	0.11	21,21,21,21	0
2	CA	А	501	1/1	0.99	0.11	$18,\!18,\!18,\!18$	0

6.5 Other polymers (i)

There are no such residues in this entry.

