WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:07 PM GMT

PDB ID : 4NUZ

Title : Crystal structure of a glycosynthase mutant (D233Q) of EndoS, an endo-beta -N-acetyl-glucosaminidase from Streptococcus pyogenes

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Deposited on : 2013-12-04

Resolution : 1.91 Å(reported)

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 1.91 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.
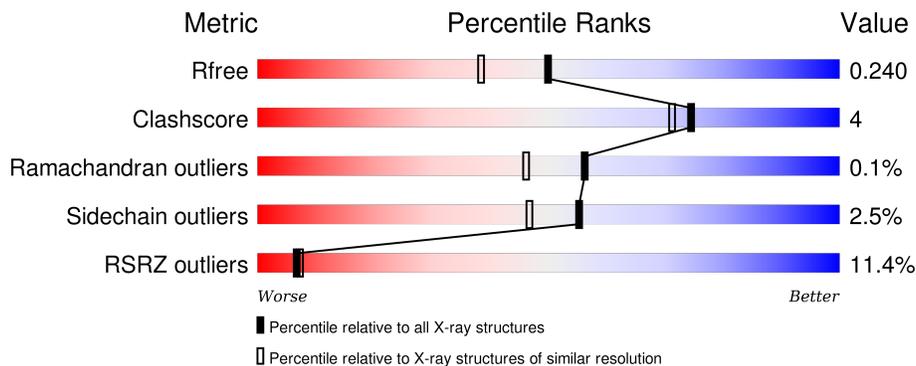
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 <=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	899	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7896 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 Endo-beta-N-acetylglucosaminidase F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	888	Total 7047	C 4457	N 1189	O 1384	S 17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLN	ASP	engineered mutation	UNP Q48WW7
A	996	LEU	-	EXPRESSION TAG	UNP Q48WW7

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	848	Total 848	O 848	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 errors 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: Endo-beta-N-acetylglucosaminidase F2

Chain A:
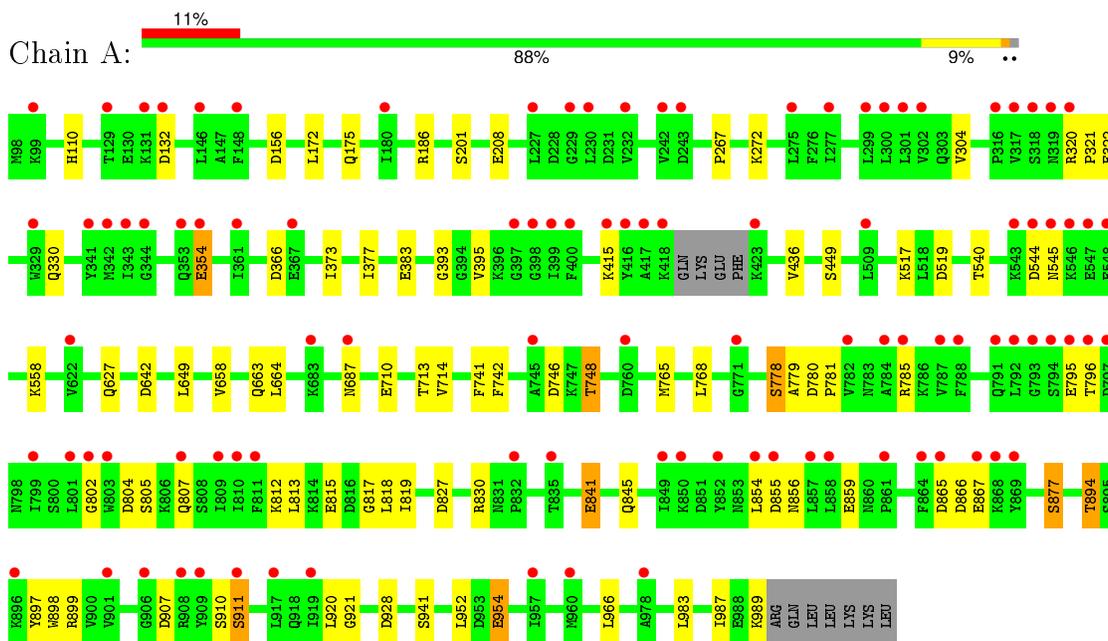
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.77Å　　96.39Å　　141.54Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	29.68　–　1.91 29.68　–　1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.68-1.91) 98.8 (29.68-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.47 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192　,　0.235 0.203　,　0.240	Depositor DCC
R_{free} test set	1987 reflections (2.06%)	DCC
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.0	EDS
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.41, <L^2> = 0.24$	Xtriage
Outliers	2 of 98640 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7896	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

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	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.75	0/7189	0.74	0/9718

There are no bond length outliers.

There are no bond angle outliers.

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	7047	0	6993	56	0
2	A	1	0	0	0	0
3	A	848	0	0	14	0
All	All	7896	0	6993	56	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 4.

All (56) 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:395:VAL:HG11	1:A:449:SER:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LYS:HE2	1:A:519:ASP:OD2	2.01	0.60
1:A:687:ASN:HB3	3:A:1419:HOH:O	2.01	0.59
1:A:894:THR:HG21	1:A:928:ASP:HA	1.83	0.59
1:A:765:MET:HE2	1:A:920:LEU:C	2.23	0.58
1:A:845:GLN:OE1	1:A:899:ARG:NH1	2.37	0.56
1:A:907:ASP:O	1:A:910:SER:OG	2.23	0.56
1:A:856:ASN:ND2	1:A:859:GLU:OE1	2.34	0.54
1:A:540:THR:OG1	1:A:545:ASN:HA	2.08	0.53
1:A:841:GLU:OE2	1:A:877:SER:HB3	2.07	0.53
1:A:866:ASP:OD1	1:A:867:GLU:N	2.42	0.52
1:A:320:ARG:HG3	1:A:321:PRO:HD2	1.92	0.52
1:A:322:GLU:HG2	3:A:1915:HOH:O	2.08	0.51
1:A:778:SER:OG	1:A:865:ASP:OD2	2.25	0.50
1:A:132:ASP:OD1	1:A:132:ASP:N	2.42	0.50
1:A:172:LEU:O	1:A:175:GLN:HG2	2.11	0.49
1:A:393:GLY:HA2	3:A:1442:HOH:O	2.13	0.48
1:A:815:GLU:HG2	3:A:1819:HOH:O	2.14	0.48
1:A:804:ASP:CG	1:A:805:SER:H	2.17	0.48
1:A:746:ASP:OD1	1:A:748:THR:HG22	2.13	0.48
1:A:373:ILE:HD12	3:A:1849:HOH:O	2.14	0.47
1:A:713:THR:OG1	1:A:742:PHE:HB2	2.14	0.47
1:A:827:ASP:CG	1:A:830:ARG:HH21	2.19	0.47
1:A:354:GLU:H	1:A:354:GLU:HG2	1.40	0.47
1:A:954:GLU:HG2	3:A:1639:HOH:O	2.15	0.46
1:A:987:ILE:O	1:A:989:LYS:HA	2.15	0.46
1:A:765:MET:HE3	1:A:921:GLY:HA2	1.98	0.46
1:A:941:SER:HA	1:A:952:LEU:HD22	1.98	0.46
1:A:804:ASP:OD1	1:A:805:SER:N	2.45	0.45
1:A:854:LEU:HD11	1:A:897:TYR:CE1	2.52	0.45
1:A:658:VAL:CG1	1:A:663:GLN:HG3	2.47	0.44
1:A:983:LEU:O	1:A:987:ILE:HG13	2.16	0.44
1:A:415:LYS:N	3:A:1580:HOH:O	2.23	0.44
1:A:377:ILE:HG22	1:A:383:GLU:HG3	2.00	0.43
1:A:714:VAL:HG12	1:A:741:PHE:CD1	2.53	0.43
1:A:819:ILE:HD13	1:A:898:TRP:HZ2	1.83	0.43
1:A:812:LYS:HB2	1:A:897:TYR:CE2	2.54	0.43
1:A:267:PRO:O	1:A:272:LYS:HE3	2.19	0.43
1:A:856:ASN:HA	1:A:859:GLU:OE1	2.19	0.43
1:A:802:GLY:O	1:A:911:SER:HB3	2.18	0.43
1:A:208:GLU:HG2	3:A:1691:HOH:O	2.18	0.42
1:A:855:ASP:OD1	1:A:856:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:ASP:OD1	1:A:866:ASP:C	2.58	0.42
1:A:807:GLN:NE2	3:A:1858:HOH:O	2.51	0.42
1:A:558:LYS:HE2	3:A:1601:HOH:O	2.18	0.42
1:A:156:ASP:HB3	3:A:1588:HOH:O	2.19	0.42
1:A:110:HIS:HE1	3:A:1651:HOH:O	2.02	0.41
1:A:186:ARG:NH1	3:A:1307:HOH:O	2.45	0.41
1:A:818:LEU:HD22	1:A:966:LEU:HD22	2.02	0.41
1:A:330:GLN:HG3	3:A:1910:HOH:O	2.20	0.41
1:A:649:LEU:HB2	1:A:664:LEU:HD21	2.03	0.40
1:A:377:ILE:CD1	1:A:436:VAL:HG13	2.51	0.40
1:A:856:ASN:O	1:A:859:GLU:HG2	2.20	0.40
1:A:768:LEU:HD13	1:A:817:GLY:HA3	2.03	0.40
1:A:894:THR:HG22	1:A:894:THR:O	2.21	0.40
1:A:780:ASP:HA	1:A:781:PRO:HD3	1.76	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	884/899 (98%)	859 (97%)	24 (3%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	779	ALA

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	A	775/786 (99%)	756 (98%)	19 (2%)	55 47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	SER
1	A	304	VAL
1	A	354	GLU
1	A	366	ASP
1	A	544	ASP
1	A	627	GLN
1	A	642	ASP
1	A	710	GLU
1	A	748	THR
1	A	778	SER
1	A	785	ARG
1	A	795	GLU
1	A	796	THR
1	A	813	LEU
1	A	841	GLU
1	A	877	SER
1	A	894	THR
1	A	911	SER
1	A	954	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS

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 1 ligands modelled in this entry, 1 is 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(Å²)	Q<0.9
1	A	888/899 (98%)	0.57	101 (11%)	7	7	15, 35, 69, 103	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	803	TRP	8.1
1	A	796	THR	7.4
1	A	544	ASP	7.3
1	A	909	TYR	6.9
1	A	864	PHE	5.8
1	A	546	LYS	5.3
1	A	317	VAL	4.9
1	A	242	VAL	4.8
1	A	545	ASN	4.6
1	A	850	LYS	4.4
1	A	301	LEU	4.4
1	A	417	ALA	4.2
1	A	799	ILE	4.2
1	A	908	ARG	4.2
1	A	316	PRO	4.0
1	A	687	ASN	3.9
1	A	855	ASP	3.8
1	A	852	TYR	3.7
1	A	793	GLY	3.7
1	A	795	GLU	3.6
1	A	277	ILE	3.6
1	A	785	ARG	3.6
1	A	415	LYS	3.5
1	A	849	ILE	3.5
1	A	320	ARG	3.5
1	A	543	LYS	3.5
1	A	857	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	180	ILE	3.4
1	A	367	GLU	3.4
1	A	299	LEU	3.4
1	A	794	SER	3.4
1	A	801	LEU	3.3
1	A	129	THR	3.2
1	A	400	PHE	3.2
1	A	423	LYS	3.1
1	A	835	THR	3.1
1	A	341	TYR	3.0
1	A	867	GLU	3.0
1	A	342	MET	3.0
1	A	906	GLY	2.9
1	A	243	ASP	2.9
1	A	547	GLU	2.9
1	A	354	GLU	2.9
1	A	399	ILE	2.9
1	A	416	TYR	2.8
1	A	343	ILE	2.8
1	A	319	ASN	2.8
1	A	810	ILE	2.7
1	A	854	LEU	2.7
1	A	418	LYS	2.7
1	A	901	VAL	2.7
1	A	869	TYR	2.7
1	A	978	ALA	2.7
1	A	807	GLN	2.7
1	A	782	VAL	2.7
1	A	760	ASP	2.6
1	A	809	ILE	2.6
1	A	797	ASP	2.6
1	A	787	VAL	2.6
1	A	398	GLY	2.6
1	A	917	LEU	2.6
1	A	318	SER	2.5
1	A	548	GLU	2.5
1	A	146	LEU	2.5
1	A	683	LYS	2.5
1	A	911	SER	2.5
1	A	802	GLY	2.5
1	A	622	VAL	2.5
1	A	300	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	361	ILE	2.4
1	A	960	MET	2.4
1	A	771	GLY	2.4
1	A	148	PHE	2.4
1	A	275	LEU	2.4
1	A	784	ALA	2.3
1	A	788	PHE	2.3
1	A	861	PRO	2.3
1	A	509	LEU	2.3
1	A	232	VAL	2.3
1	A	791	GLN	2.3
1	A	811	PHE	2.3
1	A	792	LEU	2.2
1	A	919	ILE	2.2
1	A	858	LEU	2.2
1	A	229	GLY	2.2
1	A	131	LYS	2.2
1	A	302	VAL	2.2
1	A	957	ILE	2.2
1	A	865	ASP	2.2
1	A	896	LYS	2.2
1	A	832	PRO	2.1
1	A	868	LYS	2.1
1	A	230	LEU	2.1
1	A	132	ASP	2.1
1	A	344	GLY	2.1
1	A	745	ALA	2.1
1	A	353	GLN	2.1
1	A	397	GLY	2.1
1	A	329	TRP	2.0
1	A	227	LEU	2.0
1	A	99	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors($Å^2$)	Q<0.9
2	CA	A	1001	1/1	0.99	0.08	-2.36	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.