



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2023 – 05:52 AM EDT

PDB ID : 3LK6
Title : Beta-N-hexosaminidase N318D mutant (YBBD_N318D) from bacillus subtilis
Authors : Krug, M.
Deposited on : 2010-01-27
Resolution : 2.88 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

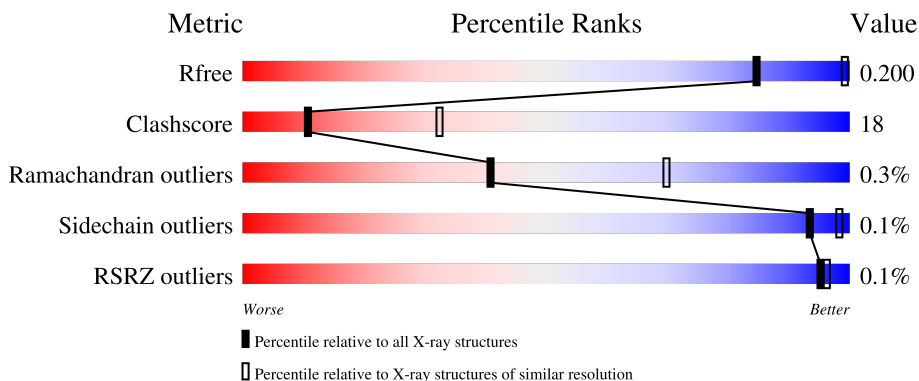
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 of 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 $\leq 5\%$. 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	616	67% 32%
1	B	616	66% 33%
1	C	616	68% 32%
1	D	616	66% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19416 atoms, of which 188 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 Lipoprotein ybbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	615	4767	3019	829	900	19	0	2	0
1	B	612	4738	3002	824	893	19	0	1	0
1	C	616	4758	3013	829	897	19	0	0	0
1	D	614	4753	3011	827	896	19	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	ASN	ASP	engineered mutation	UNP P40406
B	318	ASN	ASP	engineered mutation	UNP P40406
C	318	ASN	ASP	engineered mutation	UNP P40406
D	318	ASN	ASP	engineered mutation	UNP P40406

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	15	4	8	3	0	0
2	A	1	17	4	10	3	0	0
2	A	1	17	4	10	3	0	0
2	A	1	17	4	10	3	0	0
2	B	1	17	4	10	3	0	0
2	B	1	17	4	10	3	0	0
2	B	1	17	4	10	3	0	0
2	B	1	17	4	10	3	0	0
2	B	1	17	4	10	3	0	0
2	B	1	17	4	10	3	0	0
2	C	1	17	4	10	3	0	0
2	C	1	17	4	10	3	0	0
2	C	1	17	4	10	3	0	0
2	C	1	17	4	10	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	23	Total	O	0	0
			23	23		
4	C	19	Total	O	0	0
			19	19		
4	D	15	Total	O	0	0
			15	15		



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.31Å 99.15Å 139.86Å 90.11° 90.05° 89.94°	Depositor
Resolution (Å)	48.99 – 2.88 48.99 – 2.88	Depositor EDS
% Data completeness (in resolution range)	93.9 (48.99-2.88) 93.8 (48.99-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.171 , 0.201 0.169 , 0.200	Depositor DCC
R_{free} test set	3270 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtrriage
Anisotropy	0.958	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.418 for h,-k,-l 0.420 for -h,k,-l 0.418 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19416	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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](#)

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

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	0.31	0/4854	0.50	0/6553
1	B	0.31	0/4825	0.50	0/6515
1	C	0.31	0/4842	0.50	0/6537
1	D	0.32	0/4840	0.50	0/6534
All	All	0.31	0/19361	0.50	0/26139

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	4767	0	4886	178	0
1	B	4738	0	4858	187	0
1	C	4758	0	4880	177	0
1	D	4753	0	4876	180	0
2	A	28	38	40	3	0
2	B	42	60	60	10	0
2	C	35	50	50	3	0
2	D	28	40	40	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	0	1	0
4	B	23	0	0	1	0
4	C	19	0	0	1	0
4	D	15	0	0	2	0
All	All	19228	188	19690	711	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 18.

The worst 5 of 711 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:482:LYS:HD3	2:B:643:PEG:H31	1.37	1.06
1:C:554:ASN:HD21	1:D:289:ASP:HB2	1.28	0.98
1:D:429:LYS:HE2	2:D:644:PEG:H32	1.43	0.95
1:C:151:ILE:O	1:C:155:GLN:HG3	1.67	0.94
1:C:554:ASN:ND2	1:D:289:ASP:HB2	1.83	0.94

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	615/616 (100%)	575 (94%)	38 (6%)	2 (0%)	41 70
1	B	611/616 (99%)	573 (94%)	36 (6%)	2 (0%)	41 70
1	C	614/616 (100%)	575 (94%)	37 (6%)	2 (0%)	41 70
1	D	613/616 (100%)	573 (94%)	38 (6%)	2 (0%)	41 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2453/2464 (100%)	2296 (94%)	149 (6%)	8 (0%)	41 70

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	HIS
1	C	61	LYS
1	C	222	HIS
1	D	222	HIS
1	A	61	LYS

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	520/519 (100%)	520 (100%)	0	100 100
1	B	517/519 (100%)	517 (100%)	0	100 100
1	C	519/519 (100%)	518 (100%)	1 (0%)	93 98
1	D	519/519 (100%)	517 (100%)	2 (0%)	91 97
All	All	2075/2076 (100%)	2072 (100%)	3 (0%)	93 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	186	PRO
1	D	449	PRO
1	D	561	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	50	GLN
1	D	101	GLN

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Mol	Chain	Res	Type
1	B	101	GLN
1	B	384	ASN
1	C	50	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 for Mogul analysis.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	A	646	-	6,6,6	0.69	0	5,5,5	0.74	0
2	PEG	B	643	-	6,6,6	0.60	0	5,5,5	1.06	1 (20%)
2	PEG	D	645	-	6,6,6	0.67	0	5,5,5	0.71	0
2	PEG	D	644	-	6,6,6	0.56	0	5,5,5	0.69	0
2	PEG	D	643	-	6,6,6	0.58	0	5,5,5	0.69	0
2	PEG	A	643	-	6,6,6	0.65	0	5,5,5	0.79	0
2	PEG	A	645	-	6,6,6	0.58	0	5,5,5	0.54	0
2	PEG	C	643	-	6,6,6	0.63	0	5,5,5	0.86	0
2	PEG	B	648	-	6,6,6	0.61	0	5,5,5	0.61	0
2	PEG	D	646	-	6,6,6	0.62	0	5,5,5	0.62	0
2	PEG	A	644	-	6,6,6	0.51	0	5,5,5	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	C	645	-	6,6,6	0.52	0	5,5,5	0.72	0
2	PEG	B	649	-	6,6,6	0.61	0	5,5,5	0.77	0
2	PEG	B	650	-	6,6,6	0.55	0	5,5,5	0.63	0
2	PEG	B	645	-	6,6,6	0.59	0	5,5,5	0.55	0
2	PEG	B	644	-	6,6,6	0.66	0	5,5,5	0.70	0
2	PEG	C	644	-	6,6,6	0.65	0	5,5,5	0.68	0
2	PEG	C	646	-	6,6,6	0.59	0	5,5,5	0.57	0
2	PEG	C	647	-	6,6,6	0.61	0	5,5,5	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	646	-	-	0/4/4/4	-
2	PEG	B	643	-	-	2/4/4/4	-
2	PEG	D	645	-	-	0/4/4/4	-
2	PEG	D	644	-	-	1/4/4/4	-
2	PEG	D	643	-	-	0/4/4/4	-
2	PEG	A	643	-	-	1/4/4/4	-
2	PEG	A	645	-	-	0/4/4/4	-
2	PEG	C	643	-	-	0/4/4/4	-
2	PEG	B	648	-	-	0/4/4/4	-
2	PEG	D	646	-	-	0/4/4/4	-
2	PEG	A	644	-	-	0/4/4/4	-
2	PEG	C	645	-	-	1/4/4/4	-
2	PEG	B	649	-	-	0/4/4/4	-
2	PEG	B	650	-	-	0/4/4/4	-
2	PEG	B	645	-	-	2/4/4/4	-
2	PEG	B	644	-	-	2/4/4/4	-
2	PEG	C	644	-	-	1/4/4/4	-
2	PEG	C	646	-	-	1/4/4/4	-
2	PEG	C	647	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	643	PEG	C3-O2-C2	2.30	123.23	113.29

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	645	PEG	O1-C1-C2-O2
2	B	643	PEG	O2-C3-C4-O4
2	B	645	PEG	O1-C1-C2-O2
2	A	643	PEG	O2-C3-C4-O4
2	B	643	PEG	C1-C2-O2-C3

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	646	PEG	2	0
2	B	643	PEG	3	0
2	D	645	PEG	1	0
2	D	644	PEG	3	0
2	A	644	PEG	1	0
2	C	645	PEG	2	0
2	B	649	PEG	1	0
2	B	650	PEG	2	0
2	B	645	PEG	2	0
2	B	644	PEG	2	0
2	C	644	PEG	1	0

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	615/616 (99%)	-0.27	0 100 100	19, 43, 80, 138	0
1	B	612/616 (99%)	-0.28	1 (0%) 95 95	17, 43, 79, 123	0
1	C	616/616 (100%)	-0.28	1 (0%) 95 95	18, 43, 82, 126	0
1	D	614/616 (99%)	-0.30	1 (0%) 95 95	19, 43, 80, 123	0
All	All	2457/2464 (99%)	-0.28	3 (0%) 95 96	17, 43, 80, 138	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	ALA	3.3
1	D	32	ALA	2.9
1	C	33	ILE	2.4

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 monosaccharides 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, 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	B-factors(Å ²)	Q<0.9
3	NA	C	648	1/1	0.85	0.38	69,69,69,69	0
3	NA	A	647	1/1	0.86	0.27	63,63,63,63	0
2	PEG	A	643	7/7	0.86	0.36	66,78,93,93	0
2	PEG	D	644	7/7	0.89	0.30	53,83,100,100	0
2	PEG	C	645	7/7	0.90	0.20	39,69,89,89	0
2	PEG	A	644	7/7	0.90	0.29	55,80,96,96	0
2	PEG	B	645	7/7	0.90	0.26	55,93,115,117	0
2	PEG	C	647	7/7	0.90	0.15	65,93,112,112	0
2	PEG	C	643	7/7	0.91	0.35	72,86,92,94	0
2	PEG	B	649	7/7	0.91	0.24	76,96,125,125	0
3	NA	B	651	1/1	0.91	0.16	51,51,51,51	0
2	PEG	D	643	7/7	0.91	0.18	50,61,73,73	0
2	PEG	B	643	7/7	0.92	0.31	62,74,88,88	0
2	PEG	B	650	7/7	0.92	0.23	53,82,99,99	0
2	PEG	C	646	7/7	0.92	0.23	32,67,81,81	0
2	PEG	A	645	7/7	0.92	0.27	50,74,98,98	0
2	PEG	A	646	7/7	0.93	0.45	74,100,127,136	0
2	PEG	C	644	7/7	0.94	0.28	70,89,107,107	0
2	PEG	B	648	7/7	0.94	0.25	47,72,87,87	0
3	NA	D	647	1/1	0.94	0.20	71,71,71,71	0
2	PEG	D	645	7/7	0.95	0.32	71,88,97,98	0
2	PEG	D	646	7/7	0.95	0.21	51,62,72,76	0
2	PEG	B	644	7/7	0.96	0.27	61,73,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.