

wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 - 06:10 am GMT

PDB ID : 2BER

Title : Y370G Active Site Mutant of the Sialidase from Micromonospora viridifaciens

in complex with beta-Neu5Ac (sialic acid).

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Deposited on : 2004-11-30

Resolution : 1.80 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018) Percentile statistics : FAILED 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) : 2.36

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 1.80 Å.

There are no overall percentile quality scores available for this entry.

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 <=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	• •				
			<mark>%</mark>				
1	A	601	91%	7%	-		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SLB	A	1648	X	-	-	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5404 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.

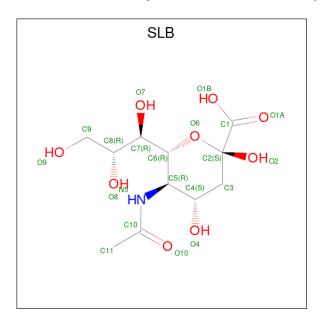
• Molecule 1 is a protein called BACTERIAL SIALIDASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	601	Total	С	N	О	S	0	6	0
1	Λ	001	4545	2813	819	905	8	0	0	U

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	GLY	TYR	engineered mutation	UNP Q02834

• Molecule 2 is N-acetyl-beta-neuraminic acid (three-letter code: SLB) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	Δ	1	Total	С	N	О	0	0
	11	1	21	11	1	9		

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



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

• Molecule 4 is water.

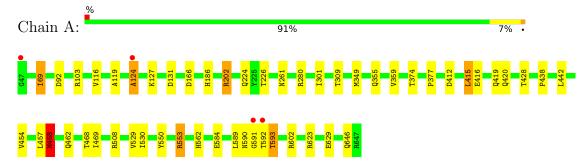
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	837	Total O 837 837	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: BACTERIAL SIALIDASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	55.44Å 49.53Å 107.04Å	Donositor
a, b, c, α , β , γ	90.00° 101.74° 90.00°	Depositor
Resolution (Å)	105.41 - 1.80	Depositor
Resolution (A)	34.93 - 1.80	EDS
% Data completeness	87.0 (105.41-1.80)	Depositor
(in resolution range)	87.1 (34.93-1.80)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.60 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.140 , 0.199	Depositor
R, R_{free}	0.155 , 0.209	DCC
R_{free} test set	2348 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 64.3	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5404	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.64% 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: NA, SLB

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	Boı	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.94	1/4675~(0.0%)	0.97	$15/6383 \ (0.2\%)$	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	124	ALA	CA-CB	-5.64	1.40	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	602	ARG	NE-CZ-NH1	14.46	127.53	120.30
1	A	602	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	A	508	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	553	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	508	ARG	NE-CZ-NH2	-7.90	116.35	120.30

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	4545	0	4360	41	0
2	A	21	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	837	0	0	20	0
All	All	5404	0	4376	41	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 5.

The worst 5 of 41 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:589:LEU:HA	4:A:2756:HOH:O	1.35	1.23
1:A:420:GLN:NE2	4:A:2566:HOH:O	2.00	0.94
1:A:589:LEU:CA	4:A:2756:HOH:O	2.03	0.84
1:A:589:LEU:O	4:A:2756:HOH:O	2.00	0.80
1:A:591:GLY:C	4:A:2759:HOH:O	2.23	0.76

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	Perc	entiles
1	A	605/601 (101%)	595 (98%)	8 (1%)	2 (0%)	41	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	THR
1	A	69	ILE



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	482/476 (101%)	472 (98%)	10 (2%)	53 42	

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468[A]	THR
1	A	468[B]	THR
1	A	593	THR
1	A	415	LEU
1	A	442	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	562	HIS
1	A	573	GLN
1	A	646	GLN
1	A	355	GLN
1	A	395	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 monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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).

Mal	Type	Chain	Res	Link	Bond lengths		Bond angles			
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SLB	A	1648	-	21,21,21	2.84	6 (28%)	25,31,31	2.31	8 (32%)

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	SLB	A	1648	-	1/1/8/9	6/20/38/38	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\mathring{A}})$	Ideal(A)
2	A	1648	SLB	O2-C2	8.20	1.50	1.39
2	A	1648	SLB	O8-C8	-7.96	1.26	1.43
2	A	1648	SLB	C7-C6	3.29	1.57	1.53
2	A	1648	SLB	C5-N5	2.57	1.50	1.45
2	A	1648	SLB	C2-C1	-2.22	1.50	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
2	A	1648	SLB	O8-C8-C9	5.63	122.36	109.14
2	A	1648	SLB	O8-C8-C7	5.60	122.72	109.10
2	A	1648	SLB	O7-C7-C8	3.96	118.37	108.81
2	A	1648	SLB	O6-C6-C5	-2.80	107.04	109.78
2	A	1648	SLB	O1A-C1-C2	-2.76	119.40	123.59

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
2	A	1648	SLB	C8

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1648	SLB	O1B-C1-C2-O6
2	A	1648	SLB	C6-C7-C8-O8
2	A	1648	SLB	O7-C7-C8-O8
2	A	1648	SLB	C7-C8-C9-O9
2	A	1648	SLB	O1A-C1-C2-C3

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.

Mo	l Chain	Analysed	<RSRZ $>$	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	601/601 (100%)	-0.58	4 (0%) 87 86	8, 14, 23, 36	8 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	4.6
1	A	592	THR	4.2
1	A	124	ALA	4.1
1	A	591	GLY	2.3

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)

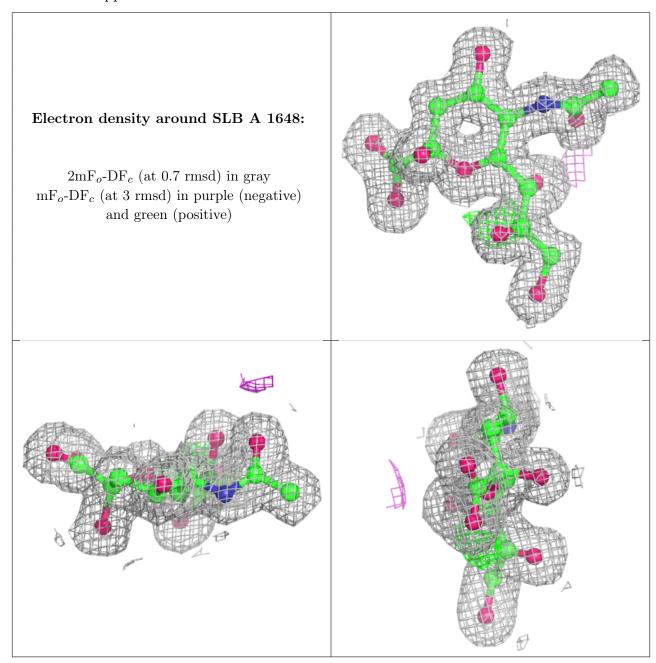
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ m B ext{-}factors(\AA^2)$	Q<0.9
2	SLB	A	1648	21/21	0.97	0.08	7,9,13,15	0
3	NA	A	1649	1/1	0.99	0.06	9,9,9,9	0

The following is a graphical depiction of the model fit to experimental electron density of all



instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

