



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 8, 2017 – 05:24 AM EST

PDB ID : 5SWA  
Title : Crystal structure of N-glycan transport solute binding protein (NgtS) from Streptococcus pneumoniae in complex with Man1GlcNAc  
Authors : Robb, M.; Boraston, A.B.  
Deposited on : 2016-08-08  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

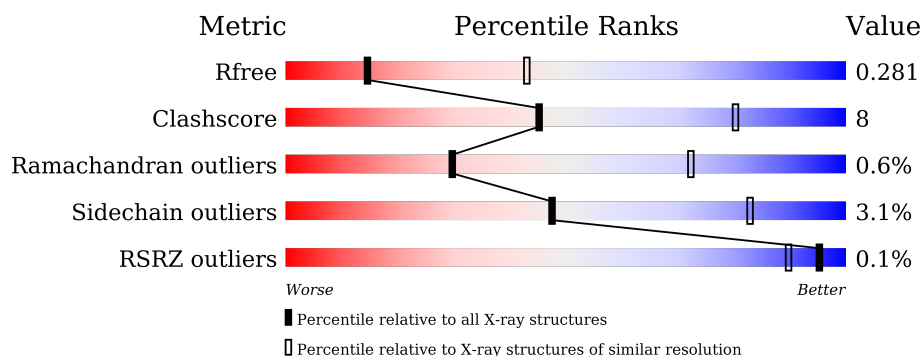
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	476	 78% 15% • 6%
1	B	476	 74% 18% • 5%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6989 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 Extracellular solute-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	1	0
			3425	2180	561	677	7			
1	B	450	Total	C	N	O	S	0	1	0
			3459	2203	566	683	7			

There are 18 discrepancies between the modelled and reference sequences:

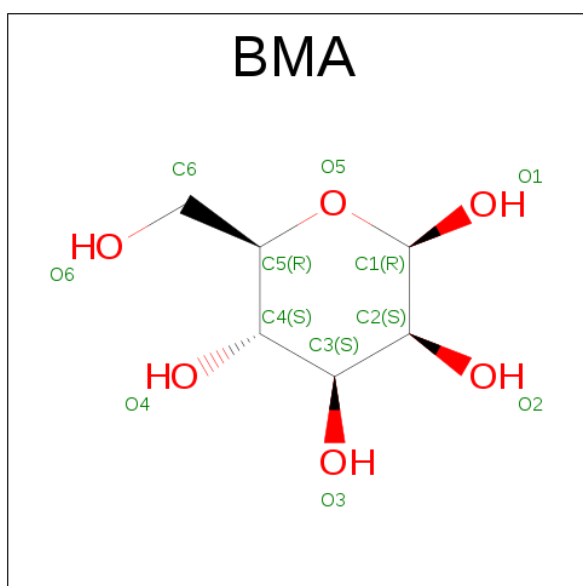
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP A0A0T7JX40
A	492	LEU	-	expression tag	UNP A0A0T7JX40
A	493	GLU	-	expression tag	UNP A0A0T7JX40
A	494	HIS	-	expression tag	UNP A0A0T7JX40
A	495	HIS	-	expression tag	UNP A0A0T7JX40
A	496	HIS	-	expression tag	UNP A0A0T7JX40
A	497	HIS	-	expression tag	UNP A0A0T7JX40
A	498	HIS	-	expression tag	UNP A0A0T7JX40
A	499	HIS	-	expression tag	UNP A0A0T7JX40
B	24	MET	-	initiating methionine	UNP A0A0T7JX40
B	492	LEU	-	expression tag	UNP A0A0T7JX40
B	493	GLU	-	expression tag	UNP A0A0T7JX40
B	494	HIS	-	expression tag	UNP A0A0T7JX40
B	495	HIS	-	expression tag	UNP A0A0T7JX40
B	496	HIS	-	expression tag	UNP A0A0T7JX40
B	497	HIS	-	expression tag	UNP A0A0T7JX40
B	498	HIS	-	expression tag	UNP A0A0T7JX40
B	499	HIS	-	expression tag	UNP A0A0T7JX40

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Br 1	0	0
4	A	1	Total 1	Br 1	0	0

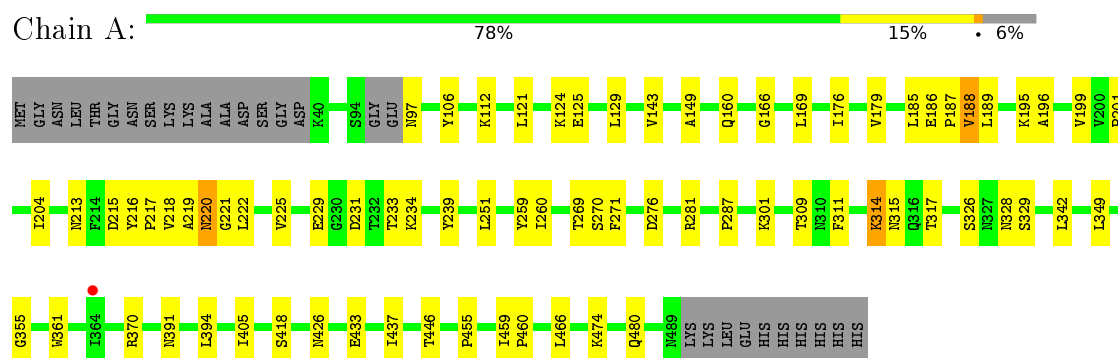
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total 29	O 29	0	0
5	B	22	Total 22	O 22	0	0

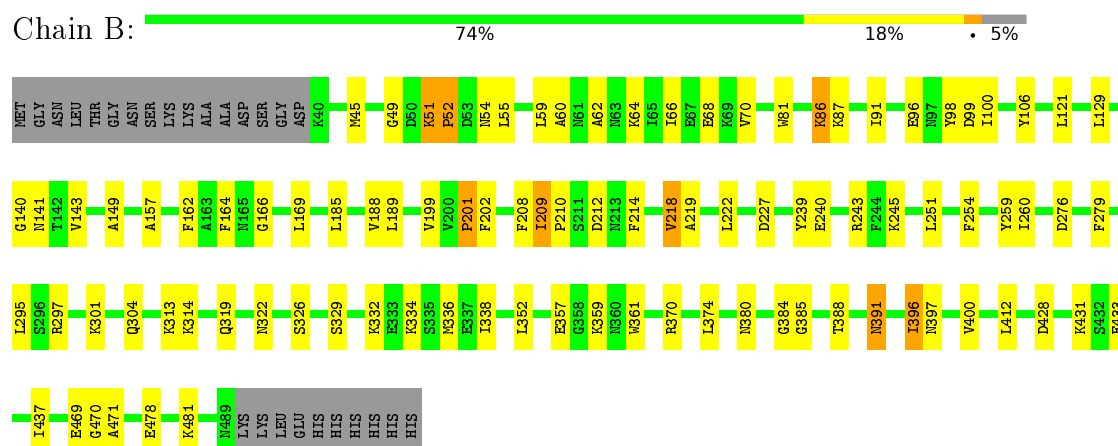
### 3 Residue-property plots

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: Extracellular solute-binding protein



- Molecule 1: Extracellular solute-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.99 Å 50.47 Å 107.89 Å 89.17° 89.02° 88.90°	Depositor
Resolution (Å)	107.86 – 3.00 45.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (107.86-3.00) 96.6 (45.46-3.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.01 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.227 , 0.281 0.227 , 0.281	Depositor DCC
$R_{free}$ test set	820 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-l 0.054 for -h,k,-l 0.047 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	6989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, BR

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	0.28	0/3496	0.44	0/4762
1	B	0.28	0/3532	0.45	0/4805
All	All	0.28	0/7028	0.45	0/9567

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

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	3425	0	3268	45	0
1	B	3459	0	3317	59	0
2	A	15	0	14	0	0
2	B	15	0	14	2	0
3	A	11	0	10	0	0
3	B	11	0	10	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	29	0	0	0	0
5	B	22	0	0	0	0
All	All	6989	0	6633	106	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 8.

The worst 5 of 106 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:51:LYS:HE3	1:B:55:LEU:HB2	1.19	1.17
1:B:254:PHE:HB3	1:B:260:ILE:HG12	1.62	0.82
2:B:501:NAG:O3	3:B:502:BMA:O5	1.98	0.81
1:A:239:TYR:HB3	1:A:459:ILE:HD11	1.63	0.79
1:B:428:ASP:HA	1:B:431:LYS:HE2	1.69	0.74

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	445/476 (94%)	410 (92%)	35 (8%)	0	100	100
1	B	449/476 (94%)	418 (93%)	26 (6%)	5 (1%)	17	58
All	All	894/952 (94%)	828 (93%)	61 (7%)	5 (1%)	30	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	ASN
1	B	219	ALA
1	B	470	GLY
1	B	52	PRO
1	B	201	PRO

### 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	357/408 (88%)	345 (97%)	12 (3%)	44	81
1	B	362/408 (89%)	352 (97%)	10 (3%)	51	84
All	All	719/816 (88%)	697 (97%)	22 (3%)	47	83

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	LYS
1	B	51	LYS
1	B	396	ILE
1	A	426	ASN
1	A	446	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	ASN
1	B	477	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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	NAG	A	501	3	15,15,15	0.63	0	17,21,21	1.61	3 (17%)
3	BMA	A	502	2	11,11,12	0.25	0	15,15,17	0.69	0
2	NAG	B	501	3	15,15,15	0.67	0	17,21,21	0.98	1 (5%)
3	BMA	B	502	2	11,11,12	0.27	0	15,15,17	0.73	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	NAG	A	501	3	-	0/6/26/26	0/1/1/1
3	BMA	A	502	2	-	0/2/19/22	0/1/1/1
2	NAG	B	501	3	-	0/6/26/26	0/1/1/1
3	BMA	B	502	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAG	C3-C2-N2	-3.48	103.44	110.67
2	B	501	NAG	O4-C4-C3	-2.68	104.31	110.36
2	A	501	NAG	C8-C7-N2	-2.01	112.24	116.10
2	A	501	NAG	O7-C7-N2	3.46	128.90	121.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAG	2	0
3	B	502	BMA	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	448/476 (94%)	-0.21	1 (0%) 95 87	23, 38, 62, 88	0
1	B	450/476 (94%)	-0.22	0 100 100	21, 38, 58, 73	0
All	All	898/952 (94%)	-0.21	1 (0%) 95 90	21, 38, 60, 88	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	ILE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	B	501	15/15	0.89	0.20	-0.03	38,40,41,42	0
2	NAG	A	501	15/15	0.92	0.18	-0.30	38,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BR	A	503	1/1	0.95	0.09	-	86,86,86,86	0
4	BR	B	503	1/1	0.98	0.04	-	44,44,44,44	0
3	BMA	B	502	11/12	0.89	0.18	-	41,42,43,43	0
3	BMA	A	502	11/12	0.92	0.19	-	37,37,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.