

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	2YK6
Title	:	Structure of Neisseria LOS-specific sialyltransferase (NST), in complex with
		CDP.
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Deposited on	:	2011-05-25
Resolution	:	2.83 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:

:	4.02b-467
:	1.13
:	FAILED
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.36
	: : : : :

Clashscore

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.83 Å.

141614

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.

1078 (2.86-2.82)

Metric	Percent	ile Ranks Value
Clashscore		11
Worse	2	Better
Perc	centile relative to all X-ray structures	
Perc	centile relative to X-ray structures of sin	nilar resolution
Matria	Whole archive	Similar resolution
wietric	(# Entries)	$(\# \text{Entries, resolution range}(\text{\AA}))$



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2764 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 CMP-N-ACETYLNEURAMINATE-BETA-GALACTOSAMI DE-ALPHA-2,3-SIALYLTRANSFERASE.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	325	Total 2637	C 1715	N 429	0 481	S 12	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	371	LEU	-	expression tag	UNP P72097
А	372	VAL	-	expression tag	UNP P72097
А	373	PRO	-	expression tag	UNP P72097
А	374	ARG	-	expression tag	UNP P72097
А	102	TRP	ARG	variant	UNP P72097
А	129	ALA	SER	variant	UNP P72097
А	168	ILE	GLY	variant	UNP P72097
А	242	ALA	THR	variant	UNP P72097
A	273	ASN	LYS	variant	UNP P72097

• Molecule 2 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
0	Δ	1	Total	С	Ν	Ο	Р	0	0
	A	L	25	9	3	11	2	0	0

• Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 16	C 10	O 6	0	0





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	А	1	Total 5	0 4	S 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	81	Total O 81 81	0	0

SEQUENCE-PLOTS INFOmissingINFO



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	86.10Å 123.51Å 41.65Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 - 2.83	Depositor
% Data completeness	99.5 (70.71-2.83)	Depositor
(in resolution range)	55.5 (10.11-2.05)	Depositor
R _{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.57 (at 2.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.190 , 0.257	Depositor
Wilson B-factor ($Å^2$)	39.9	Xtriage
Anisotropy	0.104	Xtriage
L-test for twinning ²	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2764	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.52% 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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CDP, SO4, $1\mathrm{PE}$

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	Bo	nd lengths	Bo	nd angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.75	1/2706~(0.0%)	0.80	2/3662~(0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	55	CYS	CB-SG	-7.65	1.69	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
1	А	303	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	А	131	LEU	CA-CB-CG	5.29	127.46	115.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2637	0	2638	58	1
2	А	25	0	12	2	0
3	А	16	0	22	1	0
4	А	5	0	0	0	0
5	А	81	0	0	2	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2764	0	2672	61	3

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 11.

The worst 5 of 61 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:280:HIS:HD2	1:A:282:ARG:H	1.17	0.87
1:A:141:ALA:HB3	1:A:144:GLU:HG3	1.58	0.84
1:A:165:ASP:H	1:A:169:ASN:HD21	1.26	0.84
1:A:280:HIS:H	1:A:283:GLN:HE21	1.29	0.81
1:A:280:HIS:H	1:A:283:GLN:NE2	1.84	0.75

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2004:HOH:O	5:A:2057:HOH:O[3_655]	1.68	0.52
5:A:2003:HOH:O	5:A:2080:HOH:O[3_655]	2.14	0.06
1:A:66:ARG:NH1	1:A:233:PRO:O[2_665]	2.18	0.02

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA (i)

There are no RNA molecules in this entry.



4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

3 ligands are modelled in this entry.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.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

