

wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 06:49 pm BST

PDB ID	:	2YK5
Title	:	Structure of Neisseria LOS-specific sialyltransferase (NST), in complex with
		CMP.
Authors	:	Lin, L.Y.C.; Rakic, B.; Chiu, C.P.C.; Lameignere, E.; Wakarchuk, W.W.;
		Withers, S.G.; Strynadka, N.C.J.
Deposited on	:	2011-05-25
$\operatorname{Resolution}$:	2.32 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 following versions of software and data (see references (1)) were used in the production of this report:

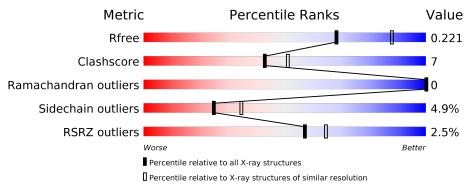
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\rm CCP4$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.32 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	5974(2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855(2.34-2.30)

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 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	Quality of chain		
			2%		
1	A	326	85%	13%	•



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 2933 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.

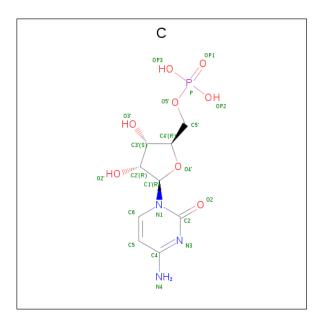
Mol	Chain	Residues		A	Atoms	5			ZeroOcc	AltConf	Trace
1	А	326	Total 2648	C 1721	N 433	O 482	S 1	Se 11	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	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
А	273	ASN	LYS	variant	UNP P72097

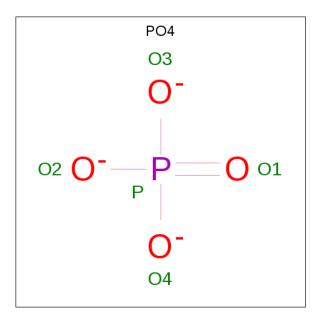
• Molecule 2 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
9	Δ	1	Total	С	Ν	0	Р	0	0
	А	L	21	9	3	8	1		0

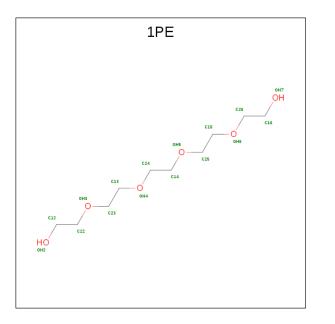
• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

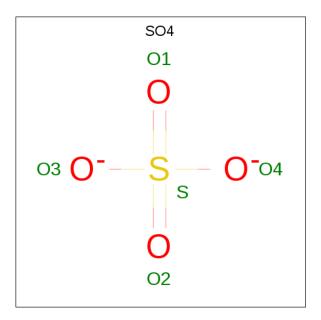
• Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).





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

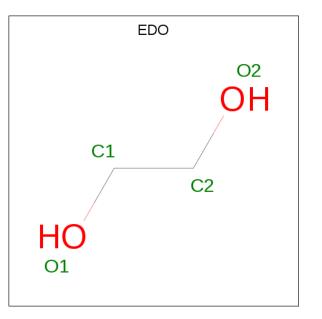
• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



- 2YK5
- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 7 is water.

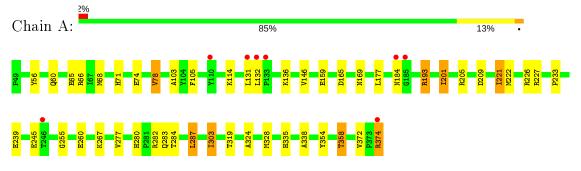
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	220	Total O 220 220	17	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

 \bullet Molecule 1: CMP-N-ACETYLNEURAMINATE-BETA-GALACTOSAMIDE-ALPHA-2,3-SIA LYLTRANSFERASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	85.75Å 124.14Å 41.93Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.53 - 2.32	Depositor
	42.87 - 2.32	EDS
% Data completeness	99.0(70.53-2.32)	Depositor
(in resolution range)	99.0(42.87-2.32)	EDS
R _{merge}	0.01	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > {}^1$	$3.55 (at 2.32 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.5.0110$	Depositor
D D.	0.176 , 0.223	Depositor
R, R_{free}	0.173 , 0.221	DCC
R_{free} test set	1013 reflections (5.09%)	wwPDB-VP
Wilson B-factor $(Å^2)$	22.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 44.7	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2933	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.44% 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.

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: PO4, 1PE, EDO, SO4

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).

Mal	Chain	Bond lengths		Bond angles	
Mol Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.89	1/2706~(0.0%)	0.81	4/3643~(0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	78	VAL	CB-CG1	5.44	1.64	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	226	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	А	303	ILE	CG1-CB-CG2	-7.45	95.02	111.40
1	А	226	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	А	131	LEU	CA-CB-CG	5.17	127.19	115.30

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	А	2648	0	2651	36	1
2	А	21	0	12	1	0
3	А	5	0	0	1	0

Continued on next page...



Mol		Non-H	H(model)	H(added)	Clashes	Symm-Clashes
	Cham		ii(iiiouci)	II(duucu)	Clashes	
4	A	16	0	22	0	0
5	А	15	0	0	0	0
6	А	8	0	12	0	0
7	А	220	0	0	4	1
All	All	2933	0	2697	37	2

Continued from previous page...

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 7.

The worst 5 of 37 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:374:ARG:HH11	1:A:374:ARG:HG2	1.14	1.10
1:A:374:ARG:CG	1:A:374:ARG:HH11	1.78	0.95
1:A:280:HIS:HD2	1:A:282:ARG:H	1.22	0.87
1:A:245:GLU:OE2	1:A:335:HIS:HE1	1.63	0.82
1:A:374:ARG:NH1	1:A:374:ARG:HG2	1.93	0.76

All (2) 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)
1:A:66:ARG:NH1	1:A:233:PRO:O[2_665]	1.97	0.23
7:A:2038:HOH:O	7:A:2071:HOH:O[2_665]	2.07	0.13

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	Perce	\mathbf{ntiles}
1	А	324/326~(99%)	319~(98%)	5(2%)	0	100	100



There are no Ramachandran outliers to report.

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.

Mo	l Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	287/276~(104%)	273~(95%)	14~(5%)	25 34

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	201	ILE
1	А	221	ILE
1	А	303	ILE
1	А	193	ARG
1	А	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	275	GLN
1	А	335	HIS
1	А	280	HIS
1	А	169	ASN
1	А	283	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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	Tune	Chain	Res	Link	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
	Type	Chain			Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	SO4	А	1378	-	4,4,4	0.27	0	6,6,6	0.75	0
4	1PE	А	1377	-	15, 15, 15	0.68	0	$14,\!14,\!14$	1.38	1 (7%)
6	EDO	А	1381	-	3,3,3	0.40	0	$2,\!2,\!2$	0.85	0
5	SO4	А	1379	-	4,4,4	0.24	0	$6,\!6,\!6$	0.49	0
5	SO4	А	1380	-	4,4,4	0.26	0	$6,\!6,\!6$	0.24	0
6	EDO	А	1382	-	3,3,3	0.34	0	$2,\!2,\!2$	0.77	0
3	PO4	А	1376	-	4,4,4	1.04	0	6,6,6	0.91	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	\mathbf{Res}	Link	Chirals	Torsions	Rings
6	EDO	А	1382	-	-	1/1/1/1	-
4	1PE	А	1377	-	-	6/13/13/13	-
6	EDO	А	1381	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	A	1377	1PE	OH5-C14-C24	-3.83	93.15	110.39

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
4	А	1377	1PE	OH6-C15-C25-OH5
4	А	1377	1PE	OH2-C12-C22-OH3
4	А	1377	1PE	OH4-C13-C23-OH3
4	А	1377	1PE	C24-C14-OH5-C25
4	А	1377	1PE	OH5-C14-C24-OH4

5 of 7 torsion outliers are listed below:

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
3	А	1376	PO4	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	А	315/326~(96%)	-0.46	8 (2%) 57 64	5, 18, 36, 48	8 (2%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	184	ASN	3.6
1	А	185	GLY	3.3
1	А	133	PRO	3.3
1	А	132	LEU	3.1
1	А	246	THR	2.8

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. 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	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	1PE	А	1377	16/16	0.95	0.13	$17,\!21,\!29,\!33$	0
5	SO4	А	1378	5/5	0.96	0.12	$36,\!39,\!39,\!43$	0

Continued on next page...



Mol	Type	Chain	Res	Atoms	RSCC	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	SO4	А	1380	5/5	0.97	0.11	55, 56, 57, 58	0
5	SO4	А	1379	5/5	0.98	0.14	$33,\!33,\!35,\!36$	0
6	EDO	А	1382	4/4	0.98	0.12	21,22,22,23	0
3	PO4	А	1376	5/5	0.98	0.11	27,29,31,31	0
6	EDO	А	1381	4/4	0.99	0.12	6,7,8,10	0
2	С	А	1375	21/21	0.99	0.10	7,11,15,20	0

Continued from previous page...

6.5 Other polymers (i)

There are no such residues in this entry.

