



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 07:58 PM EDT

PDB ID : 3JQY
Title : Crystal Structure of the polySia specific acetyltransferase NeuO
Authors : Schulz, E.-C.; Bergfeld, A.; Muehlenhoff, M.; Ficner, R.
Deposited on : 2009-09-08
Resolution : 1.70 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

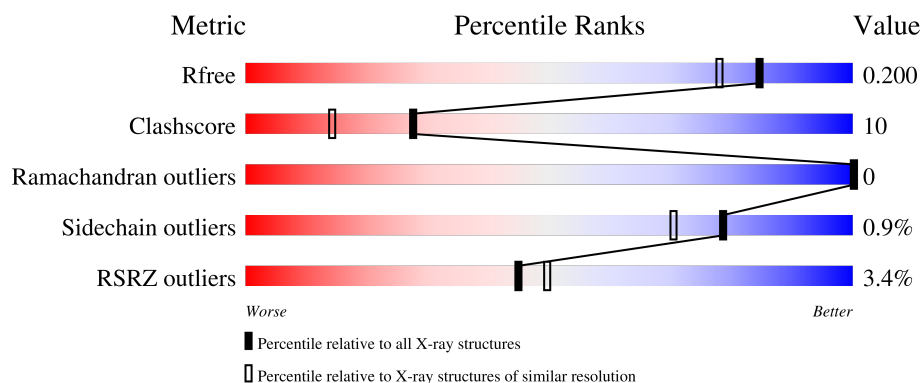
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


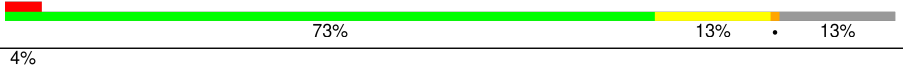
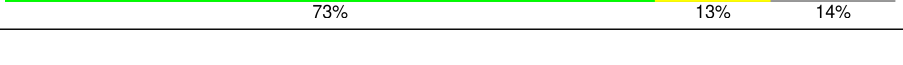
The reported resolution of this entry is 1.70 Å.

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	252	 2% 80% 12% • 8%
1	B	252	 4% 73% 13% • 13%
1	C	252	 4% 73% 13% 14%

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	PEG	B	253	-	-	X	-
2	PEG	C	253	-	-	X	-
3	CL	A	255	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6197 atoms, of which 20 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 Polysialic acid O-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	220	Total	C	N	O	S	0	5	0
			1714	1072	310	322	10			
1	A	233	Total	C	N	O	S	0	4	0
			1829	1144	337	339	9			
1	C	216	Total	C	N	O	S	0	4	0
			1685	1055	307	314	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	cloning artifact	UNP Q58WP5
B	2	LEU	-	cloning artifact	UNP Q58WP5
B	245	LEU	-	expression tag	UNP Q58WP5
B	246	GLU	-	expression tag	UNP Q58WP5
B	247	HIS	-	expression tag	UNP Q58WP5
B	248	HIS	-	expression tag	UNP Q58WP5
B	249	HIS	-	expression tag	UNP Q58WP5
B	250	HIS	-	expression tag	UNP Q58WP5
B	251	HIS	-	expression tag	UNP Q58WP5
B	252	HIS	-	expression tag	UNP Q58WP5
A	1	MET	-	cloning artifact	UNP Q58WP5
A	2	LEU	-	cloning artifact	UNP Q58WP5
A	245	LEU	-	expression tag	UNP Q58WP5
A	246	GLU	-	expression tag	UNP Q58WP5
A	247	HIS	-	expression tag	UNP Q58WP5
A	248	HIS	-	expression tag	UNP Q58WP5
A	249	HIS	-	expression tag	UNP Q58WP5
A	250	HIS	-	expression tag	UNP Q58WP5
A	251	HIS	-	expression tag	UNP Q58WP5
A	252	HIS	-	expression tag	UNP Q58WP5
C	1	MET	-	cloning artifact	UNP Q58WP5
C	2	LEU	-	cloning artifact	UNP Q58WP5
C	245	LEU	-	expression tag	UNP Q58WP5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	246	GLU	-	expression tag	UNP Q58WP5
C	247	HIS	-	expression tag	UNP Q58WP5
C	248	HIS	-	expression tag	UNP Q58WP5
C	249	HIS	-	expression tag	UNP Q58WP5
C	250	HIS	-	expression tag	UNP Q58WP5
C	251	HIS	-	expression tag	UNP Q58WP5
C	252	HIS	-	expression tag	UNP Q58WP5

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



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

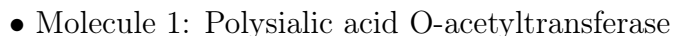
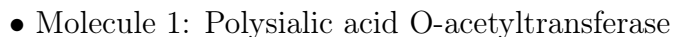
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	293	Total 293	O 293	0	0
4	A	334	Total 334	O 334	0	0
4	C	306	Total 306	O 306	0	0

- Molecule 1: Polysialic acid O-acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.83Å 88.37Å 73.00Å 90.00° 106.62° 90.00°	Depositor
Resolution (Å)	37.35 – 1.70 44.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (37.35-1.70) 99.8 (44.18-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.166 , 0.195 0.171 , 0.200	Depositor DCC
R_{free} test set	4183 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6197	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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

5.1 Standard geometry

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

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	0.33	0/1871	0.50	0/2522
1	B	0.33	0/1754	0.57	2/2365 (0.1%)
1	C	0.30	0/1719	0.51	0/2317
All	All	0.32	0/5344	0.53	2/7204 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	B	234	ARG	CG-CD-NE	5.80	123.99	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	51	LYS	Mainchain

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	1829	0	1861	37	0
1	B	1714	0	1753	40	0
1	C	1685	0	1721	31	0
2	B	7	10	10	5	0
2	C	7	10	10	4	0
3	A	2	0	0	2	0
4	A	334	0	0	4	0
4	B	293	0	0	12	0
4	C	306	0	0	4	0
All	All	6177	20	5355	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 10.

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:A:234:ARG:HG2	1:A:234:ARG:HH11	1.24	0.98
1:B:63:LYS:HG2	1:B:65:ILE:HD11	1.48	0.92
1:B:233:LYS:HE3	4:B:830:HOH:O	1.68	0.92
1:B:63:LYS:HD3	1:B:65:ILE:HD11	1.50	0.92
1:B:63:LYS:HG2	1:B:65:ILE:CD1	2.01	0.90

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	235/252 (93%)	231 (98%)	4 (2%)	0	100	100
1	B	223/252 (88%)	219 (98%)	4 (2%)	0	100	100
1	C	218/252 (86%)	213 (98%)	5 (2%)	0	100	100
All	All	676/756 (89%)	663 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	206/221 (93%)	203 (98%)	3 (2%)	65	51
1	B	194/221 (88%)	193 (100%)	1 (0%)	88	83
1	C	189/221 (86%)	188 (100%)	1 (0%)	88	83
All	All	589/663 (89%)	584 (99%)	5 (1%)	78	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	225	LYS
1	A	19	LYS
1	A	25	LEU
1	A	223	THR
1	C	228	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	153	HIS
1	C	62	ASN
1	A	126	ASN
1	A	217	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	253	-	6,6,6	0.42	0	5,5,5	0.36	0
2	PEG	C	253	-	6,6,6	0.44	0	5,5,5	0.50	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	B	253	-	-	3/4/4/4	-
2	PEG	C	253	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	253	PEG	O2-C3-C4-O4
2	C	253	PEG	C4-C3-O2-C2
2	B	253	PEG	C1-C2-O2-C3
2	B	253	PEG	O2-C3-C4-O4
2	B	253	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	253	PEG	5	0
2	C	253	PEG	4	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	233/252 (92%)	-0.23	5 (2%) 63 67	9, 16, 33, 51	0
1	B	220/252 (87%)	-0.03	9 (4%) 37 41	10, 17, 37, 52	0
1	C	216/252 (85%)	0.04	9 (4%) 36 40	10, 16, 33, 51	0
All	All	669/756 (88%)	-0.08	23 (3%) 45 50	9, 17, 34, 52	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	LEU	6.7
1	B	26	LYS	4.6
1	A	251	HIS	4.4
1	C	228	LEU	3.9
1	C	225	LYS	3.6

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(\AA^2)	Q<0.9
2	PEG	B	253	7/7	0.81	0.28	21,38,50,54	0
2	PEG	C	253	7/7	0.82	0.18	22,41,50,50	0
3	CL	A	253	1/1	0.92	0.16	50,50,50,50	0
3	CL	A	255	1/1	0.97	0.10	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.