



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2025 – 02:13 PM JST

PDB ID : 8YV7
Title : X-ray structure of Thialysine N-epsilon-acetyltransferase from *Caenorhabditis elegans*
Authors : Wang, N.; Ma, X.
Deposited on : 2024-03-28
Resolution : 3.38 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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

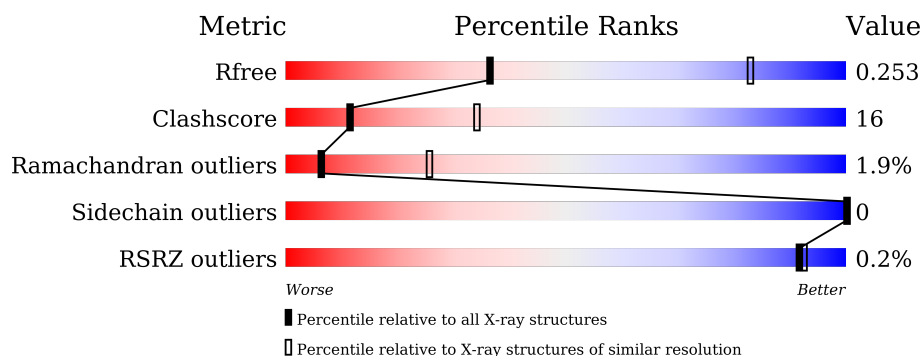
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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}	164625	1137 (3.44-3.32)
Clashscore	180529	1165 (3.44-3.32)
Ramachandran outliers	177936	1164 (3.44-3.32)
Sidechain outliers	177891	1164 (3.44-3.32)
RSRZ outliers	164620	1137 (3.44-3.32)

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	160	<div> <div></div> <div>66%33%.</div> </div>
1	B	160	<div> <div></div> <div>63%36%.</div> </div>
1	C	160	<div> <div>%</div> <div>63%34%.</div> </div>
1	D	160	<div> <div></div> <div>62%38%.</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5261 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.

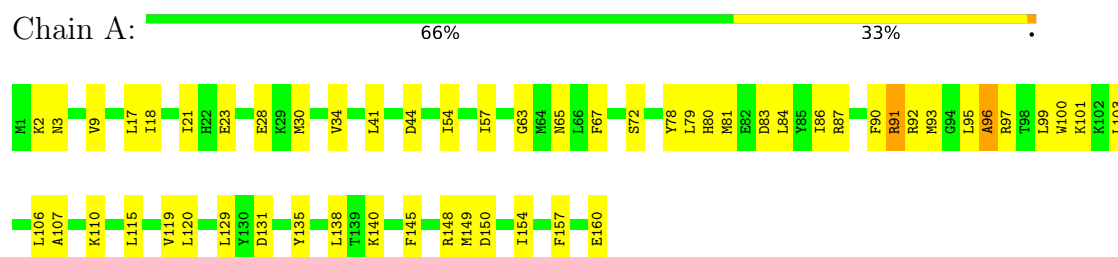
- Molecule 1 is a protein called Thialysine N-epsilon-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1315	851	220	237	7			
1	B	160	Total	C	N	O	S	0	0	0
			1316	851	220	238	7			
1	C	160	Total	C	N	O	S	0	0	0
			1315	851	220	237	7			
1	D	160	Total	C	N	O	S	0	0	0
			1315	851	220	237	7			

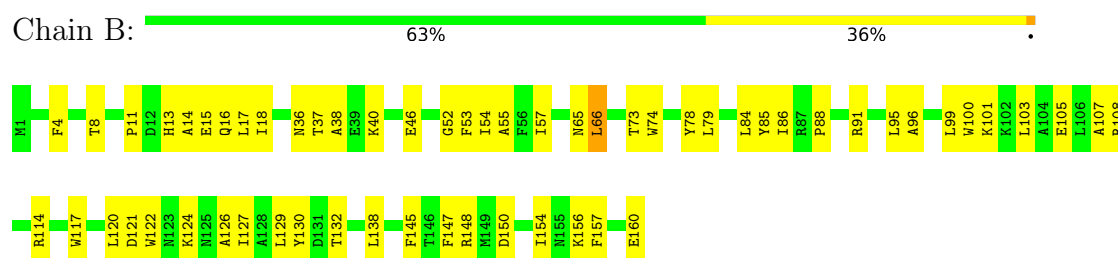
3 Residue-property plots [i](#)

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.

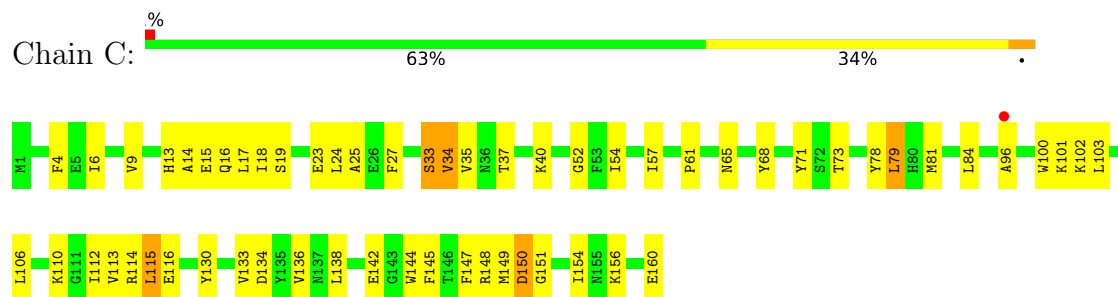
• Molecule 1: Thialysine N-epsilon-acetyltransferase



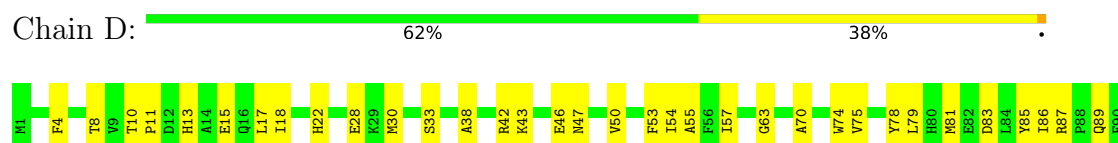
• Molecule 1: Thialysine N-epsilon-acetyltransferase



• Molecule 1: Thialysine N-epsilon-acetyltransferase



• Molecule 1: Thialysine N-epsilon-acetyltransferase



R91	
L95	
A96	
R97	
T98	
L99	
W100	
K101	
E105	
L106	
A107	
R108	
D109	
I112	
V113	
R114	
L115	
E116	
W117	
D121	
L129	
L138	
F147	
R148	
M149	
D150	
I154	
F157	
E160	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.33Å 65.10Å 65.32Å 80.62° 72.76° 63.98°	Depositor
Resolution (Å)	34.25 – 3.38 34.25 – 3.38	Depositor EDS
% Data completeness (in resolution range)	81.9 (34.25-3.38) 82.0 (34.25-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.183 , 0.252 0.183 , 0.253	Depositor DCC
R_{free} test set	544 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.954	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5261	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/1347	0.75	0/1819
1	B	0.51	0/1348	0.79	1/1819 (0.1%)
1	C	0.55	0/1347	0.80	2/1819 (0.1%)
1	D	0.49	0/1347	0.75	0/1819
All	All	0.51	0/5389	0.77	3/7276 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	115	LEU	CB-CG-CD2	-7.36	98.49	111.00
1	B	66	LEU	CA-CB-CG	-6.00	101.50	115.30
1	C	79	LEU	CB-CG-CD2	-5.45	101.74	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	95	LEU	Peptide

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	1315	0	1299	44	0
1	B	1316	0	1299	48	0
1	C	1315	0	1299	50	0
1	D	1315	0	1299	55	0
All	All	5261	0	5196	165	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 16.

The worst 5 of 165 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:2:LYS:HD2	1:A:93:MET:HE3	1.62	0.82
1:A:86:ILE:O	1:A:91:ARG:NH1	2.14	0.79
1:B:129:LEU:O	1:B:132:THR:HG22	1.89	0.72
1:D:75:VAL:HG21	1:D:114:ARG:HD3	1.72	0.71
1:A:79:LEU:HD12	1:A:107:ALA:HB2	1.74	0.70

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	158/160 (99%)	149 (94%)	6 (4%)	3 (2%)	6	26
1	B	158/160 (99%)	138 (87%)	18 (11%)	2 (1%)	10	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	158/160 (99%)	140 (89%)	13 (8%)	5 (3%)	3	17
1	D	158/160 (99%)	143 (90%)	13 (8%)	2 (1%)	10	33
All	All	632/640 (99%)	570 (90%)	50 (8%)	12 (2%)	6	26

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ALA
1	B	96	ALA
1	A	91	ARG
1	C	14	ALA
1	C	150	ASP

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	136/136 (100%)	136 (100%)	0	100	100
1	B	136/136 (100%)	136 (100%)	0	100	100
1	C	136/136 (100%)	136 (100%)	0	100	100
1	D	136/136 (100%)	136 (100%)	0	100	100
All	All	544/544 (100%)	544 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	65	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	160/160 (100%)	-0.77	0 100 100	46, 66, 91, 132	0
1	B	160/160 (100%)	-0.71	0 100 100	44, 62, 113, 140	0
1	C	160/160 (100%)	-0.68	1 (0%) 85 81	47, 65, 105, 118	0
1	D	160/160 (100%)	-0.63	0 100 100	51, 79, 117, 131	0
All	All	640/640 (100%)	-0.70	1 (0%) 92 92	44, 66, 111, 140	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	ALA	2.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.