



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 12:52 AM JST

PDB ID : 7E7A  
Title : Crystal structure of apo ENL YEATS domain T3 mutant  
Authors : Li, Y.; Li, H.  
Deposited on : 2021-02-25  
Resolution : 2.64 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

<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>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

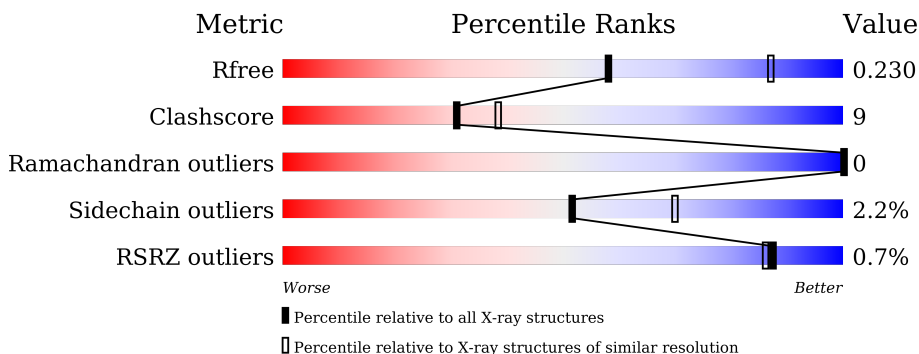
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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  $\geq 3$ , 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	155	 72% 14% • 12%
1	B	155	 74% 15% • 11%
1	C	155	 70% 17% • 11%
1	D	155	 69% 18% • 12%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4655 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 Protein ENL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	137	1142	738	202	194	8	0	0	0
1	B	138	1150	743	203	195	9	0	0	0
1	C	138	1150	743	203	195	9	0	0	0
1	D	137	1142	738	202	194	8	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q03111
A	-1	SER	-	expression tag	UNP Q03111
A	0	HIS	-	expression tag	UNP Q03111
A	111	LYS	ASN	engineered mutation	UNP Q03111
A	?	-	PRO	deletion	UNP Q03111
A	?	-	PRO	deletion	UNP Q03111
A	147	HIS	-	expression tag	UNP Q03111
A	148	HIS	-	expression tag	UNP Q03111
A	149	HIS	-	expression tag	UNP Q03111
A	150	HIS	-	expression tag	UNP Q03111
A	151	HIS	-	expression tag	UNP Q03111
A	152	HIS	-	expression tag	UNP Q03111
B	-2	GLY	-	expression tag	UNP Q03111
B	-1	SER	-	expression tag	UNP Q03111
B	0	HIS	-	expression tag	UNP Q03111
B	111	LYS	ASN	engineered mutation	UNP Q03111
B	?	-	PRO	deletion	UNP Q03111
B	?	-	PRO	deletion	UNP Q03111
B	147	HIS	-	expression tag	UNP Q03111
B	148	HIS	-	expression tag	UNP Q03111
B	149	HIS	-	expression tag	UNP Q03111

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Chain	Residue	Modelled	Actual	Comment	Reference
B	150	HIS	-	expression tag	UNP Q03111
B	151	HIS	-	expression tag	UNP Q03111
B	152	HIS	-	expression tag	UNP Q03111
C	-2	GLY	-	expression tag	UNP Q03111
C	-1	SER	-	expression tag	UNP Q03111
C	0	HIS	-	expression tag	UNP Q03111
C	111	LYS	ASN	engineered mutation	UNP Q03111
C	?	-	PRO	deletion	UNP Q03111
C	?	-	PRO	deletion	UNP Q03111
C	147	HIS	-	expression tag	UNP Q03111
C	148	HIS	-	expression tag	UNP Q03111
C	149	HIS	-	expression tag	UNP Q03111
C	150	HIS	-	expression tag	UNP Q03111
C	151	HIS	-	expression tag	UNP Q03111
C	152	HIS	-	expression tag	UNP Q03111
D	-2	GLY	-	expression tag	UNP Q03111
D	-1	SER	-	expression tag	UNP Q03111
D	0	HIS	-	expression tag	UNP Q03111
D	111	LYS	ASN	engineered mutation	UNP Q03111
D	?	-	PRO	deletion	UNP Q03111
D	?	-	PRO	deletion	UNP Q03111
D	147	HIS	-	expression tag	UNP Q03111
D	148	HIS	-	expression tag	UNP Q03111
D	149	HIS	-	expression tag	UNP Q03111
D	150	HIS	-	expression tag	UNP Q03111
D	151	HIS	-	expression tag	UNP Q03111
D	152	HIS	-	expression tag	UNP Q03111

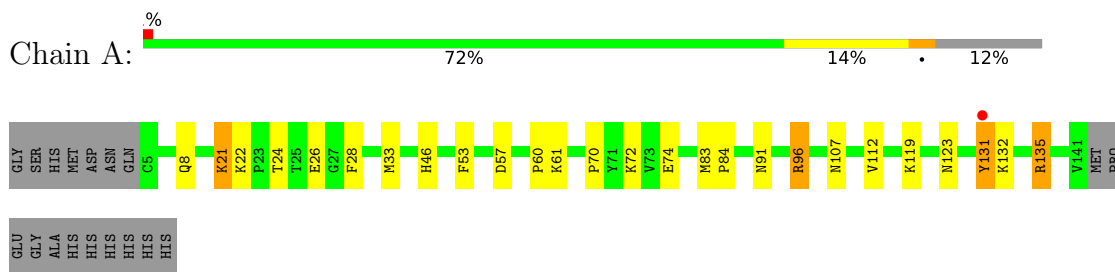
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	23	Total O 23 23	0	0
2	B	20	Total O 20 20	0	0
2	C	13	Total O 13 13	0	0
2	D	15	Total O 15 15	0	0

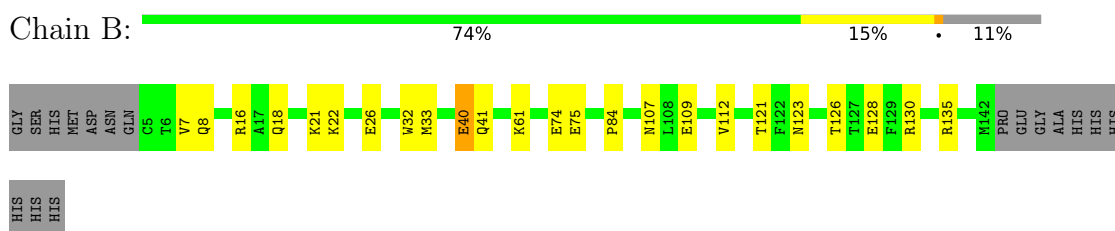
### 3 Residue-property plots [i](#)

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.

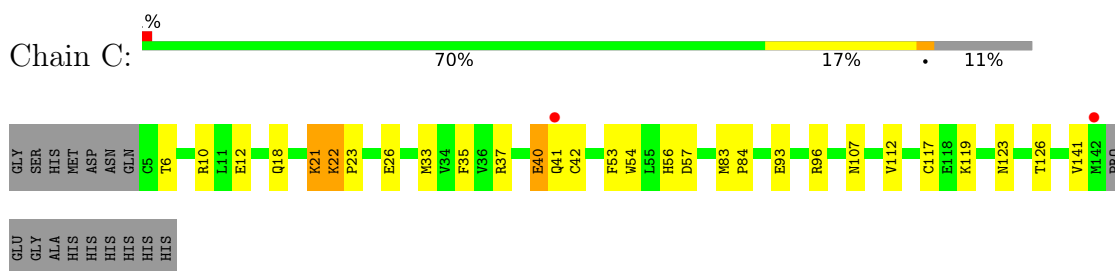
- Molecule 1: Protein ENL



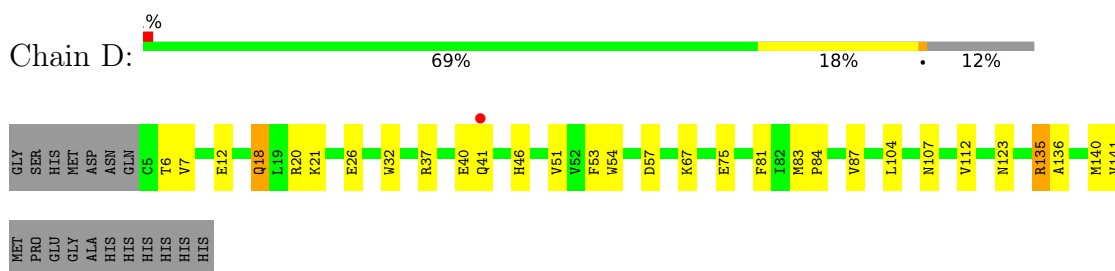
- Molecule 1: Protein ENL



- Molecule 1: Protein ENL



- Molecule 1: Protein ENL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.32Å 88.26Å 167.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.64 49.04 – 2.64	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.04-2.64) 96.1 (49.04-2.64)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.213 , 0.230 0.212 , 0.230	Depositor DCC
$R_{free}$ test set	1772 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtrriage
Anisotropy	0.640	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7043e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [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	2/1175 (0.2%)	0.66	3/1585 (0.2%)
1	B	0.35	0/1183	0.75	3/1595 (0.2%)
1	C	0.34	0/1183	0.58	1/1595 (0.1%)
1	D	0.42	1/1175 (0.1%)	0.65	1/1585 (0.1%)
All	All	0.40	3/4716 (0.1%)	0.66	8/6360 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ARG	NE-CZ	5.93	1.40	1.33
1	D	21	LYS	CG-CD	5.61	1.71	1.52
1	A	131	TYR	CD2-CE2	5.28	1.47	1.39

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ARG	NE-CZ-NH2	-19.41	110.60	120.30
1	D	135	ARG	CG-CD-NE	-7.51	96.03	111.80
1	A	131	TYR	CB-CA-C	-6.77	96.87	110.40
1	B	135	ARG	NH1-CZ-NH2	6.54	126.60	119.40
1	A	131	TYR	CA-CB-CG	6.44	125.63	113.40

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	A	1142	0	1137	21	0
1	B	1150	0	1147	17	0
1	C	1150	0	1147	28	1
1	D	1142	0	1138	25	1
2	A	23	0	0	0	0
2	B	20	0	0	2	0
2	C	13	0	0	3	0
2	D	15	0	0	2	0
All	All	4655	0	4569	83	1

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 9.

The worst 5 of 83 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:123:ASN:HD21	1:D:123:ASN:HB2	1.25	0.99
1:C:40:GLU:O	1:C:41:GLN:HG3	1.61	0.98
1:C:10:ARG:HE	1:C:119:LYS:HE3	1.27	0.96
1:D:18:GLN:NE2	2:D:202:HOH:O	2.17	0.77
1:A:46:HIS:CD2	1:A:135:ARG:HD2	2.23	0.73

All (1) 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:C:41:GLN:OE1	1:D:135:ARG:NH1[1_455]	2.11	0.09

## 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	135/155 (87%)	131 (97%)	4 (3%)	0	100	100
1	B	136/155 (88%)	133 (98%)	3 (2%)	0	100	100
1	C	136/155 (88%)	134 (98%)	2 (2%)	0	100	100
1	D	135/155 (87%)	134 (99%)	1 (1%)	0	100	100
All	All	542/620 (87%)	532 (98%)	10 (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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/141 (89%)	124 (98%)	2 (2%)	62	78
1	B	127/141 (90%)	123 (97%)	4 (3%)	40	58
1	C	127/141 (90%)	123 (97%)	4 (3%)	40	58
1	D	126/141 (89%)	125 (99%)	1 (1%)	81	89
All	All	506/564 (90%)	495 (98%)	11 (2%)	52	70

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	22	LYS
1	C	57	ASP
1	D	18	GLN
1	C	93	GLU
1	B	61	LYS

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

Mol	Chain	Res	Type
1	C	41	GLN
1	C	123	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 monosaccharides 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, 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	137/155 (88%)	-0.02	1 (0%) 87 86	32, 49, 72, 84	0
1	B	138/155 (89%)	-0.07	0 100 100	35, 50, 77, 86	0
1	C	138/155 (89%)	-0.02	2 (1%) 75 73	37, 53, 80, 102	0
1	D	137/155 (88%)	0.08	1 (0%) 87 86	40, 58, 87, 103	0
All	All	550/620 (88%)	-0.01	4 (0%) 87 86	32, 52, 80, 103	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	GLN	4.2
1	D	41	GLN	3.8
1	A	131	TYR	3.7
1	C	142	MET	3.3

### 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.