



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 09:27 AM EDT

PDB ID : 2EY2  
Title : Crystal structure of Staphylococcal nuclease mutant T41C  
Authors : Lu, J.Z.; Sakon, J.; Stites, W.E.  
Deposited on : unknown  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

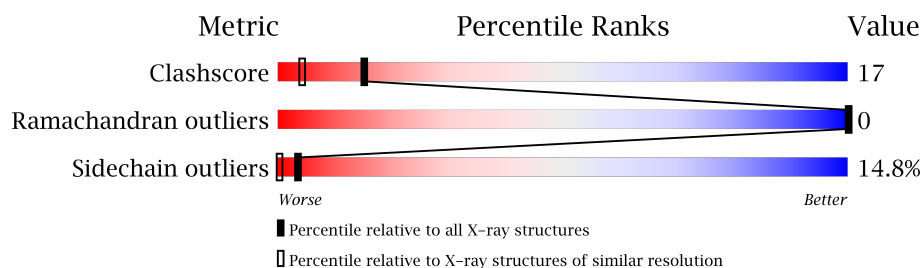
# 1 Overall quality at a glance

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))
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	149	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1141 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 Staphylococcal nuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	4	0
			1103	704	196	198	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	CYS	THR	ENGINEERED	UNP P00644
A	124	HIS	LEU	VARIANT	UNP P00644

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		

**i**

Note EDS was not executed.

- Molecule 1: Staphylococcal nuclease



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.17Å 48.17Å 63.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.70	Depositor
% Data completeness (in resolution range)	94.9 (8.00-1.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	XTALVIEW, SHELXL-97	Depositor
R, $R_{free}$	0.208 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 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	0.41	0/1146	1.05	2/1535 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	105	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	35	ARG	CD-NE-CZ	5.04	130.65	123.60

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	1103	0	1146	38	0
2	A	38	0	0	2	0
All	All	1141	0	1146	38	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 17.

All (38) 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:49:LYS:HD3	1:A:52:GLU:HG2	1.41	1.03
1:A:130:ALA:HA	1:A:133:LYS:HE3	1.69	0.74
1:A:60:ALA:O	1:A:64:LYS:HG2	1.91	0.70
1:A:43:GLU:HG2	1:A:46:HIS:HA	1.76	0.67
1:A:63:LYS:O	1:A:67:GLU:HG3	1.96	0.66
1:A:49:LYS:HZ1	1:A:52:GLU:HA	1.64	0.62
1:A:43:GLU:HB3	1:A:46:HIS:HB2	1.82	0.62
1:A:97:LYS:HD2	2:A:212:HOH:O	1.99	0.61
1:A:49:LYS:NZ	1:A:52:GLU:HA	2.17	0.59
1:A:46:HIS:HB3	1:A:50:GLY:H	1.66	0.59
1:A:130:ALA:HA	1:A:133:LYS:CE	2.33	0.59
1:A:12:ALA:O	1:A:72[A]:ILE:HG23	2.03	0.58
1:A:84:LYS:HE2	1:A:85:TYR:CZ	2.39	0.58
1:A:84:LYS:HE2	1:A:85:TYR:CE2	2.40	0.56
1:A:46:HIS:CD2	1:A:47:PRO:HD2	2.42	0.55
1:A:72[A]:ILE:HG22	2:A:202:HOH:O	2.10	0.50
1:A:43:GLU:CB	1:A:46:HIS:HB2	2.43	0.48
1:A:116:LYS:HG2	1:A:119:ASN:OD1	2.14	0.48
1:A:45:LYS:HB3	1:A:45:LYS:HE3	1.36	0.48
1:A:53:LYS:O	1:A:54:TYR:HB2	2.13	0.47
1:A:64:LYS:HA	1:A:64:LYS:HD2	1.81	0.47
1:A:78:LYS:HB3	1:A:78:LYS:HE3	1.36	0.47
1:A:71:LYS:HE2	1:A:71:LYS:HB3	1.48	0.46
1:A:78:LYS:HG3	1:A:117:PRO:HB2	2.00	0.44
1:A:43:GLU:HG2	1:A:46:HIS:CA	2.45	0.44
1:A:119:ASN:N	1:A:119:ASN:HD22	2.16	0.43
1:A:46:HIS:HB3	1:A:50:GLY:N	2.30	0.43
1:A:76:PHE:CG	1:A:81[B]:ARG:HD3	2.55	0.42
1:A:119:ASN:H	1:A:119:ASN:HD22	1.68	0.41
1:A:6:LYS:HZ2	1:A:7:LEU:H	1.68	0.41
1:A:16:LYS:HE2	1:A:16:LYS:HB2	1.46	0.41
1:A:43:GLU:HA	1:A:43:GLU:OE2	2.21	0.41
1:A:81[B]:ARG:HH11	1:A:81[B]:ARG:HG2	1.86	0.41
1:A:23[B]:VAL:HG12	1:A:25:LEU:HD13	2.02	0.41
1:A:49:LYS:HG2	1:A:50:GLY:N	2.34	0.41
1:A:6:LYS:HD2	1:A:6:LYS:HA	1.80	0.40
1:A:130:ALA:HA	1:A:133:LYS:NZ	2.37	0.40
1:A:6:LYS:HE3	1:A:7:LEU:O	2.22	0.40

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	138/149 (93%)	128 (93%)	10 (7%)	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	119/125 (95%)	100 (84%)	19 (16%)	3	0

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	9	LYS
1	A	16	LYS
1	A	19	ASP
1	A	25	LEU
1	A	43	GLU
1	A	45	LYS
1	A	53	LYS
1	A	64	LYS
1	A	71	LYS
1	A	72[A]	ILE
1	A	72[B]	ILE
1	A	78	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	80[A]	GLN
1	A	80[B]	GLN
1	A	116	LYS
1	A	119	ASN
1	A	123	GLN
1	A	134	LYS

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

Mol	Chain	Res	Type
1	A	68	ASN
1	A	131	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](#)

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.