



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2021 – 02:14 PM JST

PDB ID : 6LWQ  
Title : Crystal structure of human NEIL1(R242) bound to duplex DNA containing a C:T mismatch  
Authors : Liu, M.H.; Zhang, J.; Zhu, C.X.; Zhang, X.X.; Gao, Y.Q.; Yi, C.Q.  
Deposited on : 2020-02-07  
Resolution : 2.89 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.

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

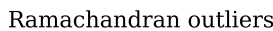
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.19
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.19

**i**

## X-RAY DIFFRACTION







A.

Metric	Percentile Rank	Value
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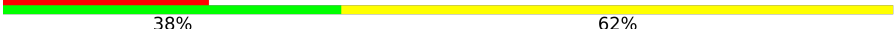
R <sub>free</sub>
Clashscore
Ramachandran outliers
Sidechain outliers
RSRZ outliers

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.

1	A	295	
1	D	295	
1	G	295	
2	B	13	
2	E	13	
2	H	13	

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Mol	Chain	Length	Quality of chain
3	C	13	 46% 54%
3	F	13	 62% 38%
3	I	13	 23% 38% 62%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7521 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 Endonuclease 8-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2142	1365	390	377	10			
1	D	260	Total	C	N	O	S	0	0	0
			2047	1306	374	358	9			
1	G	229	Total	C	N	O	S	0	0	0
			1659	1028	322	302	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	ARG	LYS	variant	UNP Q96FI4
D	242	ARG	LYS	variant	UNP Q96FI4
G	242	ARG	LYS	variant	UNP Q96FI4

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*TP\*GP\*TP\*CP\*TP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			258	125	43	78	12			
2	E	13	Total	C	N	O	P	0	0	0
			258	125	43	78	12			
2	H	13	Total	C	N	O	P	0	0	0
			258	125	43	78	12			

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*GP\*AP\*CP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	P	0	0	0
			267	127	53	75	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	13	Total 267	C 127	N 53	O 75	P 12	0	0	0
3	I	13	Total 267	C 127	N 53	O 75	P 12	0	0	0

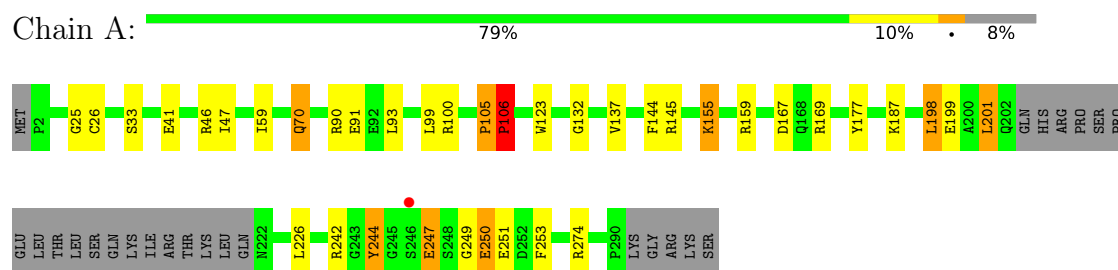
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total 49	O 49	0	0
4	B	5	Total 5	O 5	0	0
4	C	1	Total 1	O 1	0	0
4	D	39	Total 39	O 39	0	0
4	E	4	Total 4	O 4	0	0

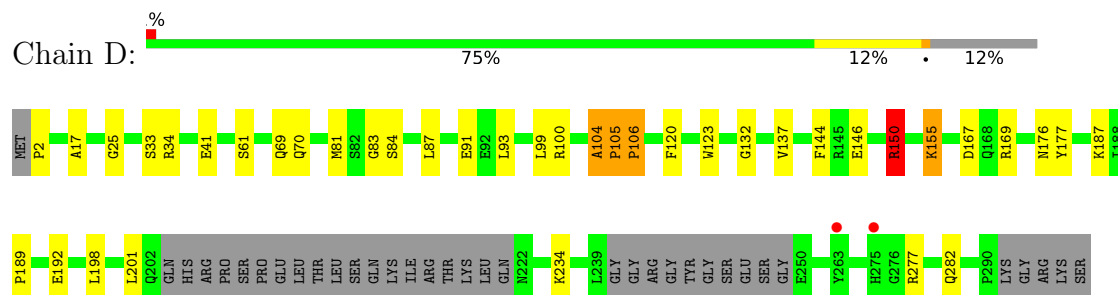
### 3 Residue-property plots [i](#)

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.

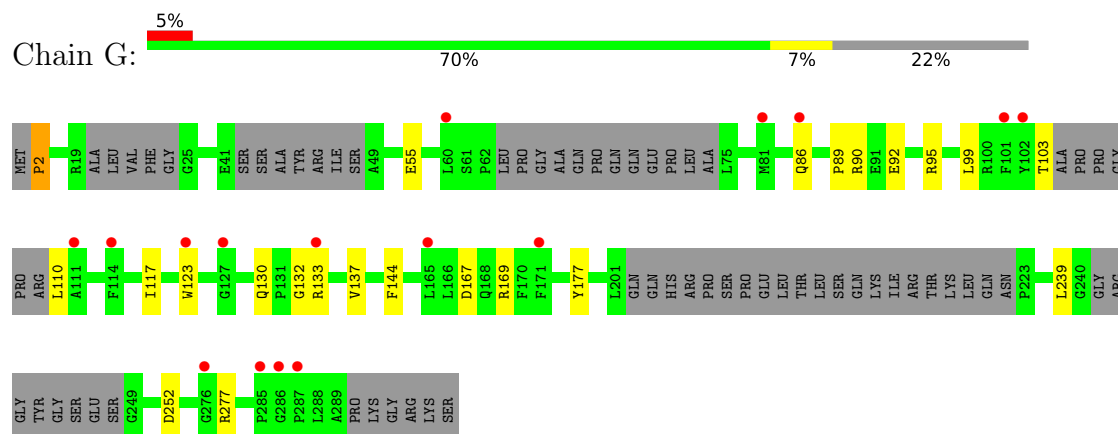
- Molecule 1: Endonuclease 8-like 1



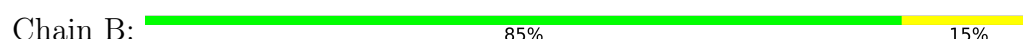
- Molecule 1: Endonuclease 8-like 1



- Molecule 1: Endonuclease 8-like 1

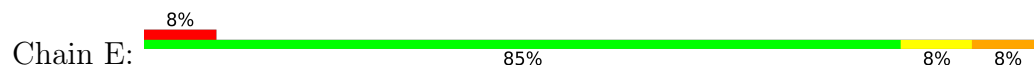


- Molecule 2: DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*TP\*GP\*TP\*CP\*TP\*AP\*C)-3')

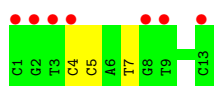
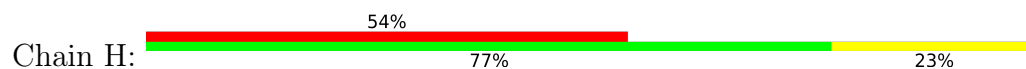




- Molecule 2: DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*TP\*GP\*TP\*CP\*TP\*AP\*C)-3')



- Molecule 2: DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*TP\*GP\*TP\*CP\*TP\*AP\*C)-3')



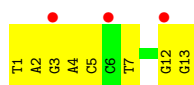
- Molecule 3: DNA (5'-D(\*TP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*GP\*AP\*CP\*GP\*G)-3')



- Molecule 3: DNA (5'-D(\*TP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*GP\*AP\*CP\*GP\*G)-3')



- Molecule 3: DNA (5'-D(\*TP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*GP\*AP\*CP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.08Å 109.23Å 171.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.03 – 2.89 43.00 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.5 (43.03-2.89) 97.5 (43.00-2.89)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.237 , 0.283 0.237 , 0.283	Depositor DCC
$R_{free}$ test set	1529 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7521	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<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	0.79	1/2201 (0.0%)	0.96	1/2977 (0.0%)
1	D	0.82	5/2102 (0.2%)	0.95	1/2843 (0.0%)
1	G	0.71	0/1695	0.86	0/2267
2	B	0.58	0/287	0.93	0/440
2	E	0.65	0/287	1.40	2/440 (0.5%)
2	H	0.53	0/287	0.90	0/440
3	C	0.66	0/300	0.87	1/462 (0.2%)
3	F	0.60	0/300	0.86	0/462
3	I	0.58	0/300	1.02	2/462 (0.4%)
All	All	0.74	6/7759 (0.1%)	0.95	7/10793 (0.1%)

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	A	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	150	ARG	CD-NE	10.12	1.63	1.46
1	D	150	ARG	NE-CZ	9.54	1.45	1.33
1	A	91	GLU	CG-CD	9.20	1.65	1.51
1	D	91	GLU	CD-OE2	7.04	1.33	1.25
1	D	91	GLU	CG-CD	6.45	1.61	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	DG	O5'-P-OP1	-18.65	88.32	110.70
1	D	105	PRO	C-N-CD	-11.03	96.34	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	DG	O5'-P-OP2	11.02	123.92	110.70
3	C	5	DC	C1'-O4'-C4'	-6.28	103.82	110.10
3	I	3	DG	C1'-O4'-C4'	-6.19	103.91	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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	2142	0	2110	24	1
1	D	2047	0	2005	33	1
1	G	1659	0	1473	12	0
2	B	258	0	149	2	0
2	E	258	0	149	4	0
2	H	258	0	149	3	0
3	C	267	0	147	7	0
3	F	267	0	147	4	0
3	I	267	0	147	8	0
4	A	49	0	0	4	0
4	B	5	0	0	1	0
4	C	1	0	0	0	0
4	D	39	0	0	4	0
4	E	4	0	0	0	0
All	All	7521	0	6476	84	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 6.

The worst 5 of 84 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:D:105:PRO:CB	1:D:106:PRO:HD2	1.65	1.15
1:D:105:PRO:HB3	1:D:106:PRO:HD2	1.27	1.10
1:D:104:ALA:HB1	1:D:105:PRO:CD	1.81	1.09
1:D:104:ALA:CB	1:D:105:PRO:HD2	1.85	1.06
1:A:47:ILE:O	1:D:150:ARG:NH1	1.92	1.02

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:A:199:GLU:OE1	1:D:34:ARG:NH2[3_445]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	266/295 (90%)	247 (93%)	17 (6%)	2 (1%)	19	51
1	D	254/295 (86%)	235 (92%)	16 (6%)	3 (1%)	13	40
1	G	215/295 (73%)	198 (92%)	16 (7%)	1 (0%)	29	61
All	All	735/885 (83%)	680 (92%)	49 (7%)	6 (1%)	19	51

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	106	PRO
1	A	244	TYR
1	A	106	PRO
1	D	104	ALA
1	G	90	ARG

### 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	224/248 (90%)	213 (95%)	11 (5%)	25	57
1	D	213/248 (86%)	205 (96%)	8 (4%)	33	67
1	G	151/248 (61%)	146 (97%)	5 (3%)	38	72
All	All	588/744 (79%)	564 (96%)	24 (4%)	30	64

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	70	GLN
1	D	177	TYR
1	D	155	LYS
1	D	234	LYS
1	A	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	D	70	GLN
1	D	130	GLN
1	G	130	GLN

### 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 [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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	270/295 (91%)	0.07	1 (0%) 92 93	39, 61, 95, 131	0
1	D	260/295 (88%)	0.21	2 (0%) 86 86	41, 75, 122, 142	0
1	G	229/295 (77%)	0.50	16 (6%) 16 12	88, 115, 151, 174	0
2	B	13/13 (100%)	-0.05	0 100 100	64, 95, 139, 148	0
2	E	13/13 (100%)	0.22	1 (7%) 13 10	68, 90, 111, 122	0
2	H	13/13 (100%)	1.80	7 (53%) 0 0	124, 137, 143, 146	0
3	C	13/13 (100%)	0.10	0 100 100	72, 95, 123, 126	0
3	F	13/13 (100%)	0.08	0 100 100	57, 79, 109, 114	0
3	I	13/13 (100%)	1.21	3 (23%) 0 0	101, 127, 146, 150	0
All	All	837/963 (86%)	0.28	30 (3%) 42 37	39, 85, 140, 174	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	9	DT	3.8
1	G	81	MET	3.5
1	G	86	GLN	3.3
1	A	246	SER	3.0
2	H	1	DC	2.8

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

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

### 6.3 Carbohydrates ⓘ

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.