



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:07 AM UTC

PDB ID : 1Q39 / pdb_00001q39
Title : Crystal structure of the DNA repair enzyme endonuclease-VIII (Nei) from E. coli: The WT enzyme at 2.8 resolution.
Authors : Golan, G.; Zharkov, D.O.; Feinberg, H.; Fernandes, A.S.; Zaika, E.I.; Kycia, J.H.; Grollman, A.P.; Shoham, G.
Deposited on : 2003-07-29
Resolution : 2.80 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

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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

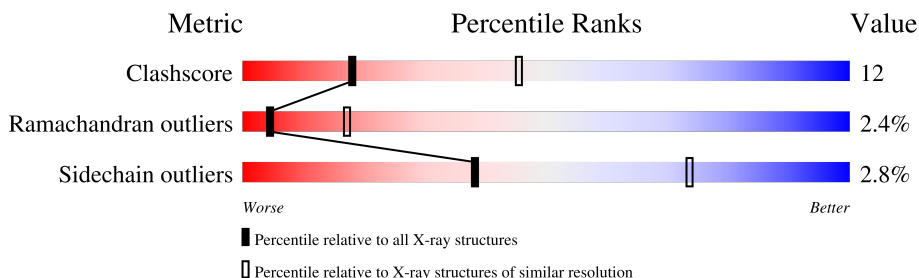
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	262	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2044 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 VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2026	1293	368	360	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	THR	PRO	SEE REMARK 999	UNP P50465
A	112	ARG	THR	SEE REMARK 999	UNP P50465

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		

Note EDS was not executed.

Chain A: 72% 24% 4%

Node	Category
P40	Green
GLJ	Green
GLY	Green
P4	Green
R7	Green
E14	Green
K18	Green
G19	Green
K20	Green
T40	Green
R50	Green
G51	Green
N60	Green
D61	Green
L62	Green
T63	Green
L64	Green
H67	Green
M68	Green
Q69	Green
V73	Green
D78	Green
T79	Green
G80	Green
E81	Green
E82	Green
P80	Green
GLN	Green
T85	Green
V88	Green
L89	Green
K92	Green
L93	Green
Q94	Green
T95	Green
A96	Green
D97	Green
I100	Green
L101	Green
S104	Green
E109	Green
F121	Yellow
L122	Yellow
Q123	Yellow
R124	Yellow
V125	Yellow
R147	Yellow
F148	Yellow
R149	Yellow
N150	Yellow
L158	Yellow
D159	Yellow
Q160	Yellow
L170	Yellow
I174	Yellow
L175	Yellow
W176	Yellow
Q177	Yellow
W178	Yellow
T181	Yellow
K185	Yellow
A186	Yellow
K187	Yellow
D188	Yellow
L189	Yellow
Q193	Yellow
L201	Yellow
L202	Yellow
E203	Yellow
T204	Yellow
P205	Yellow
Q214	Yellow
A223	Yellow
R226	Yellow
F227	Yellow
K228	Yellow
C237	Yellow
E238	Yellow
R239	Yellow
K246	Yellow
T247	Yellow
T248	Yellow
L249	Yellow
C260	Red
Q261	Red
H262	Red

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	57.72Å 79.58Å 169.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.02 – 2.80	Depositor
% Data completeness (in resolution range)	81.7 (29.02-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2044	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.51	1/2075 (0.0%)	1.03	9/2820 (0.3%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	THR	C-N	5.53	1.41	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	SER	N-CA-C	10.84	125.00	108.52
1	A	248	THR	CA-C-N	7.04	135.00	121.54
1	A	248	THR	C-N-CA	7.04	135.00	121.54
1	A	249	LEU	CA-C-N	-6.64	106.99	121.87
1	A	249	LEU	C-N-CA	-6.64	106.99	121.87
1	A	249	LEU	N-CA-C	-6.42	97.14	110.80
1	A	94	GLN	N-CA-C	5.80	118.56	108.76
1	A	104	SER	N-CA-C	5.47	122.45	110.80
1	A	51	GLY	N-CA-C	-5.04	101.59	110.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	THR	Mainchain

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	2026	0	1989	49	0
2	A	1	0	0	0	0
3	A	3	0	0	0	0
4	A	14	0	0	0	0
All	All	2044	0	1989	49	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 12.

All (49) 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:204:ILE:HG13	1:A:205:PRO:HD3	1.43	0.99
1:A:174:ILE:HD13	1:A:201:LEU:HD23	1.61	0.81
1:A:7:ARG:O	1:A:7:ARG:HG3	1.81	0.79
1:A:67:HIS:HD2	1:A:69:GLN:H	1.32	0.77
1:A:201:LEU:O	1:A:205:PRO:HG2	1.87	0.73
1:A:93:LEU:HD12	1:A:100:ILE:HD11	1.77	0.66
1:A:170:LEU:O	1:A:174:ILE:HG13	1.95	0.66
1:A:176:TRP:CZ3	1:A:228:LYS:HG3	2.31	0.65
1:A:202:LEU:C	1:A:205:PRO:HD2	2.27	0.58
1:A:204:ILE:C	1:A:204:ILE:HD12	2.29	0.58
1:A:92:LYS:HE2	1:A:94:GLN:OE1	2.05	0.57
1:A:181:THR:HG23	1:A:262:HIS:HA	1.87	0.56
1:A:239:ARG:HH12	1:A:260:CYS:HB2	1.70	0.56
1:A:174:ILE:HG12	1:A:204:ILE:HG12	1.89	0.55
1:A:189:LEU:HD22	1:A:193:GLN:HB3	1.89	0.54
1:A:60:ASN:HD21	1:A:62:LEU:HD12	1.71	0.54
1:A:204:ILE:CG1	1:A:205:PRO:HD3	2.29	0.54
1:A:14:GLU:HB3	1:A:18:LYS:HE3	1.90	0.54
1:A:170:LEU:HD22	1:A:204:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLN:HG2	1:A:160:GLN:O	2.08	0.53
1:A:181:THR:HG23	1:A:262:HIS:CA	2.42	0.49
1:A:78:ASP:O	1:A:80:GLY:N	2.46	0.48
1:A:148:PHE:O	1:A:150:ASN:N	2.46	0.48
1:A:181:THR:CG2	1:A:262:HIS:HA	2.43	0.47
1:A:239:ARG:NH1	1:A:260:CYS:HB2	2.29	0.47
1:A:237:CYS:O	1:A:239:ARG:N	2.47	0.47
1:A:119:HIS:HB3	1:A:122:LEU:HB2	1.97	0.47
1:A:177:GLN:HG3	1:A:178:VAL:HG13	1.97	0.47
1:A:125:VAL:O	1:A:125:VAL:HG13	2.15	0.46
1:A:89:LEU:HD11	1:A:101:LEU:HD22	1.97	0.46
1:A:64:LEU:HD12	1:A:109:GLU:O	2.16	0.46
1:A:204:ILE:N	1:A:205:PRO:CD	2.79	0.46
1:A:73:VAL:HG13	1:A:73:VAL:O	2.15	0.45
1:A:246:LYS:HB2	1:A:254:PHE:O	2.16	0.45
1:A:170:LEU:HD22	1:A:204:ILE:HD12	1.98	0.45
1:A:123:GLN:O	1:A:147:ARG:NH2	2.50	0.45
1:A:204:ILE:HD12	1:A:205:PRO:N	2.32	0.45
1:A:237:CYS:C	1:A:239:ARG:N	2.76	0.44
1:A:150:ASN:OD1	1:A:187:LYS:HE2	2.17	0.44
1:A:20:LYS:HB2	1:A:95:THR:HG21	2.00	0.43
1:A:238:GLU:O	1:A:238:GLU:HG2	2.19	0.42
1:A:50:ARG:O	1:A:121:PHE:HE2	2.02	0.42
1:A:80:GLY:O	1:A:81:GLU:C	2.62	0.42
1:A:97:ASP:OD1	1:A:97:ASP:N	2.42	0.42
1:A:67:HIS:HD2	1:A:69:GLN:N	2.09	0.42
1:A:40:ILE:HD12	1:A:40:ILE:N	2.34	0.41
1:A:114:GLU:H	1:A:114:GLU:CD	2.28	0.41
1:A:67:HIS:CD2	1:A:69:GLN:H	2.24	0.41
1:A:223:ALA:O	1:A:226:ARG:NE	2.50	0.41

There are no symmetry-related clashes.

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	253/262 (97%)	226 (89%)	21 (8%)	6 (2%)	4	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LEU
1	A	79	THR
1	A	149	ARG
1	A	238	GLU
1	A	214	GLN
1	A	251	SER

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	211/226 (93%)	205 (97%)	6 (3%)	38	73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	158	LEU
1	A	160	GLN
1	A	177	GLN
1	A	185	LYS
1	A	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	43	HIS

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Mol	Chain	Res	Type
1	A	67	HIS
1	A	68	ASN
1	A	69	GLN
1	A	123	GLN
1	A	152	GLN
1	A	160	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.