



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 09:00 AM GMT

PDB ID : 2OQ4
Title : Crystal structure of the DNA repair enzyme endonuclease-VIII (Nei) from E. coli (E2Q) in complex with AP-site containing DNA substrate
Authors : Golan, G.; Zharkov, D.O.; Grollman, A.P.; Shoahm, G.
Deposited on : 2007-01-31
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

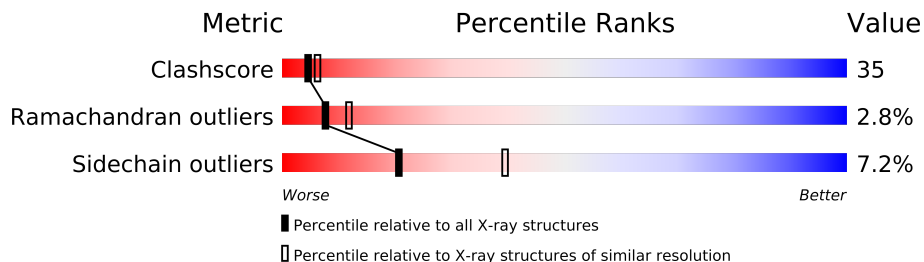
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	13	
1	E	13	
2	D	13	
2	F	13	
3	A	262	
3	B	262	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4976 atoms, of which 0 are hydrogen and 0 are deuterium.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	11	Total	C	N	O	P	0	0	0
			218	106	35	67	10			
1	E	9	Total	C	N	O	P	0	0	0
			177	87	27	55	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			237	112	49	65	11			
2	F	11	Total	C	N	O	P	0	0	0
			218	103	46	59	10			

- Molecule 3 is a protein called Endonuclease VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	252	Total	C	N	O	S	0	0	0
			2014	1286	362	361	5			
3	B	250	Total	C	N	O	S	0	0	0
			2000	1275	363	357	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLN	GLU	ENGINEERED	UNP P50465
A	34	THR	PRO	SEE REMARK 999	UNP P50465
A	112	ARG	THR	SEE REMARK 999	UNP P50465
B	2	GLN	GLU	ENGINEERED	UNP P50465
B	34	THR	PRO	SEE REMARK 999	UNP P50465
B	112	ARG	THR	SEE REMARK 999	UNP P50465

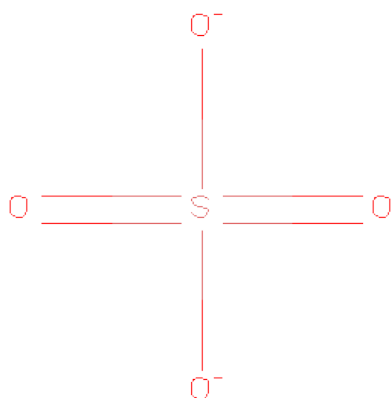
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total 2	O 2	0	0
7	D	6	Total 6	O 6	0	0
7	E	2	Total 2	O 2	0	0
7	F	6	Total 6	O 6	0	0
7	A	38	Total 38	O 38	0	0
7	B	39	Total 39	O 39	0	0

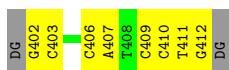
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: 5'-D(*G*GP*CP*TP*TP*CP*AP*TP*CP*CP*TP*GP*G)-3'

Chain C: 



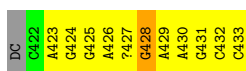
- Molecule 1: 5'-D(*G*GP*CP*TP*TP*CP*AP*TP*CP*CP*TP*GP*G)-3'

Chain E: 



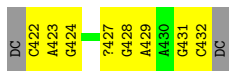
- Molecule 2: 5'-D(*C*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

Chain D: 



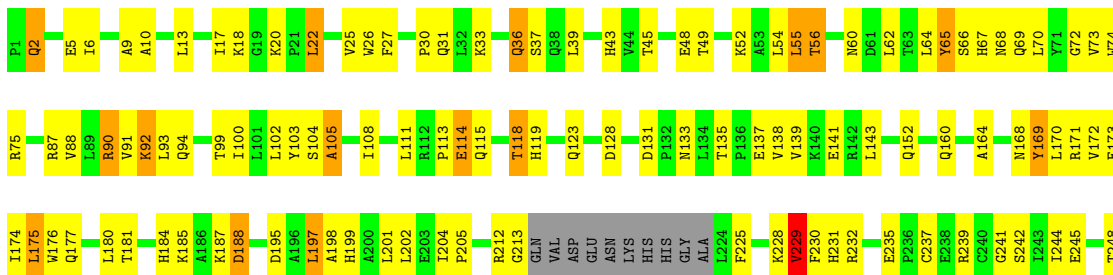
- Molecule 2: 5'-D(*C*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

Chain F: 



- Molecule 3: Endonuclease VIII

Chain A: 



L249
S250
S251
R252
P253
F254
Y255
W256
C257
P258
G259
C260
Q261
H262

● Molecule 3: Endonuclease VIII

Chain B: 

Lys	HIS	HIS	GLY	A223	L224	F225	R226	F227	K228	V229	F230	H231	R232	E235	F236	C237	S242	I243	I244	E245	K246	T247	T248	L249	R252	P253	F254	Y255	W256	C257	PRO	GLY	C260	Q261	H262																	
M150	R151	Q152	F153	A154	G155	L156	Q160	A161	F162	G165	L166	G167	N168	Y169	L170	R171	V172	E173	I174	L175	W176	L180	T181	G182	N183	H184	K185	A186	D187	L188	L189	L194	D195	A196	L197	A198	H199	A200	L201	L202	E203	I204	P205	R206	Y209	R212	GLY	GLN	VAL	ASP	GLU	ASN
G72	V73	W74	F77	D78	E81	T86	L89	R90	V91	Q94	D97	K98	T99	I100	L101	L102	Y103	S104	A105	S106	D107	I108	E109	R112	Q115	L116	T117	T118	H119	L122	V125	D128	V129	L130	D131	P132	N133	L134	T135	V138	V139	K140	E141	R142	L143	L144	S145					
P1	Q2	G3	P4	E5	I6	R7	R8	L13	I17	K20	P21	L22	T23	D24	V25	W26	F27	A28	F29	P30	Q31	L32	K33	Q36	L39	Q42	T45	H46	V47	E48	T49	K52	A53	L54	L55	T56	H57	F58	S59	N60	D61	L62	T63	L64	Y65	S66	H67	H68	Q69	L70	Y71	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.13Å 107.13Å 164.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.5 (16.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.374 , 0.432	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4976	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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: PED, NA, ZN, SO4

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	C	0.40	0/242	0.77	0/371
1	E	0.34	0/196	0.71	0/300
2	D	0.38	0/254	0.66	0/388
2	F	0.36	0/233	0.68	0/356
3	A	0.44	0/2063	0.68	0/2801
3	B	0.43	0/2046	0.68	1/2774 (0.0%)
All	All	0.42	0/5034	0.68	1/6990 (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	E	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	104	SER	N-CA-C	5.25	125.18	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	428	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	411	DT	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	218	0	127	17	0
1	E	177	0	105	13	0
2	D	237	0	131	25	0
2	F	218	0	121	18	0
3	A	2014	0	2002	126	0
3	B	2000	0	1998	146	0
4	B	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	10	0	0	1	0
7	A	38	0	0	4	0
7	B	39	0	0	7	0
7	C	2	0	0	0	0
7	D	6	0	0	0	0
7	E	2	0	0	0	0
7	F	6	0	0	2	0
All	All	4976	0	4484	322	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

The worst 5 of 322 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:6:ILE:HD13	3:B:52:LYS:HA	1.38	1.05
3:A:56:THR:HG23	3:A:64:LEU:HB3	1.35	1.04
3:B:13:LEU:HD22	3:B:100:ILE:HD12	1.44	0.97
1:C:411:DT:H2"	1:C:412:DG:C8	2.01	0.95
3:A:239:ARG:HD2	3:A:260:CYS:SG	2.10	0.91

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	
3	A	248/262 (95%)	223 (90%)	20 (8%)	5 (2%)	11	21
3	B	244/262 (93%)	209 (86%)	26 (11%)	9 (4%)	5	7
All	All	492/524 (94%)	432 (88%)	46 (9%)	14 (3%)	8	12

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	105	ALA
3	A	114	GLU
3	B	104	SER
3	B	116	LEU
3	B	247	THR

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	
3	A	215/226 (95%)	200 (93%)	15 (7%)	21	41
3	B	214/226 (95%)	198 (92%)	16 (8%)	19	36
All	All	429/452 (95%)	398 (93%)	31 (7%)	21	39

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	260	CYS

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Mol	Chain	Res	Type
3	B	56	THR
3	B	197	LEU
3	B	2	GLN
3	B	64	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	199	HIS
3	A	231	HIS
3	B	115	GLN
3	A	160	GLN
3	B	94	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	601	-	4,4,4	0.15	0	6,6,6	0.13	0
6	SO4	B	602	-	4,4,4	0.25	0	6,6,6	0.06	0
6	SO4	B	603	-	4,4,4	0.64	0	6,6,6	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	A	601	-	-	0/0/0/0	0/0/0/0
6	SO4	B	602	-	-	0/0/0/0	0/0/0/0
6	SO4	B	603	-	-	0/0/0/0	0/0/0/0

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.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.