



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:50 PM GMT

PDB ID : 4Q0Z  
Title : The catalytic core of Rad2 in complex with DNA substrate (complex III)  
Authors : Mietus, M.; Nowak, E.; Jaciuk, M.; Kustos, P.; Nowotny, M.  
Deposited on : 2014-04-02  
Resolution : 2.40 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

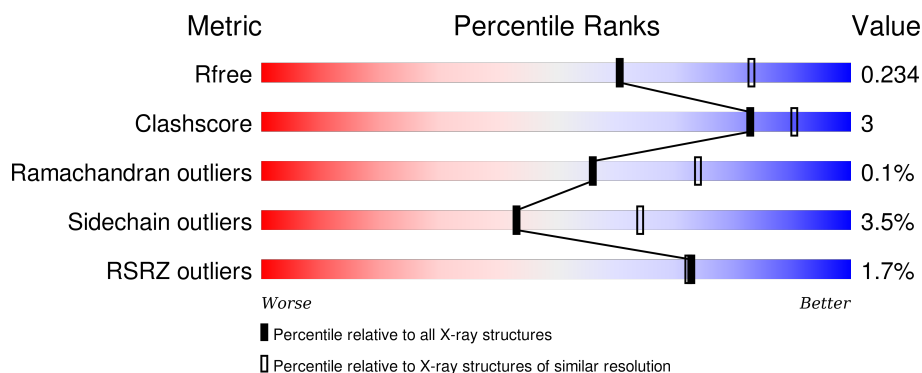
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	365	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>12%</div> </div> </div>
1	B	365	<div> <div></div> <div>77%</div> <div>7%</div> <div>16%</div> </div>
1	E	365	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>17%</div> </div> </div>
1	F	365	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>7%</div> <div>16%</div> </div> </div>
2	C	17	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>41%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	17	
3	D	17	
3	H	17	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13433 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 Rad2p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	3	0
			2581	1657	426	485	13			
1	B	307	Total	C	N	O	S	0	1	0
			2460	1590	400	457	13			
1	E	304	Total	C	N	O	S	0	2	0
			2406	1557	397	439	13			
1	F	307	Total	C	N	O	S	0	2	0
			2495	1608	412	462	13			

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*GP\*CP\*TP\*CP\*CP\*CP\*TP\*TP\*GP\*TP\*CP\*TP\*CP\*AP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	17	0
			660	318	102	208	32			
2	G	17	Total	C	N	O	P	0	17	0
			644	308	100	204	32			

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*GP\*AP\*CP\*AP\*AP\*GP\*GP\*GP\*AP\*GP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	17	Total	C	N	O	P	0	17	0
			686	324	138	192	32			
3	H	17	Total	C	N	O	P	0	17	0
			670	314	136	188	32			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	F	1	Total 1	Ca 1	0	0
4	E	1	Total 1	Ca 1	0	0

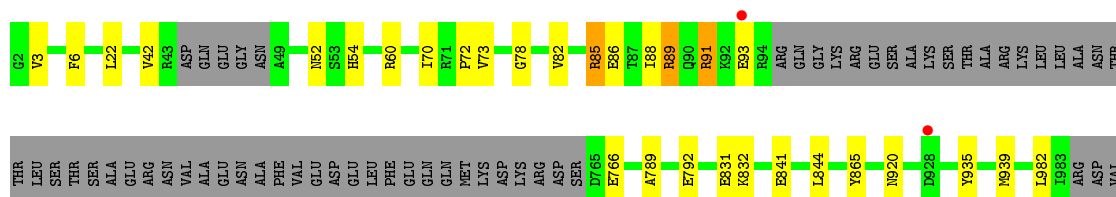
- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	K 1	0	0
5	A	1	Total 1	K 1	0	0
5	F	1	Total 1	K 1	0	0
5	E	1	Total 1	K 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	205	Total 205	O 205	0	0
6	B	184	Total 184	O 184	0	0
6	C	43	Total 43	O 43	0	0
6	D	25	Total 25	O 25	0	0
6	E	117	Total 117	O 117	0	0
6	F	198	Total 198	O 198	0	0
6	G	31	Total 31	O 31	0	0
6	H	20	Total 20	O 20	0	0

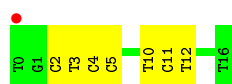




● Molecule 2: DNA (5'-D(\*TP\*GP\*CP\*TP\*CP\*CP\*CP\*TP\*TP\*GP\*TP\*CP\*TP\*CP\*AP\*GP\*T)-3')



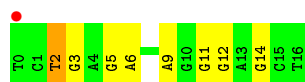
● Molecule 2: DNA (5'-D(\*TP\*GP\*CP\*TP\*CP\*CP\*CP\*TP\*TP\*GP\*TP\*CP\*TP\*CP\*AP\*GP\*T)-3')



● Molecule 3: DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*GP\*AP\*CP\*AP\*AP\*GP\*GP\*GP\*AP\*GP\*CP\*T)-3')



● Molecule 3: DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*GP\*AP\*CP\*AP\*AP\*GP\*GP\*GP\*AP\*GP\*CP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.28 Å   86.04 Å   134.44 Å 90.00°   110.95°   90.00°	Depositor
Resolution (Å)	34.33 – 2.40 39.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.33-2.40) 99.8 (39.70-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.39 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.178 , 0.235 0.176 , 0.234	Depositor DCC
$R_{free}$ test set	4603 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	5 of 92191 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0/2645	0.56	0/3575
1	B	0.40	0/2518	0.54	0/3405
1	E	0.38	0/2465	0.54	0/3339
1	F	0.39	0/2556	0.54	0/3453
2	C	0.61	0/750	1.19	0/1152
2	G	0.52	0/714	1.21	4/1098 (0.4%)
3	D	98.61	2/790 (0.3%)	1.22	4/1218 (0.3%)
3	H	0.53	0/754	1.03	2/1164 (0.2%)
All	All	24.14	2/13192 (0.0%)	0.75	10/18404 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	16[A]	DT	O5'-C5'	1959.87	50.41	1.42
3	D	16[B]	DT	O5'-C5'	1959.87	50.41	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	16[A]	DT	P-O5'-C5'	-11.07	103.18	120.90
3	D	16[B]	DT	P-O5'-C5'	-11.07	103.18	120.90
2	G	12[A]	DT	N3-C4-O4	5.74	123.34	119.90
2	G	12[B]	DT	N3-C4-O4	5.74	123.34	119.90
2	G	3[A]	DT	O4'-C1'-N1	-5.64	104.05	108.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2581	0	2514	16	0
1	B	2460	0	2401	10	0
1	E	2406	0	2317	17	0
1	F	2495	0	2452	12	0
2	C	660	0	352	6	0
2	G	644	0	339	7	0
3	D	686	0	350	5	0
3	H	670	0	338	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	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
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	205	0	0	1	0
6	B	184	0	0	0	0
6	C	43	0	0	1	0
6	D	25	0	0	0	0
6	E	117	0	0	3	0
6	F	198	0	0	1	0
6	G	31	0	0	0	0
6	H	20	0	0	1	0
All	All	13433	0	11063	73	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 3.

The worst 5 of 73 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)
3:D:2[B]:DT:H2'	3:D:3[B]:DG:C8	2.32	0.65
1:F:86:GLU:OE1	1:F:89:ARG:NH1	2.32	0.62
2:G:5[A]:DC:N4	3:H:11[A]:DG:O6	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5[B]:DC:N4	3:H:11[B]:DG:O6	2.36	0.58
2:G:4[A]:DC:N4	3:H:12[A]:DG:O6	2.37	0.57

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	321/365 (88%)	314 (98%)	7 (2%)	0	100	100
1	B	302/365 (83%)	293 (97%)	9 (3%)	0	100	100
1	E	296/365 (81%)	281 (95%)	14 (5%)	1 (0%)	46	63
1	F	303/365 (83%)	295 (97%)	8 (3%)	0	100	100
All	All	1222/1460 (84%)	1183 (97%)	38 (3%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	885	GLY

### 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	276/324 (85%)	267 (97%)	9 (3%)	45	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	263/324 (81%)	257 (98%)	6 (2%)	58	78
1	E	251/324 (78%)	241 (96%)	10 (4%)	38	58
1	F	270/324 (83%)	258 (96%)	12 (4%)	35	53
All	All	1060/1296 (82%)	1023 (96%)	37 (4%)	43	64

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	42	VAL
1	E	890	PHE
1	F	841	GLU
1	E	54	HIS
1	E	71	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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 ⓘ

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	322/365 (88%)	-0.07	3 (0%) 85 85	11, 23, 63, 98	0
1	B	307/365 (84%)	-0.36	0 100 100	10, 25, 52, 85	0
1	E	304/365 (83%)	-0.03	13 (4%) 39 40	18, 34, 72, 102	0
1	F	307/365 (84%)	-0.18	2 (0%) 89 88	12, 26, 56, 98	0
2	C	17/17 (100%)	-0.42	1 (5%) 26 26	17, 36, 46, 72	1 (5%)
2	G	17/17 (100%)	-0.32	1 (5%) 26 26	25, 38, 74, 80	0
3	D	17/17 (100%)	-0.35	1 (5%) 26 26	18, 34, 46, 72	1 (5%)
3	H	17/17 (100%)	-0.32	1 (5%) 26 26	25, 37, 74, 80	0
All	All	1308/1528 (85%)	-0.17	22 (1%) 73 72	10, 28, 63, 102	2 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	980	ILE	4.2
1	A	95	ARG	4.2
2	G	0[A]	DT	3.9
3	H	0[A]	DT	3.9
1	E	910	PHE	3.6

### 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	K	F	1002	1/1	0.87	0.11	0.15	65,65,65,65	0
5	K	A	1002	1/1	0.90	0.11	-0.30	54,54,54,54	0
4	CA	F	1001	1/1	0.97	0.11	-0.70	62,62,62,62	0
5	K	E	1002	1/1	0.93	0.10	-0.83	66,66,66,66	0
4	CA	B	1001	1/1	0.96	0.08	-1.64	56,56,56,56	0
4	CA	A	1001	1/1	0.95	0.08	-2.09	53,53,53,53	0
5	K	B	1002	1/1	0.95	0.07	-2.61	53,53,53,53	0
4	CA	E	1001	1/1	0.98	0.08	-3.66	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.