



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:21 am BST

PDB ID : 2F4Q
Title : Crystal Structure of Deinococcus radiodurans topoisomerase IB
Authors : Patel, A.; Shuman, S.; Mondragon, A.
Deposited on : 2005-11-23
Resolution : 1.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

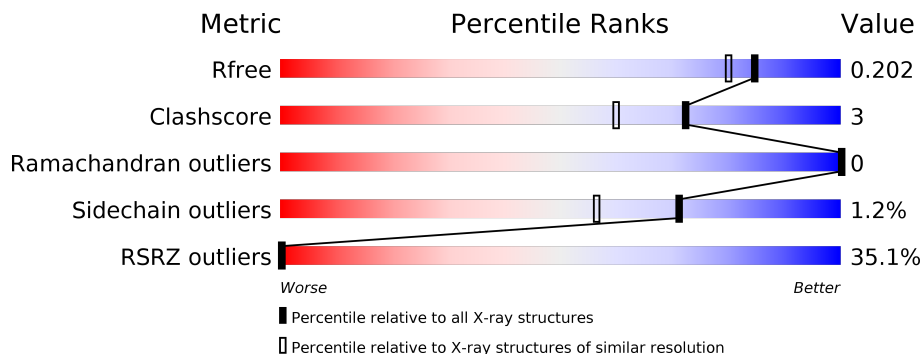
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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 $\leq 5\%$. 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	346	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2849 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 type I topoisomerase, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	309	2507	1581	464	456	2	4	0	12	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	GB 15805717
A	124	MSE	MET	MODIFIED RESIDUE	GB 15805717
A	127	MSE	MET	MODIFIED RESIDUE	GB 15805717
A	192	MSE	MET	MODIFIED RESIDUE	GB 15805717
A	331	MSE	MET	MODIFIED RESIDUE	GB 15805717

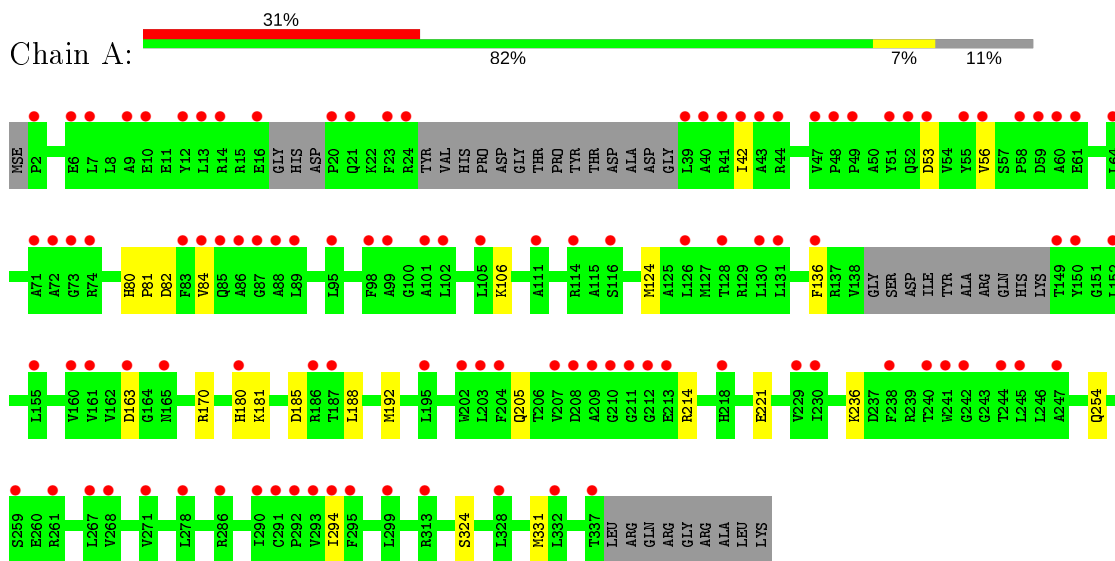
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	341	Total	O	0	1
			342	342		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: type I topoisomerase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.09Å 64.97Å 76.62Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	27.50 – 1.75 27.43 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.5 (27.50-1.75) 96.5 (27.43-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.231 0.198 , 0.202	Depositor DCC
R_{free} test set	1790 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2849	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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	0.38	0/2599	0.52	0/3500

There are no bond length outliers.

There are no bond angle outliers.

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	2507	0	2529	17	0
2	A	342	0	0	3	0
All	All	2849	0	2529	17	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.

All (17) 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:236:LYS:HG3	2:A:682:HOH:O	1.78	0.84
1:A:205:GLN:HE22	1:A:214:ARG:HH11	1.31	0.77
1:A:80:HIS:HD2	1:A:82:ASP:H	1.35	0.73
1:A:136:PHE:CE1	1:A:181:LYS:HG3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HH11	1:A:180[A]:HIS:CD2	2.19	0.60
1:A:254:GLN:HG2	2:A:449:HOH:O	2.02	0.60
1:A:170:ARG:HH11	1:A:180[A]:HIS:HD2	1.53	0.55
1:A:106:LYS:HG3	2:A:409:HOH:O	2.05	0.55
1:A:205:GLN:NE2	1:A:214:ARG:HH11	2.04	0.53
1:A:294[B]:ILE:HG13	1:A:331:MSE:SE	2.59	0.52
1:A:188:LEU:O	1:A:192:MSE:HG2	2.10	0.52
1:A:42:ILE:HG23	1:A:56:VAL:HG11	1.93	0.50
1:A:205:GLN:HE22	1:A:214:ARG:NH1	2.06	0.49
1:A:185:ASP:HB3	1:A:188:LEU:HB3	1.95	0.48
1:A:81:PRO:HA	1:A:84:VAL:HG22	1.96	0.47
1:A:124:MSE:SE	1:A:221:GLU:HG2	2.70	0.42
1:A:170:ARG:HG2	1:A:180[A]:HIS:HD2	1.84	0.42

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	313/346 (90%)	311 (99%)	2 (1%)	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	267/279 (96%)	263 (98%)	4 (2%)	65 49

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	163	ASP
1	A	324[A]	SER
1	A	324[B]	SER

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	80	HIS
1	A	205	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

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, 95th 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 ²)	Q<0.9
1	A	305/346 (88%)	1.81	107 (35%) 0 0	27, 34, 42, 53	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	ALA	10.3
1	A	84	VAL	9.6
1	A	23	PHE	8.6
1	A	210	GLY	8.1
1	A	85	GLN	6.9
1	A	40	ALA	6.1
1	A	337	THR	5.9
1	A	186	ARG	5.9
1	A	10	GLU	5.7
1	A	16	GLU	5.7
1	A	43	ALA	5.7
1	A	58	PRO	5.7
1	A	13	LEU	5.4
1	A	241	TRP	5.1
1	A	294[A]	ILE	5.0
1	A	20	PRO	4.9
1	A	14	ARG	4.8
1	A	290	ILE	4.7
1	A	98	PHE	4.7
1	A	52	GLN	4.6
1	A	126	LEU	4.5
1	A	209	ALA	4.4
1	A	87	GLY	4.4
1	A	39	LEU	4.4
1	A	88	ALA	4.4
1	A	295	PHE	4.3
1	A	102	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	61	GLU	4.1
1	A	53	ASP	4.0
1	A	7	LEU	3.9
1	A	261	ARG	3.9
1	A	12	TYR	3.9
1	A	2	PRO	3.9
1	A	59	ASP	3.9
1	A	267	LEU	3.9
1	A	208	ASP	3.8
1	A	203	LEU	3.8
1	A	74	ARG	3.7
1	A	24	ARG	3.6
1	A	72	ALA	3.6
1	A	187	THR	3.6
1	A	116	SER	3.6
1	A	105	LEU	3.6
1	A	238	PHE	3.5
1	A	293	VAL	3.4
1	A	83	PHE	3.4
1	A	95	LEU	3.4
1	A	48	PRO	3.3
1	A	150	TYR	3.3
1	A	152	LEU	3.3
1	A	130	LEU	3.2
1	A	313	ARG	3.1
1	A	291	CYS	3.1
1	A	211	GLY	3.1
1	A	101	ALA	3.1
1	A	244	THR	3.1
1	A	49	PRO	3.1
1	A	180[A]	HIS	3.0
1	A	64	LEU	3.0
1	A	155	LEU	3.0
1	A	160	VAL	3.0
1	A	292	PRO	2.9
1	A	204	PHE	2.9
1	A	161	VAL	2.9
1	A	42	ILE	2.9
1	A	230	ILE	2.9
1	A	195	LEU	2.8
1	A	60	ALA	2.8
1	A	242	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	71	ALA	2.8
1	A	131	LEU	2.8
1	A	99	ALA	2.7
1	A	259	SER	2.7
1	A	9	ALA	2.7
1	A	332	LEU	2.7
1	A	218	HIS	2.7
1	A	240	THR	2.7
1	A	245	LEU	2.7
1	A	299	LEU	2.7
1	A	41	ARG	2.7
1	A	21	GLN	2.6
1	A	128	THR	2.6
1	A	202	TRP	2.6
1	A	51	TYR	2.6
1	A	247	ALA	2.6
1	A	165	ASN	2.6
1	A	212	GLY	2.6
1	A	328	LEU	2.6
1	A	213	GLU	2.5
1	A	271	VAL	2.5
1	A	114	ARG	2.5
1	A	278	LEU	2.5
1	A	89	LEU	2.4
1	A	44	ARG	2.4
1	A	73	GLY	2.4
1	A	229	VAL	2.4
1	A	207	VAL	2.3
1	A	163	ASP	2.3
1	A	149	THR	2.2
1	A	111	ALA	2.2
1	A	6	GLU	2.2
1	A	136	PHE	2.1
1	A	56	VAL	2.1
1	A	268	VAL	2.0
1	A	286	ARG	2.0
1	A	55	TYR	2.0
1	A	47	VAL	2.0

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 [i](#)

There are no carbohydrates 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.