



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:02 AM UTC

PDB ID : 6CA8 / pdb_00006ca8
Title : Crystal structure of Plasmodium falciparum topoisomerase II DNA-binding, cleavage and re-ligation domain
Authors : Kumar, S.; Kandavelu, P.; Rathod, P.K.
Deposited on : 2018-01-29
Resolution : 2.33 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

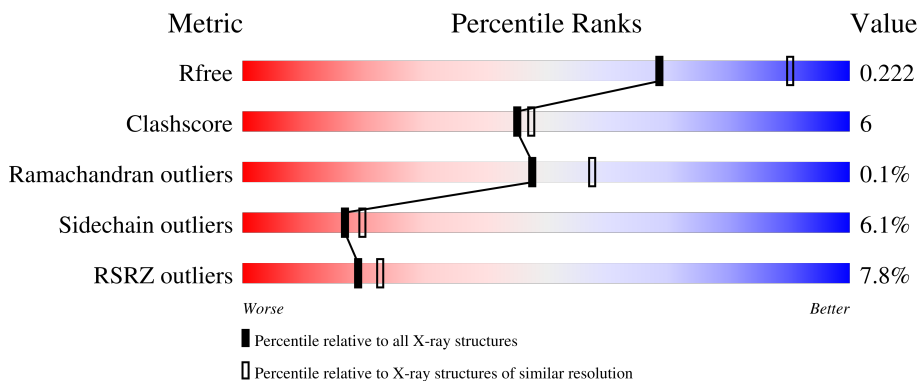
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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 $\leq 5\%$. 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	751	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6462 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 DNA topoisomerase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	731	5926	3800	977	1127	22	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	468	MET	-	initiating methionine	UNP Q7Z2D0
A	1213	HIS	-	expression tag	UNP Q7Z2D0
A	1214	HIS	-	expression tag	UNP Q7Z2D0
A	1215	HIS	-	expression tag	UNP Q7Z2D0
A	1216	HIS	-	expression tag	UNP Q7Z2D0
A	1217	HIS	-	expression tag	UNP Q7Z2D0
A	1218	HIS	-	expression tag	UNP Q7Z2D0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	536	Total	O	0	0
			536	536		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.03Å 104.48Å 114.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.22 – 2.33 44.22 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.22-2.33) 98.0 (44.22-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.188 , 0.223 0.190 , 0.222	Depositor DCC
R_{free} test set	2135 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtrriage
Anisotropy	0.463	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6462	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.40	0/6042	0.87	6/8141 (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	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	881	GLY	N-CA-C	-6.07	103.81	112.55
1	A	556	ILE	N-CA-C	6.00	116.74	110.62
1	A	1157	LEU	N-CA-C	5.51	116.97	111.07
1	A	643	GLY	N-CA-C	5.49	123.01	115.27
1	A	777	GLU	N-CA-C	5.30	117.13	111.36
1	A	724	ASN	N-CA-C	5.07	116.88	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1136	ILE	Peptide
1	A	642	LEU	Peptide

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	5926	0	5853	69	0
2	A	536	0	0	5	0
All	All	6462	0	5853	69	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 6.

All (69) 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:1066:LYS:NZ	1:A:1171:GLU:OE1	1.94	0.99
1:A:1165:THR:HA	1:A:1168:LYS:NZ	1.92	0.84
1:A:642:LEU:H	1:A:644:TRP:HD1	1.33	0.76
1:A:924:GLU:OE2	2:A:1301:HOH:O	2.03	0.76
1:A:939:LYS:HD2	1:A:1002:GLU:OE2	1.89	0.72
1:A:1165:THR:HA	1:A:1168:LYS:HZ3	1.56	0.69
1:A:633:GLU:O	1:A:637:GLU:HG2	1.94	0.68
1:A:561:LYS:NZ	1:A:565:LYS:O	2.17	0.67
1:A:994:ASP:HB3	1:A:997:LYS:HB2	1.76	0.66
1:A:539:LEU:HD21	1:A:596:PHE:CZ	2.31	0.65
1:A:1165:THR:HA	1:A:1168:LYS:HZ2	1.60	0.65
1:A:677:THR:N	1:A:681:ASP:OD2	2.25	0.64
1:A:790:GLN:NE2	2:A:1306:HOH:O	2.30	0.64
1:A:680:ARG:NH2	2:A:1307:HOH:O	2.31	0.62
1:A:642:LEU:H	1:A:644:TRP:CD1	2.19	0.60
1:A:539:LEU:HD21	1:A:596:PHE:HZ	1.69	0.57
1:A:1149:SER:OG	2:A:1302:HOH:O	2.17	0.57
1:A:1067:ARG:HD3	1:A:1109:ILE:HG23	1.87	0.56
1:A:600:LEU:HD13	1:A:606:PHE:CZ	2.40	0.56
1:A:1151:PRO:O	1:A:1154:SER:OG	2.20	0.56
1:A:554:LEU:HD22	1:A:597:TRP:CE2	2.41	0.56
1:A:1085:ILE:O	1:A:1089:LYS:NZ	2.32	0.55
1:A:852:TYR:HA	1:A:862:PRO:HA	1.89	0.55
1:A:1052:GLU:HG3	1:A:1182:VAL:HG11	1.88	0.55
1:A:1135:ILE:HG22	1:A:1136:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:GLU:OE1	1:A:1138:GLY:HA2	2.07	0.54
1:A:483:ASN:HB2	1:A:517:ASP:HA	1.88	0.54
1:A:556:ILE:H	1:A:556:ILE:HD12	1.73	0.54
1:A:473:ILE:HG21	1:A:476:ILE:HD12	1.90	0.53
1:A:626:PHE:HD1	1:A:631:GLU:HG2	1.72	0.53
1:A:602:LYS:HE3	1:A:676:TRP:NE1	2.23	0.53
1:A:700:TRP:CE2	1:A:728:ILE:HD12	2.43	0.53
1:A:804:ASN:ND2	1:A:890:ASN:HB3	2.25	0.52
1:A:819:GLU:O	1:A:822:LYS:HE3	2.11	0.50
1:A:1130:GLU:O	1:A:1131:ASP:HB2	2.10	0.50
1:A:943:ASP:OD1	1:A:995:PRO:HG3	2.12	0.50
1:A:561:LYS:O	1:A:599:SER:OG	2.28	0.49
1:A:549:PHE:CE1	1:A:597:TRP:HH2	2.31	0.49
1:A:1136:ILE:O	1:A:1139:ILE:HB	2.13	0.48
1:A:1165:THR:O	1:A:1168:LYS:HG3	2.13	0.48
1:A:614:ILE:HG23	1:A:615:VAL:HG23	1.95	0.48
1:A:480:GLU:OE2	1:A:504:LYS:HE3	2.15	0.47
1:A:1180:ILE:HD13	1:A:1185:MET:HG3	1.97	0.46
1:A:554:LEU:HD22	1:A:597:TRP:CD2	2.51	0.46
1:A:898:ASP:HB3	1:A:902:ARG:NH1	2.31	0.46
1:A:544:GLU:O	1:A:548:ILE:HG13	2.16	0.45
1:A:473:ILE:HD11	1:A:568:ARG:CZ	2.47	0.45
1:A:859:LYS:HB2	1:A:1118:PHE:CG	2.53	0.44
1:A:1154:SER:HA	1:A:1159:LYS:HG2	1.98	0.44
1:A:822:LYS:NZ	2:A:1329:HOH:O	2.50	0.44
1:A:496:ILE:HG12	1:A:573:MET:HE2	2.00	0.43
1:A:642:LEU:N	1:A:644:TRP:HD1	2.10	0.43
1:A:531:VAL:HG21	1:A:592:MET:HA	2.00	0.43
1:A:658:ARG:O	1:A:662:GLN:HG3	2.18	0.43
1:A:940:ILE:HD11	1:A:946:GLU:HG2	2.00	0.43
1:A:772:VAL:HG13	1:A:788:LEU:HD23	2.01	0.42
1:A:839:ARG:HD3	1:A:839:ARG:HA	1.93	0.42
1:A:514:VAL:HG11	1:A:519:TYR:CD2	2.54	0.42
1:A:572:LEU:HB3	1:A:607:LEU:HD12	2.00	0.42
1:A:484:ASP:OD2	1:A:518:LYS:NZ	2.48	0.42
1:A:888:ILE:HA	1:A:889:PRO:HD3	1.90	0.42
1:A:1135:ILE:O	1:A:1136:ILE:HB	2.20	0.42
1:A:752:LYS:HB3	1:A:779:SER:HB3	2.01	0.41
1:A:687:MET:HE3	1:A:687:MET:HB3	1.74	0.41
1:A:1047:ARG:O	1:A:1047:ARG:HD2	2.20	0.41
1:A:1130:GLU:CB	1:A:1141:VAL:HG11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:MET:O	1:A:697:ARG:NH1	2.53	0.41
1:A:530:ASN:OD1	1:A:591:ASN:ND2	2.54	0.40
1:A:1139:ILE:HG21	1:A:1144:TYR:HE2	1.86	0.40

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	725/751 (96%)	704 (97%)	20 (3%)	1 (0%)	48 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1136	ILE

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	642/685 (94%)	603 (94%)	39 (6%)	17 20

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	GLU
1	A	472	ARG
1	A	474	ILE
1	A	514	VAL
1	A	528	LEU
1	A	539	LEU
1	A	544	GLU
1	A	578	GLN
1	A	618	GLN
1	A	628	THR
1	A	629	ILE
1	A	646	ILE
1	A	684	SER
1	A	699	LEU
1	A	738	SER
1	A	763	ARG
1	A	828	ARG
1	A	880	ILE
1	A	882	THR
1	A	909	LEU
1	A	920	LYS
1	A	924	GLU
1	A	954	LYS
1	A	960	LYS
1	A	965	GLU
1	A	967	LEU
1	A	969	ASP
1	A	997	LYS
1	A	1040	LEU
1	A	1047	ARG
1	A	1056	SER
1	A	1064	LYS
1	A	1080	VAL
1	A	1109	ILE
1	A	1117	ILE
1	A	1154	SER
1	A	1168	LYS
1	A	1169	GLU
1	A	1175	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	790	GLN
1	A	938	ASN
1	A	1087	ASN

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 oligosaccharides 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, 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	731/751 (97%)	0.24	57 (7%) 19 23	12, 29, 62, 82	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	GLU	4.8
1	A	470	ARG	4.7
1	A	1137	ALA	4.5
1	A	641	LEU	4.4
1	A	882	THR	4.3
1	A	556	ILE	4.0
1	A	555	ASP	3.8
1	A	474	ILE	3.8
1	A	707	GLY	3.8
1	A	881	GLY	3.7
1	A	622	GLN	3.7
1	A	472	ARG	3.6
1	A	1115	GLU	3.6
1	A	560	ASN	3.5
1	A	1210	GLU	3.4
1	A	1130	GLU	3.4
1	A	562	ASP	3.4
1	A	620	GLY	3.4
1	A	642	LEU	3.3
1	A	563	ASP	3.3
1	A	1117	ILE	3.3
1	A	1122	LEU	3.2
1	A	618	GLN	3.1
1	A	1136	ILE	3.1
1	A	564	ILE	3.1
1	A	880	ILE	3.0
1	A	1168	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1131	ASP	3.0
1	A	644	TRP	3.0
1	A	643	GLY	2.9
1	A	706	LEU	2.9
1	A	1134	GLU	2.9
1	A	557	THR	2.8
1	A	602	LYS	2.8
1	A	566	GLY	2.8
1	A	621	SER	2.8
1	A	640	ASN	2.7
1	A	969	ASP	2.7
1	A	1167	LEU	2.7
1	A	1138	GLY	2.6
1	A	1133	GLU	2.5
1	A	558	ASP	2.5
1	A	1111	LYS	2.4
1	A	624	TYR	2.3
1	A	673	MET	2.3
1	A	1169	GLU	2.3
1	A	559	LYS	2.3
1	A	898	ASP	2.2
1	A	1047	ARG	2.2
1	A	712	HIS	2.2
1	A	554	LEU	2.2
1	A	1099	TYR	2.2
1	A	635	TRP	2.2
1	A	1132	ASN	2.2
1	A	972	HIS	2.1
1	A	973	GLN	2.0
1	A	629	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.