



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2016 – 06:08 PM EDT

PDB ID : 5IJL  
Title : D-family DNA polymerase - DP2 subunit (catalytic subunit)  
Authors : Sauguet, L.; Raia, P.; De Larue, M.  
Deposited on : 2016-03-02  
Resolution : 2.19 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](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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

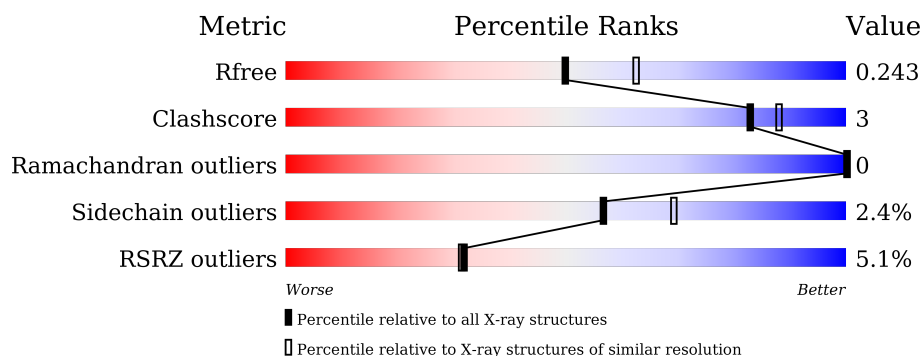
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	1066	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7769 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 polymerase II large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	943	7525	4844	1266	1388	27	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9V2F4
A	-3	THR	-	expression tag	UNP Q9V2F4
A	-2	GLY	-	expression tag	UNP Q9V2F4
A	-1	ASP	-	expression tag	UNP Q9V2F4
A	0	GLY	-	expression tag	UNP Q9V2F4
A	1	SER	-	expression tag	UNP Q9V2F4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

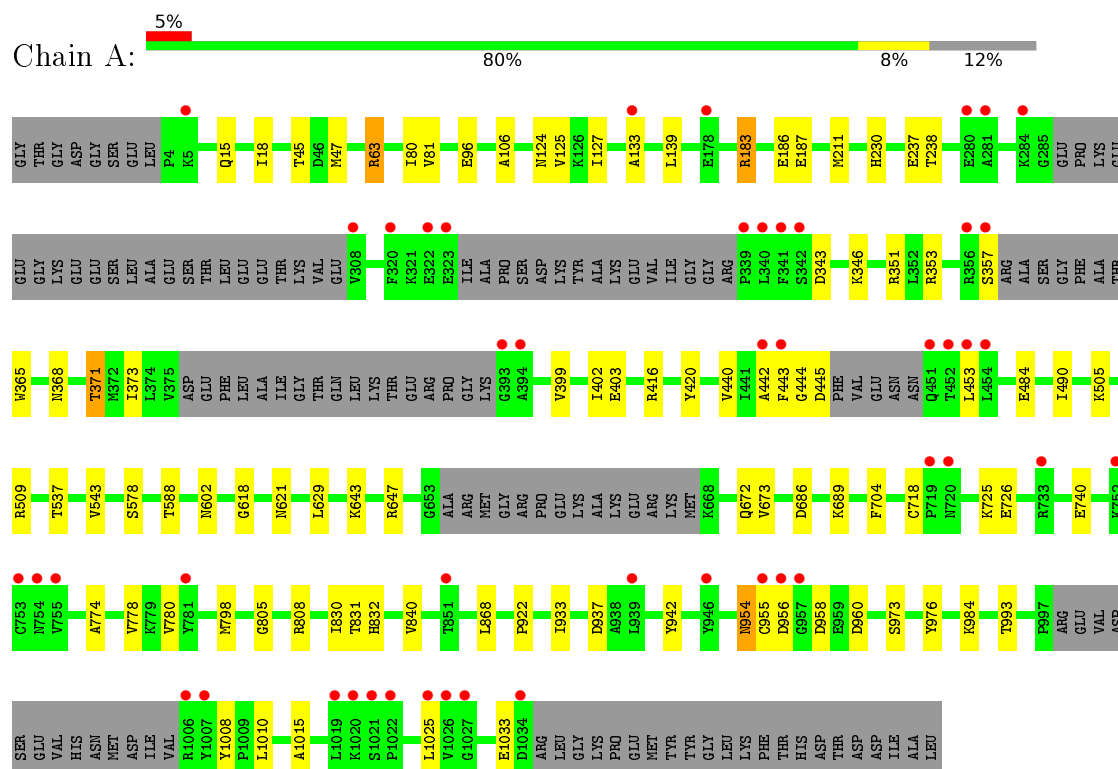
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	242	Total	O	0	0
			242	242		

### 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 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.

- Molecule 1: DNA polymerase II large subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.82Å 106.20Å 110.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.80 – 2.19 49.15 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.80-2.19) 98.9 (49.15-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.199 , 0.235 0.205 , 0.243	Depositor DCC
$R_{free}$ test set	3165 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.53	0/7695	0.69	3/10408 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	955	CYS	C-N-CA	7.32	140.00	121.70
1	A	133	ALA	N-CA-C	6.46	128.46	111.00
1	A	444	GLY	N-CA-C	-5.91	98.32	113.10

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	7525	0	7562	46	0
2	A	2	0	0	0	0
3	A	242	0	0	3	0
All	All	7769	0	7562	46	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 (46) 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:183:ARG:NH2	1:A:238:THR:O	2.12	0.81
1:A:357:SER:OG	1:A:442:ALA:HB2	1.85	0.77
1:A:831:THR:HG23	1:A:832:HIS:ND1	2.04	0.72
1:A:96:GLU:HG3	1:A:127:ILE:HG12	1.74	0.69
1:A:183:ARG:NH1	1:A:187:GLU:OE2	2.29	0.65
1:A:186:GLU:OE1	1:A:230:HIS:HD2	1.82	0.63
1:A:830:ILE:HG12	1:A:942:TYR:HB3	1.81	0.63
1:A:373:ILE:HD11	1:A:420:TYR:CD2	2.35	0.61
1:A:673:VAL:HB	1:A:805:GLY:HA3	1.84	0.59
1:A:371:THR:HG21	3:A:1237:HOH:O	2.04	0.57
1:A:778:VAL:HG23	1:A:780:VAL:HG22	1.87	0.57
1:A:443:PHE:HB3	1:A:1008:TYR:OH	2.06	0.56
1:A:484:GLU:HG3	1:A:509:ARG:HH21	1.72	0.55
1:A:357:SER:OG	1:A:442:ALA:CB	2.54	0.54
1:A:954:ASN:C	1:A:956:ASP:H	2.08	0.54
1:A:647:ARG:O	1:A:647:ARG:HG2	2.07	0.54
1:A:351:ARG:HD2	1:A:647:ARG:O	2.09	0.53
1:A:81:VAL:HG23	1:A:106:ALA:HB2	1.91	0.52
1:A:726:GLU:HG2	1:A:740:GLU:HB2	1.92	0.52
1:A:403:GLU:HG2	1:A:416:ARG:HH22	1.73	0.52
1:A:343:ASP:HB3	1:A:346:LYS:HB2	1.92	0.51
1:A:922:PRO:HB3	1:A:984:LYS:HG2	1.91	0.51
1:A:63:ARG:HB3	1:A:80:ILE:HD11	1.94	0.47
1:A:211:MET:HE1	3:A:1227:HOH:O	2.15	0.47
1:A:840:VAL:HG21	1:A:933:ILE:O	2.15	0.46
1:A:402:ILE:HD13	1:A:440:VAL:HG23	1.98	0.46
1:A:537:THR:O	1:A:647:ARG:HD2	2.17	0.45
1:A:830:ILE:HG13	1:A:868:LEU:HD22	1.99	0.45
1:A:973:SER:HB3	1:A:976:TYR:CD2	2.52	0.45
1:A:490:ILE:HG21	1:A:505:LYS:HG3	1.98	0.44
1:A:1015:ALA:HB3	1:A:1025:LEU:HD21	1.99	0.44
1:A:371:THR:CG2	3:A:1237:HOH:O	2.65	0.44
1:A:543:VAL:HG11	1:A:588:THR:HG23	1.99	0.44
1:A:353:ARG:O	1:A:440:VAL:HA	2.19	0.43
1:A:673:VAL:HB	1:A:805:GLY:CA	2.48	0.42
1:A:368:ASN:HA	1:A:399:VAL:O	2.19	0.42
1:A:686:ASP:HB3	1:A:689:LYS:HB2	2.01	0.42
1:A:672:GLN:O	1:A:808:ARG:HD2	2.20	0.41
1:A:125:VAL:CG1	1:A:139:LEU:HD11	2.51	0.41
1:A:18:ILE:HD13	1:A:993:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG12	1:A:139:LEU:HD11	2.03	0.41
1:A:578:SER:HA	1:A:602:ASN:HD22	1.85	0.41
1:A:704:PHE:HZ	1:A:798:MET:HG3	1.86	0.41
1:A:774:ALA:O	1:A:778:VAL:HG22	2.21	0.41
1:A:618:GLY:O	1:A:621:ASN:HB2	2.20	0.40
1:A:718:CYS:HA	1:A:725:LYS:HD2	2.03	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	928/1066 (87%)	902 (97%)	26 (3%)	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	801/907 (88%)	782 (98%)	19 (2%)	57	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	45	THR
1	A	47	MET
1	A	63	ARG
1	A	124	ASN
1	A	183	ARG
1	A	237	GLU
1	A	365	TRP
1	A	371	THR
1	A	445	ASP
1	A	453	LEU
1	A	629	LEU
1	A	643	LYS
1	A	937	ASP
1	A	954	ASN
1	A	958	ASP
1	A	960	ASP
1	A	1010	LEU
1	A	1033	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	43	GLN
1	A	124	ASN
1	A	180	HIS
1	A	230	HIS
1	A	421	ASN
1	A	602	ASN
1	A	711	HIS
1	A	747	ASN
1	A	852	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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, 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	943/1066 (88%)	0.23	48 (5%)	32 31	31, 49, 83, 119	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	VAL	8.9
1	A	956	ASP	7.9
1	A	320	PHE	7.0
1	A	1019	LEU	6.9
1	A	452	THR	5.0
1	A	451	GLN	4.9
1	A	284	LYS	4.4
1	A	340	LEU	4.4
1	A	955	CYS	4.3
1	A	1022	PRO	4.3
1	A	357	SER	4.2
1	A	394	ALA	4.1
1	A	946	TYR	4.0
1	A	453	LEU	4.0
1	A	393	GLY	4.0
1	A	753	CYS	3.9
1	A	733	ARG	3.9
1	A	1021	SER	3.9
1	A	720	ASN	3.8
1	A	781	TYR	3.7
1	A	322	GLU	3.6
1	A	755	VAL	3.6
1	A	752	LYS	3.4
1	A	443	PHE	3.3
1	A	341	PHE	3.3
1	A	754	ASN	3.1
1	A	1020	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	3.0
1	A	957	GLY	2.9
1	A	323	GLU	2.9
1	A	851	THR	2.8
1	A	1034	ASP	2.8
1	A	1006	ARG	2.8
1	A	719	PRO	2.8
1	A	133	ALA	2.8
1	A	1025	LEU	2.6
1	A	356	ARG	2.5
1	A	178	GLU	2.5
1	A	442	ALA	2.5
1	A	5	LYS	2.4
1	A	339	PRO	2.4
1	A	280	GLU	2.3
1	A	939	LEU	2.3
1	A	342	SER	2.3
1	A	1027	GLY	2.3
1	A	1007	TYR	2.2
1	A	454	LEU	2.1
1	A	1026	VAL	2.1

## 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 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(Å <sup>2</sup> )	Q<0.9
2	ZN	A	1102	1/1	0.91	0.04	-1.64	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	1101	1/1	0.99	0.03	-1.71	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.