



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2016 – 06:09 PM EDT

PDB ID : 5J0P
Title : Binary complex crystal structure of DNA polymerase Beta with A:C mismatch at the primer terminus
Authors : Batra, V.K.; Wilson, S.H.
Deposited on : 2016-03-28
Resolution : 2.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
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-20028320

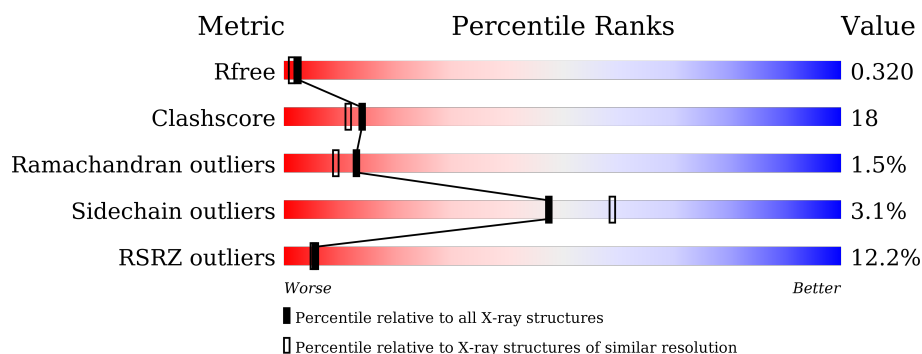
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 ≥ 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	335	<div> <div>13%</div> <div>65%</div> <div>31%</div> <div>..</div> </div>
2	T	16	<div> <div>75%</div> <div>25%</div> </div>
3	P	10	<div> <div>10%</div> <div>50%</div> <div>50%</div> </div>
4	D	5	<div> <div>60%</div> <div>40%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3533 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 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2640	1667	461	503	9			

- Molecule 2 is a DNA chain called Template Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	16	Total	C	N	O	P	0	0	0
			321	153	63	90	15			

- Molecule 3 is a DNA chain called Primer Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

- Molecule 4 is a DNA chain called Downstream Primer Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	P	0	0	0
			106	49	20	32	5			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	181	Total	O	0	0
			181	181		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	46	Total 46	O 46	0	0
6	P	21	Total 21	O 21	0	0
6	D	13	Total 13	O 13	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.14Å 79.62Å 54.57Å 90.00° 105.55° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 20.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	81.2 (50.00-2.20) 81.4 (20.88-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.320 0.253 , 0.320	Depositor DCC
R_{free} test set	1823 reflections (9.87%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.056 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3533	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% 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](#)

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

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	0.36	0/2690	0.57	0/3617
2	T	0.42	0/360	0.84	0/552
3	P	0.49	0/227	0.76	0/349
4	D	0.91	1/118 (0.8%)	0.87	0/179
All	All	0.41	1/3395 (0.0%)	0.64	0/4697

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
4	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	DG	OP3-P	-7.24	1.52	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	2	DT	Sidechain

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	2640	0	2650	104	0
2	T	321	0	179	5	0
3	P	203	0	114	8	0
4	D	106	0	57	0	0
5	A	2	0	0	0	0
6	A	181	0	0	7	0
6	D	13	0	0	0	0
6	P	21	0	0	2	0
6	T	46	0	0	1	0
All	All	3533	0	3000	115	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 18.

The worst 5 of 115 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:HH12	1:A:275:SER:HB3	1.32	0.94
1:A:209:LYS:HA	1:A:212:HIS:HB3	1.51	0.90
1:A:209:LYS:HG2	1:A:213:GLN:HG3	1.56	0.88
1:A:201:THR:H	1:A:204:SER:HB3	1.38	0.87
3:P:10:DC:H2"	6:P:111:HOH:O	1.82	0.77

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	328/335 (98%)	289 (88%)	34 (10%)	5 (2%)	13 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	LYS
1	A	265	TYR
1	A	130	ASP
1	A	207	GLN
1	A	208	PRO

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
1	A	289/295 (98%)	280 (97%)	9 (3%)	47 59

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	GLU
1	A	327	TYR
1	A	267	CYS
1	A	48	LYS
1	A	258	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	A	217	GLN
1	A	252	HIS
1	A	207	GLN
1	A	245	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	330/335 (98%)	0.76	43 (13%) 5 4	18, 42, 80, 94	0
2	T	16/16 (100%)	0.23	0 100 100	26, 41, 64, 65	0
3	P	10/10 (100%)	0.40	1 (10%) 9 8	23, 32, 50, 64	0
4	D	5/5 (100%)	-0.30	0 100 100	25, 26, 37, 39	0
All	All	361/366 (98%)	0.71	44 (12%) 5 5	18, 42, 79, 94	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	ALA	7.6
1	A	287	LEU	7.0
1	A	246	ASP	7.0
1	A	205	THR	6.1
1	A	208	PRO	6.0

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 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, 95th 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(\AA^2)	Q<0.9
5	NA	A	402	1/1	0.93	0.16	0.27	44,44,44,44	0
5	NA	A	401	1/1	0.96	0.17	0.07	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.