

# wwPDB X-ray Structure Validation Summary Report (i)

#### Jul 31, 2023 – 01:14 AM EDT

:	1NOM
:	DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7), 31-KD DOMAIN;
	SOAKED IN THE PRESENCE OF MNCL2 (5 MILLIMOLAR)
:	Pelletier, H.; Sawaya, M.R.
	1996-04-19
:	3.00  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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

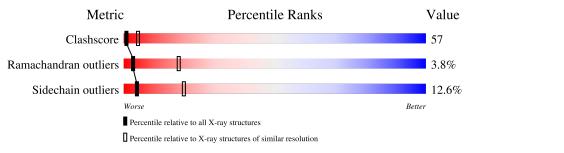
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)		
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.34

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.00 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Mol	Chain	Length	Quality of chain					
1	А	248	29%	47%	18%	•••		



#### 1NOM

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2046 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	А	242	Total	C 1991	N 242	0	S °	4	1	0
			1939	1221	343	367	0			

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	А	1	Total 1	Mn 1	0	0

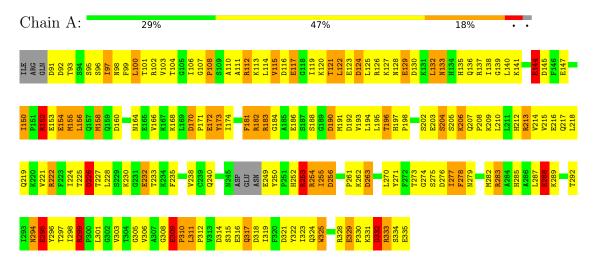
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	106	Total O 106 106	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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 BETA



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	120.18Å $62.88$ Å $38.29$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	20.00 - 3.00	Depositor
Resolution (A)	43.44 – $2.60$	EDS
% Data completeness	97.0 (20.00-3.00)	Depositor
(in resolution range)	87.8 (43.44 - 2.60)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$< I/\sigma(I) > 1$	$1.68 (at 2.61 \text{\AA})$	Xtriage
Refinement program	TNT 5-D	Depositor
$R, R_{free}$	(Not available) , (Not available)	Depositor
II, II, <i>free</i>	0.172 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	28.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.30 , $189.4$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2046	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MN

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		Bo	nd lengths	Bond angles		
Mol Cha	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.12	17/1977~(0.9%)	1.71	44/2666~(1.7%)	

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	154	GLU	CD-OE1	6.69	1.33	1.25
1	А	203	GLU	CD-OE1	6.40	1.32	1.25
1	А	144	GLU	CD-OE1	6.22	1.32	1.25
1	А	117	GLU	CD-OE1	6.13	1.32	1.25
1	А	309	GLU	CD-OE1	5.99	1.32	1.25

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	182	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	А	263	ASP	CB-CG-OD1	-9.07	110.14	118.30
1	А	190	ASP	CB-CG-OD2	-8.79	110.38	118.30
1	А	253	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	А	145	ASP	CB-CG-OD1	-8.44	110.70	118.30

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	А	1939	0	1875	218	0
2	А	1	0	0	0	0
3	А	106	0	0	11	2
All	All	2046	0	1875	218	2

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 57.

The worst 5 of 218 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:317:GLN:H	1:A:317:GLN:NE2	1.42	1.18
1:A:158:MET:HB2	1:A:191:MET:HE3	1.31	1.08
1:A:317:GLN:HE21	1:A:317:GLN:N	1.56	1.03
1:A:103:VAL:HB	1:A:106:ILE:HD13	1.38	1.02
1:A:294:ASN:HD22	1:A:296:TYR:H	1.02	0.93

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:468:HOH:O	3:A:468:HOH:O[2_565]	0.71	1.49
3:A:502:HOH:O	3:A:502:HOH:O[2_555]	1.73	0.47

## 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	А	239/248~(96%)	197 (82%)	33 (14%)	9~(4%)	3 18

5 of 9 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	204	SER
1	А	206	LYS
1	А	309	GLU
1	А	306	VAL
1	А	108	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	207/226~(92%)	180 (87%)	27~(13%)	4 19

5 of 27 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	226	ASP
1	А	277	ILE
1	А	317	GLN
1	А	255	ILE
1	А	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	252	HIS
1	А	281	ASN
1	А	317	GLN
1	А	285	HIS
1	А	157	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

