



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 05:37 PM BST

PDB ID : 6MP3  
Title : Binary structure of DNA polymerase eta in complex with templating hypoxanthine  
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Deposited on : 2018-10-05  
Resolution : 1.91 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

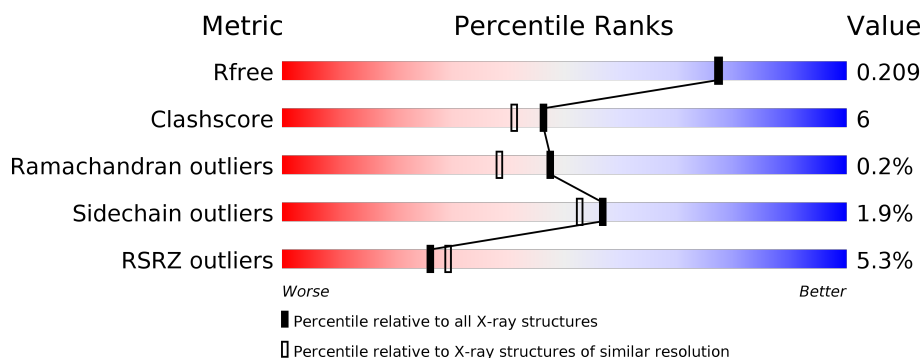
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	435	<div> <div>6%</div> <div>89%</div> <div>8%</div> <div>••</div> </div>
2	T	12	<div> <div>50%</div> <div>42%</div> <div>8%</div> </div>
3	P	8	<div> <div>63%</div> <div>38%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7963 atoms, of which 3759 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 eta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	430	Total	C	H	N	O	S	11	22	0
			7003	2166	3544	623	640	30			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9Y253
A	-1	PRO	-	expression tag	UNP Q9Y253
A	0	HIS	-	expression tag	UNP Q9Y253

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*AP\*TP\*IP\*AP\*TP\*GP\*AP\*CP\*GP\*CP\*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	T	12	Total	C	H	N	O	P	0	0	1
			350	108	123	41	67	11			

- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*GP\*CP\*GP\*TP\*CP\*AP\*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	P	8	Total	C	H	N	O	P	0	0	0
			253	78	92	30	46	7			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

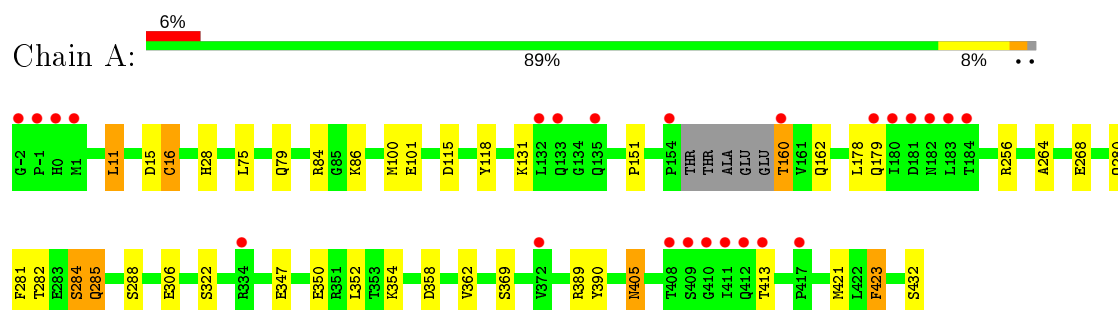
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	299	Total 299	O 299	0	0
5	T	27	Total 27	O 27	0	0
5	P	29	Total 29	O 29	0	0

### 3 Residue-property plots

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 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 eta



- Molecule 2: DNA (5'-D(\*CP\*AP\*TP\*IP\*AP\*TP\*GP\*AP\*CP\*GP\*CP\*T)-3')



- Molecule 3: DNA (5'-D(\*AP\*GP\*CP\*GP\*TP\*CP\*AP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.65Å 98.65Å 81.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.72 – 1.91 42.72 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.72-1.91) 99.9 (42.72-1.91)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.168 , 0.209 0.168 , 0.209	Depositor DCC
$R_{free}$ test set	2021 reflections (5.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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 ⓘ

### 5.1 Standard geometry ⓘ

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	0.38	0/3595	0.59	1/4845 (0.0%)
2	T	1.46	2/229 (0.9%)	1.32	3/350 (0.9%)
3	P	1.25	0/180	1.27	1/276 (0.4%)
All	All	0.57	2/4004 (0.0%)	0.71	5/5471 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	6	DT	C5-C7	-6.08	1.46	1.50
2	T	6	DT	C4'-O4'	-5.01	1.40	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	7	DA	O4'-C4'-C3'	-7.42	101.53	104.50
2	T	7	DG	O4'-C1'-N9	6.58	112.61	108.00
2	T	9	DC	O4'-C1'-N1	6.28	112.40	108.00
2	T	7	DG	O4'-C4'-C3'	-5.56	102.28	104.50
1	A	11	LEU	CA-CB-CG	-5.23	103.27	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284[A]	SER	Peptide

## 5.2 Too-close contacts ⓘ

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	3459	3544	3528	43	3
2	T	227	123	124	3	0
3	P	161	92	92	2	0
4	A	2	0	0	1	0
5	A	299	0	0	21	1
5	P	29	0	0	1	0
5	T	27	0	0	2	0
All	All	4204	3759	3744	48	4

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 (48) 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:256:ARG:NH2	5:A:602:HOH:O	1.78	1.17
1:A:100[B]:MET:SD	5:A:847:HOH:O	2.04	1.16
1:A:100[A]:MET:SD	5:A:847:HOH:O	2.05	1.14
1:A:178:LEU:O	5:A:601:HOH:O	1.73	1.05
1:A:282:THR:N	1:A:285:GLN:OE1	1.87	1.05
1:A:28:HIS:NE2	5:A:603:HOH:O	1.89	1.04
2:T:8:DA:OP2	5:T:101:HOH:O	1.91	0.88
1:A:100[B]:MET:HB3	5:A:847:HOH:O	1.73	0.88
1:A:306:GLU:OE2	5:A:604:HOH:O	1.98	0.82
1:A:179:GLN:CD	5:A:608:HOH:O	2.19	0.79
1:A:101:GLU:OE1	5:A:605:HOH:O	2.01	0.78
1:A:179:GLN:HG3	5:A:828:HOH:O	1.83	0.78
1:A:282:THR:OG1	1:A:285:GLN:HG3	1.84	0.77
1:A:79:GLN:OE1	5:A:606:HOH:O	2.02	0.77
4:A:501:NA:NA	5:A:842:HOH:O	1.57	0.76
1:A:322[B]:SER:HB2	1:A:421[B]:MET:HE2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100[A]:MET:CG	5:A:847:HOH:O	2.34	0.72
1:A:179:GLN:OE1	5:A:607:HOH:O	2.10	0.69
1:A:264:ALA:O	1:A:268:GLU:OE1	2.14	0.65
1:A:100[A]:MET:HB3	5:A:847:HOH:O	1.98	0.64
1:A:179:GLN:CG	5:A:828:HOH:O	2.42	0.61
1:A:179:GLN:CG	5:A:608:HOH:O	2.49	0.61
1:A:179:GLN:OE1	5:A:608:HOH:O	2.18	0.57
1:A:84[A]:ARG:NH2	1:A:350:GLU:OE2	2.37	0.57
2:T:2:DA:OP2	5:T:102:HOH:O	2.18	0.57
1:A:264:ALA:C	1:A:268:GLU:OE1	2.45	0.55
3:P:5:DT:OP2	5:P:101:HOH:O	2.18	0.53
1:A:405:ASN:N	1:A:405:ASN:OD1	2.34	0.51
1:A:281:PHE:HA	1:A:285:GLN:OE1	2.11	0.50
1:A:282:THR:OG1	1:A:285:GLN:CG	2.59	0.49
1:A:11:LEU:HD13	1:A:118:TYR:CE1	2.49	0.48
1:A:354:LYS:HE2	1:A:358:ASP:OD2	2.14	0.48
1:A:11:LEU:HD13	1:A:118:TYR:CZ	2.48	0.47
2:T:5:DA:H2''	2:T:6:DT:O5'	2.16	0.46
1:A:28:HIS:CD2	5:A:603:HOH:O	2.55	0.46
1:A:280[A]:GLN:NE2	5:A:617:HOH:O	2.49	0.45
1:A:369:SER:HB3	1:A:423:PHE:HB3	1.97	0.44
1:A:115:ASP:OD1	3:P:8:DT:O3'	2.36	0.44
1:A:421[A]:MET:SD	1:A:423:PHE:HB2	2.59	0.43
1:A:84[B]:ARG:NH2	1:A:350:GLU:OE2	2.48	0.43
1:A:281:PHE:CA	1:A:285:GLN:OE1	2.67	0.42
1:A:178:LEU:HD12	1:A:179:GLN:H	1.85	0.42
1:A:86:LYS:CE	1:A:347:GLU:OE1	2.68	0.42
1:A:15:ASP:O	1:A:16:CYS:C	2.58	0.42
1:A:179:GLN:CB	5:A:608:HOH:O	2.68	0.41
1:A:362:VAL:HG13	1:A:432:SER:HB2	2.03	0.41
1:A:352:LEU:HB3	1:A:390:TYR:CE2	2.56	0.40
1:A:160:THR:HG23	1:A:162:GLN:HG2	2.03	0.40

All (4) 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)
1:A:151:PRO:O	1:A:389:ARG:NH1[4_565]	1.79	0.41
1:A:151:PRO:O	1:A:389:ARG:HH12[4_565]	1.36	0.24
5:A:792:HOH:O	5:A:829:HOH:O[6_555]	2.05	0.15
1:A:75:LEU:O	1:A:288[B]:SER:HG[6_555]	1.52	0.08

## 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	448/435 (103%)	439 (98%)	8 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	CYS

### 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	389/372 (105%)	381 (98%)	8 (2%)	53	48

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	160	THR
1	A	284[A]	SER
1	A	284[B]	SER
1	A	285	GLN
1	A	405	ASN
1	A	413	THR
1	A	423	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 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	430/435 (98%)	0.05	24 (5%) 24 27	18, 31, 66, 99	0
2	T	11/12 (91%)	-0.37	0 100 100	30, 36, 51, 71	0
3	P	8/8 (100%)	-0.62	0 100 100	29, 34, 38, 39	0
All	All	449/455 (98%)	0.02	24 (5%) 26 29	18, 31, 66, 99	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	GLN	9.5
1	A	183	LEU	5.6
1	A	180	ILE	5.2
1	A	1	MET	4.8
1	A	410	GLY	4.6
1	A	132	LEU	4.5
1	A	184	THR	4.5
1	A	-1	PRO	4.1
1	A	182	ASN	3.8
1	A	181	ASP	3.5
1	A	160	THR	3.4
1	A	133	GLN	3.3
1	A	0	HIS	3.2
1	A	417	PRO	3.0
1	A	372	VAL	3.0
1	A	408	THR	3.0
1	A	409	SER	2.8
1	A	179	GLN	2.8
1	A	-2	GLY	2.8
1	A	411	ILE	2.7
1	A	413	THR	2.3
1	A	154	PRO	2.1
1	A	135	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	334	ARG	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	A	502	1/1	0.92	0.16	43,43,43,43	0
4	NA	A	501	1/1	0.96	0.13	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.