

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

#### Oct 15, 2023 – 12:26 PM EDT

PDB ID	:	8DH3
Title	:	T7 RNA polymerase elongation complex with unnatural base dPa
Authors	:	Oh, J.; Wang, D.
Deposited on	:	2022-06-24
Resolution	:	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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

# 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	Whole archive	Similar resolution
	(# Entries)	$(\# { m Entries},  { m resolution}  { m range}({ m A}))$
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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% 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	В	883	% <b>7</b> 9%	18'	% •
1	Е	883	7%	17%	• 7%
1	Ι	883	9%	21%	• 6%
1	М	883	68%	19%	12%

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Mol	Chain	Length	Quality of chain					
2	А	18	6% 78%		11%	11%		
2	F	18	72%		22%	6%		
2	J	18	56%	33%		11%		
2	Ν	18	17%		17%	6%		
3	С	12	<u>8%</u> 58%	17%	25%			
3	G	12	67%		33%			
3	K	12	8%	;%	33%			
3	0	12	8%	17%	33%			
4	D	9	33% 4.	4%	22%			
4	Н	9	11%		11%	11%		
4	L.	9	44%	33%	22%			
4	P	9	11%	44%	2270	11%		

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## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28298 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.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
1	В	856	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	D	000	6728	4284	1169	1239	36	0		0
1	F	825	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	Ľ	825	6472	4130	1119	1189	34	0		
1	т	831	Total	С	Ν	Ο	S	0	0	0
1	1	001	6530	4163	1142	1190	35	0	0	0
1	М	775	Total	С	Ν	Ο	S	0	0	0
	1 IVI	(()	5912	3755	1037	1088	32			0

• Molecule 1 is a protein called T7 RNA polymerase.

• Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
0	Δ	16	Total	С	Ν	Ο	Р	0	0	0
	A	10	325	155	60	94	16	0	0	0
0	Б	17	Total	С	Ν	Ο	Р	0	0	0
	Г	17	344	165	65	98	16	0	0	
0	т	16	Total	С	Ν	0	Р	0	0	0
	J	10	325	155	60	94	16	0		U
0	9 N	17	Total	С	Ν	Ο	Р	0	0	0
	11	344	165	65	98	16		U	0	

• Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	C	0	Total	С	Ν	Ο	Р	0	0	0
່ <u>ບ</u>	U	9	194	86	35	64	9	0	0	
2	С	0	Total	С	Ν	Ο	Р	0	0	0
່ <u>ບ</u>	G	0	174	77	33	56	8	0		0
2	K	0	Total	С	Ν	Ο	Р	0	0	0
່ <u>ບ</u>	Γ	κ δ	174	77	33	56	8	0	0	0
2	3 O	0	Total	С	Ν	Ο	Р	0	0	0
3		8	174	77	33	56	8			U



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	л	7	Total	С	Ν	Ο	Р	0	0	0
4	D	4	141	68	22	44	7	0	0	0
4	Ц	8	Total	С	Ν	Ο	Р	0	0	0
	11	8	160	77	25	50	8	0		
4	т	7	Total	С	Ν	Ο	Р	0	0	0
4	4 L	1	141	68	22	44	7	0	0	U
4	A D	8	Total	С	Ν	Ο	Р	0	0	0
4 F	0	160	77	25	50	8			0	

• Molecule 4 is a DNA chain called Non-template strand DNA.



## 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 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: T7 RNA polymerase

LYS GLY LEU LEU GLY GLY ALA



ARG GLN ASN ALA GLY VAL VAL VAL SLY















• Molecule 4: Non-template strand DNA

Chain L:	44%	33%	22%
25 25 25 25 25 25 25 25 25 25 25 25 25 2			
• Molecule 4:	Non-template stran	d DNA	
Chain P:	44%	44%	11%
12 17 17 17 17 17 17 17 17 17 17 17 17 17			



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	79.07Å 86.27Å 201.97Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$89.70^{\circ}$ $86.01^{\circ}$ $69.45^{\circ}$	Depositor
Bosolution(A)	47.98 - 3.00	Depositor
Resolution (A)	47.98 - 3.00	EDS
% Data completeness	98.3 (47.98-3.00)	Depositor
(in resolution range)	98.3 (47.98-3.00)	EDS
$R_{merge}$	0.11	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.09 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19	Depositor
P. P.	0.247 , $0.276$	Depositor
$n, n_{free}$	0.246 , $0.273$	DCC
$R_{free}$ test set	1850 reflections $(1.88%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	90.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29,81.8	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28298	wwPDB-VP
Average B, all atoms $(Å^2)$	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.97% 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:  ${\rm S8U}$ 

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	В	0.26	0/6878	0.49	1/9304~(0.0%)	
1	Е	0.26	0/6617	0.50	2/8952~(0.0%)	
1	Ι	0.26	0/6679	0.50	0/9030	
1	М	0.26	0/6039	0.50	1/8181~(0.0%)	
2	А	0.53	0/343	0.89	0/524	
2	F	0.50	0/365	0.87	0/559	
2	J	0.47	0/343	0.84	0/524	
2	N	0.50	0/365	0.90	0/559	
3	С	0.18	0/216	0.75	0/335	
3	G	0.17	0/194	0.73	0/301	
3	K	0.16	0/194	0.73	0/301	
3	0	0.21	0/194	0.83	0/301	
4	D	0.52	0/156	1.07	0/238	
4	Н	0.48	0/177	1.06	0/270	
4	L	0.52	0/156	1.08	0/238	
4	Р	0.47	0/177	1.07	0/270	
All	All	0.28	0/29093	0.56	4/39887~(0.0%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	М	787	ASP	CB-CG-OD1	6.18	123.86	118.30
1	В	787	ASP	CB-CG-OD1	6.18	123.86	118.30
1	Е	787	ASP	CB-CG-OD1	6.06	123.76	118.30
1	Е	39	LEU	CA-CB-CG	5.15	127.15	115.30

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	В	6728	0	6694	96	0
1	Е	6472	0	6402	95	0
1	Ι	6530	0	6480	107	0
1	М	5912	0	5684	97	1
2	А	325	0	168	1	0
2	F	344	0	180	3	0
2	J	325	0	168	3	0
2	Ν	344	0	180	2	0
3	С	194	0	98	2	0
3	G	174	0	88	0	0
3	Κ	174	0	88	3	0
3	0	174	0	88	0	0
4	D	141	0	81	3	0
4	Н	160	0	92	1	0
4	L	141	0	81	4	0
4	Р	160	0	92	3	0
All	All	28298	0	26664	407	1

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 7.

The worst 5 of 407 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:E:347:CYS:CB	1:E:350:GLU:HG3	1.80	1.12
1:E:347:CYS:HB3	1:E:350:GLU:HG3	1.28	1.11
1:E:347:CYS:SG	1:E:350:GLU:HG3	2.03	0.96
1:E:179:LYS:NZ	1:E:750:MET:SD	2.50	0.85
1:B:35:GLU:HG2	1:B:272:VAL:HG21	1.66	0.77

All (1) 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:M:31:ARG:NH2	1:M:90:GLU:O[1_655]	2.16	0.04

### 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	Perce	ntiles
1	В	850/883~(96%)	834 (98%)	15 (2%)	1 (0%)	51	85
1	Е	813/883~(92%)	798~(98%)	15 (2%)	0	100	100
1	Ι	823/883~(93%)	815 (99%)	8 (1%)	0	100	100
1	М	761/883~(86%)	750 (99%)	11 (1%)	0	100	100
All	All	3247/3532~(92%)	3197~(98%)	49 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	811	HIS

#### 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	В	701/729~(96%)	693~(99%)	8 (1%)	73 90
1	Ε	670/729~(92%)	651 (97%)	19 (3%)	43 77
1	Ι	674/729~(92%)	652 (97%)	22 (3%)	38 73
1	М	582/729~(80%)	572 (98%)	10 (2%)	60 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2627/2916~(90%)	2568~(98%)	59~(2%)	52 81

5 of 59 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	Ι	96	ARG
1	М	514	PHE
1	Ι	506	ASP
1	М	438	ASP
1	М	150	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	58	GLN
1	Е	339	ASN

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	С	8/12~(66%)	0	0
3	G	7/12~(58%)	0	0
3	K	7/12~(58%)	0	0
3	0	7/12~(58%)	2(28%)	0
All	All	29/48~(60%)	2(6%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	0	2	С
3	0	3	G

There are no RNA pucker outliers to report.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul



statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Res	Tink	Bo	ond leng	$_{\rm sths}$	Bond angles		
	Type	Ullalli			Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	S8U	F	10	2	15,19,20	4.36	7 (46%)	16,26,29	1.40	2 (12%)
2	S8U	А	10	2	15,19,20	4.39	7 (46%)	16,26,29	1.23	1 (6%)
2	S8U	J	10	2	15,19,20	4.37	7 (46%)	16,26,29	1.35	2 (12%)
2	S8U	N	10	2	15,19,20	4.37	7 (46%)	16,26,29	1.44	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S8U	F	10	2	-	0/3/23/24	0/2/2/2
2	S8U	А	10	2	-	3/3/23/24	0/2/2/2
2	S8U	J	10	2	-	3/3/23/24	0/2/2/2
2	S8U	Ν	10	2	-	0/3/23/24	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	10	S8U	C2'-C3'	-11.53	1.22	1.52
2	Ν	10	S8U	C2'-C3'	-11.37	1.22	1.52
2	J	10	S8U	C2'-C3'	-11.37	1.22	1.52
2	F	10	S8U	C2'-C3'	-11.34	1.22	1.52
2	F	10	S8U	O4'-C4'	-8.11	1.26	1.45

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	N	10	S8U	C2'-C3'-C4'	2.96	108.93	102.76
2	J	10	S8U	O14-C13-C12	-2.91	120.04	124.17
2	F	10	S8U	C2'-C3'-C4'	2.91	108.82	102.76
2	J	10	S8U	C2'-C3'-C4'	2.41	107.78	102.76
2	F	10	S8U	O14-C13-C12	-2.40	120.77	124.17



There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	А	10	S8U	O4'-C4'-C5'-O5'
2	J	10	S8U	C3'-C4'-C5'-O5'
2	J	10	S8U	O4'-C4'-C5'-O5'
2	А	10	S8U	C3'-C4'-C5'-O5'
2	J	10	S8U	C4'-C5'-O5'-P

5 of 6 torsion outliers are listed below:

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.5 Carbohydrates (i)

There are no monosaccharides 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 (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,  $95^{th}$  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 $>$	#RSF	RZ>	2	$OWAB(A^2)$	Q<0.9
1	В	856/883~(96%)	0.02	11 (1%)	77	51	46, 89, 172, 247	0
1	Е	825/883~(93%)	0.28	59 (7%)	15	4	54, 100, 243, 301	0
1	Ι	831/883~(94%)	0.41	77 (9%)	8	3	70, 137, 216, 307	0
1	М	775/883~(87%)	0.42	66 (8%)	10	3	97, 155, 236, 309	0
2	А	15/18~(83%)	0.50	1 (6%)	17	5	65, 97, 305, 307	0
2	F	16/18~(88%)	0.11	0 100	10	0	97, 148, 228, 231	0
2	J	15/18~(83%)	0.69	1 (6%)	17	5	99, 128, 332, 358	0
2	Ν	16/18~(88%)	0.61	3 (18%)	1	0	110, 198, 390, 393	0
3	С	9/12~(75%)	1.23	1 (11%)	5	1	67, 77, 127, 185	0
3	G	8/12~(66%)	0.94	0 100	10	0	87, 106, 157, 158	0
3	K	8/12~(66%)	0.81	1 (12%)	3	1	96, 115, 163, 181	0
3	Ο	8/12~(66%)	0.65	1 (12%)	3	1	117, 142, 206, 219	0
4	D	7/9~(77%)	0.31	0 100	10	0	208, 254, 295, 309	0
4	Н	8/9~(88%)	0.21	1 (12%)	3	1	221, 228, 281, 295	0
4	L	7/9~(77%)	0.46	0 100	10	0	271, 281, 301, 303	0
4	Р	8/9~(88%)	0.47	1 (12%)	3	1	291, 298, 333, 336	0
All	All	3412/3688~(92%)	0.29	223(6%)	18	5	46, 127, 233, 393	0

The worst 5 of 223 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ι	671	ASN	10.4
1	Е	142	GLY	7.4
1	Е	131	ASN	6.5
1	Ι	680	LEU	6.0
1	М	216	CYS	6.0



### 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	$B-factors(Å^2)$	Q<0.9
2	S8U	N	10	18/19	0.87	0.27	119,144,161,170	0
2	S8U	F	10	18/19	0.89	0.26	105,116,135,147	0
2	S8U	J	10	18/19	0.92	0.30	126,150,175,183	0
2	S8U	А	10	18/19	0.94	0.24	71,90,110,124	0

#### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

There are no ligands in this entry.

### 6.5 Other polymers (i)

There are no such residues in this entry.

