



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:10 AM UTC

PDB ID : 6DT8 / pdb_00006dt8
Title : Bacteriophage N4 RNA polymerase II elongation complex 1
Authors : Molodtsov, V.; Murakami, K.S.
Deposited on : 2018-06-15
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

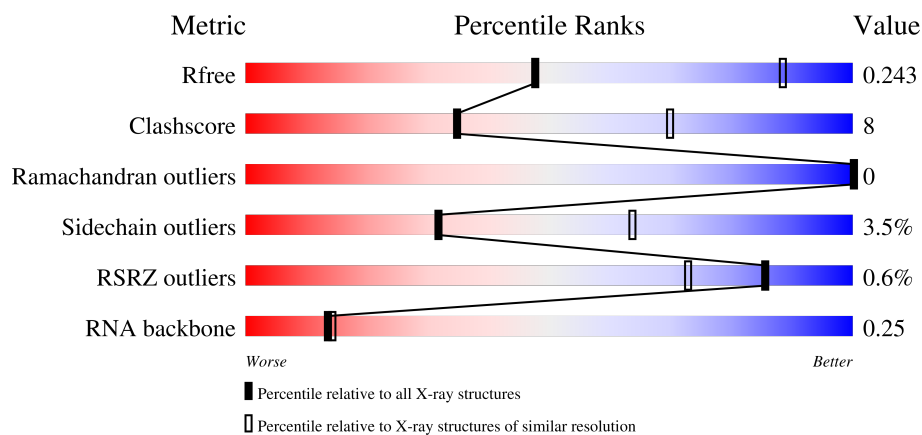
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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 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 $\leq 5\%$. 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	269	
2	B	404	
3	C	49	
4	D	12	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5672 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 RNAP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2042	1295	352	382	13			

- Molecule 2 is a protein called RNAP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3256	2073	545	617	21			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*CP*CP*CP*AP*CP*CP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			242	115	50	65	12			

- Molecule 4 is a RNA chain called RNA (5'-R(P*UP*GP*GP*UP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	P	0	0	0
			132	58	24	44	6			

- Molecule 1: RNAP1

[illegible]

- Molecule 2: RNAP2

L317	E178	N1
L324	L179	R7
R345	N180	N16
P348	K181	N17
R356	N188	Y18
N360	A191	G19
A366	F192	L20
V378	V193	E23
K387	Y194	R44
L392	H195	E47
V396	V204	A54
S404	Y205	P71
	I206	V72
	M209	R92
	V213	E95
	E214	Y102
	T215	R112
	V216	I118
	H217	Y119
	F218	M122
	C225	L126
	R237	I132
	M238	R133
	L239	R134
	S240	N135
	A241	D136
	N242	Q139
	H245	Y146
	D248	G147
	R253	S148
	D260	V155
	C273	F156
	E278	V164
	S282	S167
	E283	T168
	K284	M169
	K288	N170
	A289	V171
	M290	E172
	E291	
	Y309	
	L310	
	T311	

- Molecule 3: DNA (5'-D(P*AP*CP*CP*CP*AP*CP*CP*AP*AP*AP*AP*A)-3')

[illegible]

- Molecule 4: RNA (5'-R(P*UP*GP*GP*UP*GP*G)-3')

A A A A U U U2 G3 G4 U5 G6 G7

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	174.76Å 174.76Å 76.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.19 – 3.20 41.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.19-3.20) 99.8 (41.19-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.190 , 0.243 0.190 , 0.243	Depositor DCC
R_{free} test set	1966 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	107.8	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5672	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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](#)

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	0.50	0/2089	0.82	0/2821
2	B	0.47	0/3323	0.82	2/4496 (0.0%)
3	C	0.42	0/272	0.58	0/415
4	D	0.37	0/147	0.61	0/228
All	All	0.47	0/5831	0.80	2/7960 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	237	ARG	CA-CB-CG	6.32	126.73	114.10
2	B	237	ARG	CG-CD-NE	5.11	123.23	112.00

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	2042	0	1964	29	0
2	B	3256	0	3214	58	0
3	C	242	0	133	8	0
4	D	132	0	65	2	0
All	All	5672	0	5376	82	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 8.

All (82) 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)
2:B:237:ARG:HH11	2:B:237:ARG:HB3	1.39	0.86
3:C:5:DC:H2''	3:C:6:DA:H5'	1.59	0.84
2:B:237:ARG:HB3	2:B:237:ARG:NH1	2.05	0.71
2:B:136:ASP:HB3	2:B:155:VAL:HG13	1.73	0.69
2:B:238:MET:HG3	2:B:242:ASN:ND2	2.08	0.68
1:A:115:HIS:CE1	1:A:214:THR:HG22	2.29	0.68
2:B:290:MET:HG2	2:B:317:LEU:HD22	1.76	0.67
1:A:4:ILE:H	1:A:4:ILE:HD12	1.61	0.66
1:A:253:THR:OG1	1:A:256:ASN:HB2	1.97	0.64
1:A:19:LEU:HD21	1:A:58:LEU:HD21	1.81	0.62
1:A:181:MET:O	1:A:185:GLU:HG2	1.99	0.62
2:B:237:ARG:HH21	3:C:-1:DA:H1'	1.64	0.62
2:B:310:LEU:HA	2:B:314:THR:CG2	2.31	0.61
4:D:2:U:O2'	4:D:3:G:OP1	2.18	0.61
1:A:68:VAL:HG21	2:B:225:CYS:SG	2.40	0.60
2:B:119:TYR:CD1	2:B:134:ARG:HA	2.37	0.60
3:C:6:DA:H2''	3:C:7:DA:O4'	2.01	0.59
2:B:148:SER:HA	3:C:0:DC:H5'	1.86	0.57
2:B:178:GLU:O	2:B:181:LYS:HB3	2.03	0.57
2:B:95:GLU:O	2:B:112:ARG:HD3	2.05	0.55
2:B:238:MET:HG3	2:B:242:ASN:HD22	1.72	0.55
1:A:269:ASP:OXT	2:B:7:ARG:NH1	2.40	0.55
2:B:132:ILE:HD12	2:B:156:PHE:HE1	1.73	0.54
2:B:239:LEU:HD13	2:B:378:VAL:HG11	1.90	0.54
2:B:366:ALA:O	2:B:387:LYS:HE2	2.07	0.53
2:B:72:VAL:O	2:B:345:ARG:HA	2.07	0.53
2:B:118:ILE:HD13	2:B:169:MET:SD	2.49	0.53
2:B:237:ARG:HH11	2:B:237:ARG:CB	2.17	0.52
1:A:233:HIS:NE2	1:A:250:TYR:OH	2.43	0.51
2:B:309:TYR:O	2:B:314:THR:HG21	2.10	0.51
2:B:310:LEU:HA	2:B:314:THR:HG22	1.91	0.51
1:A:28:GLU:HG2	1:A:46:TYR:OH	2.11	0.51
2:B:310:LEU:HA	2:B:314:THR:HG21	1.93	0.50
2:B:392:LEU:O	2:B:396:VAL:HG23	2.12	0.50
1:A:35:PHE:HB3	1:A:39:PHE:CE2	2.47	0.49
2:B:18:TYR:O	2:B:47:GLU:N	2.32	0.49
1:A:268:ILE:CD1	2:B:348:PRO:HG2	2.43	0.49
1:A:26:GLU:HA	1:A:30:ASN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:U:H2'	4:D:3:G:C8	2.48	0.49
1:A:79:GLN:HA	2:B:216:VAL:HG22	1.94	0.48
2:B:282:SER:OG	2:B:284:LYS:HG2	2.14	0.48
3:C:5:DC:H2'	3:C:6:DA:C8	2.47	0.48
2:B:122:MET:O	2:B:126:LEU:HB2	2.13	0.48
1:A:49:GLY:O	1:A:53:MET:HG2	2.14	0.47
2:B:195:HIS:HA	2:B:204:VAL:O	2.14	0.47
2:B:134:ARG:HD3	2:B:134:ARG:C	2.40	0.47
2:B:20:LEU:HB3	2:B:23:GLU:HG3	1.97	0.47
2:B:167:SER:O	2:B:171:VAL:HG12	2.15	0.47
2:B:238:MET:HG2	2:B:239:LEU:N	2.16	0.46
1:A:268:ILE:O	1:A:269:ASP:HB2	2.16	0.46
2:B:237:ARG:CD	3:C:0:DC:H5''	2.45	0.46
2:B:102:TYR:CB	2:B:112:ARG:HD2	2.46	0.46
1:A:181:MET:HG2	1:A:185:GLU:OE2	2.16	0.46
2:B:136:ASP:HB3	2:B:155:VAL:CG1	2.44	0.46
2:B:288:LYS:HE3	2:B:291:GLU:OE1	2.15	0.46
3:C:6:DA:H3'	3:C:6:DA:OP2	2.16	0.45
1:A:86:PHE:HB2	2:B:218:PHE:CE2	2.51	0.45
2:B:290:MET:HE3	2:B:290:MET:HB3	1.83	0.45
1:A:262:PHE:CE2	2:B:71:PRO:HB3	2.52	0.45
1:A:238:ARG:NH1	2:B:245:HIS:CD2	2.85	0.45
1:A:268:ILE:HA	1:A:268:ILE:HD13	1.75	0.45
1:A:23:MET:HE2	1:A:58:LEU:HG	2.00	0.44
1:A:171:PRO:HB2	1:A:263:ALA:HB3	1.99	0.44
1:A:176:TRP:CH2	1:A:219:MET:HE2	2.53	0.44
1:A:240:ARG:NH1	2:B:248:ASP:OD1	2.51	0.44
2:B:188:ASN:ND2	2:B:191:ALA:HB2	2.33	0.44
1:A:189:LEU:CD2	2:B:44:ARG:HA	2.47	0.44
2:B:126:LEU:HD12	2:B:164:VAL:HG11	2.00	0.44
3:C:1:DC:H2'	3:C:2:DC:O4'	2.18	0.44
1:A:178:VAL:HG21	2:B:54:ALA:HB2	2.00	0.44
2:B:16:ASN:O	2:B:19:GLY:HA3	2.17	0.43
2:B:314:THR:O	2:B:317:LEU:HG	2.19	0.43
2:B:193:VAL:HA	2:B:206:ILE:O	2.19	0.42
2:B:356:ARG:NH1	2:B:360:ASN:OD1	2.41	0.41
1:A:174:ILE:HD12	1:A:229:PHE:CE2	2.56	0.41
2:B:273:CYS:HB2	2:B:324:LEU:HD21	2.03	0.41
2:B:146:TYR:HD1	2:B:241:ALA:HA	1.86	0.41
2:B:92:ARG:NH1	2:B:172:GLU:OE1	2.54	0.41
1:A:166:ARG:HD3	2:B:260:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:TYR:N	2:B:19:GLY:HA2	2.36	0.41
1:A:163:HIS:CD2	2:B:253:ARG:HA	2.56	0.40
2:B:209:MET:HE3	2:B:209:MET:HB3	1.91	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	248/269 (92%)	240 (97%)	8 (3%)	0	100	100
2	B	402/404 (100%)	391 (97%)	11 (3%)	0	100	100
All	All	650/673 (97%)	631 (97%)	19 (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	222/243 (91%)	217 (98%)	5 (2%)	44	70
2	B	351/351 (100%)	336 (96%)	15 (4%)	26	59
All	All	573/594 (96%)	553 (96%)	20 (4%)	32	64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	29	GLU
1	A	174	ILE
1	A	228	LYS
1	A	268	ILE
2	B	20	LEU
2	B	92	ARG
2	B	126	LEU
2	B	132	ILE
2	B	139	GLN
2	B	171	VAL
2	B	180	ASN
2	B	213	VAL
2	B	215	THR
2	B	216	VAL
2	B	237	ARG
2	B	238	MET
2	B	278	GLU
2	B	288	LYS
2	B	314	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	18	GLN
1	A	115	HIS
1	A	121	GLN
1	A	244	GLN
1	A	256	ASN
2	B	35	ASN
2	B	203	ASN
2	B	357	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	6/12 (50%)	3 (50%)	1 (16%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	3	G
4	D	4	G
4	D	6	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	2	U

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 oligosaccharides 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, 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	252/269 (93%)	-0.36	1 (0%) 88 79	62, 104, 164, 214	0
2	B	404/404 (100%)	-0.52	1 (0%) 91 85	58, 97, 153, 187	0
3	C	12/49 (24%)	-0.01	0 100 100	105, 150, 241, 242	0
4	D	6/12 (50%)	1.57	2 (33%) 1 1	43, 57, 73, 91	6 (100%)
All	All	674/734 (91%)	-0.43	4 (0%) 85 73	43, 99, 159, 242	6 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	146	TYR	3.8
1	A	207	ALA	3.0
4	D	4	G	2.2
4	D	2	U	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 oligosaccharides 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.