



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2018 – 06:03 PM EST

PDB ID : 6C2P
Title : Bacteriophage N4 RNA polymerase II elongation complex 2
Authors : Molodtsov, V.; Murakami, K.S.
Deposited on : 2018-01-08
Resolution : 2.70 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

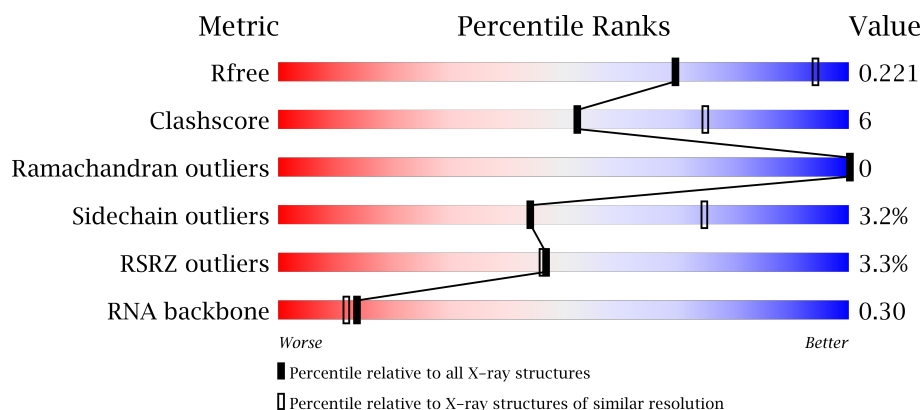
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)
RNA backbone	2435	1011 (3.06-2.34)

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	269	<div> <div>3%</div> <div>82% 10% 7%</div> </div>
2	B	404	<div> <div>2%</div> <div>84% 14% .</div> </div>
3	C	48	<div> <div>4%</div> <div>10% 13% 77%</div> </div>
4	D	8	<div> <div>25%</div> <div>38% 50% 13%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5678 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	249	Total	C	N	O	S	0	0	0
			2012	1278	347	374	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
			3250	2070	542	617	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	P	0	0	0
			221	105	45	60	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	P	0	0	0
			149	67	26	50	6			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O	0	0
			8 8		
6	B	5	Total O	0	0
			5 5		
6	C	1	Total O	0	0
			1 1		

- Molecule 1: RNAP1



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	175.05Å 175.05Å 76.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.70 29.92 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.92-2.70) 97.9 (29.92-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.68Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.191 , 0.221 0.188 , 0.221	Depositor DCC
R_{free} test set	1982 reflections (6.32%)	DCC
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5678	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0/2059	0.77	3/2781 (0.1%)
2	B	0.50	0/3317	0.74	2/4489 (0.0%)
3	C	1.00	0/248	0.96	1/378 (0.3%)
4	D	0.71	0/166	1.45	2/258 (0.8%)
All	All	0.54	0/5790	0.79	8/7906 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	238	MET	CA-CB-CG	7.54	126.12	113.30
1	A	211	TYR	CA-CB-CG	6.45	125.65	113.40
1	A	211	TYR	CB-CG-CD1	-5.96	117.43	121.00
4	D	1	U	C2-N1-C1'	5.90	124.78	117.70
2	B	239	LEU	CB-CG-CD2	-5.35	101.91	111.00
3	C	9	DA	O4'-C1'-N9	5.33	111.73	108.00
4	D	7	G	N1-C6-O6	-5.22	116.77	119.90
1	A	240	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2012	0	1932	22	0
2	B	3250	0	3203	43	0
3	C	221	0	122	11	0
4	D	149	0	76	0	0
5	B	32	0	12	0	0
6	A	8	0	0	0	0
6	B	5	0	0	0	0
6	C	1	0	0	0	0
All	All	5678	0	5345	68	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 6.

All (68) 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:211:TYR:OH	1:A:256:ASN:ND2	2.01	0.93
2:B:132:ILE:HD11	2:B:137:CYS:HB2	1.64	0.78
2:B:290:MET:HG2	2:B:317:LEU:HD22	1.68	0.74
2:B:145:LEU:O	2:B:180:ASN:ND2	2.21	0.73
2:B:366:ALA:O	2:B:387:LYS:HE2	1.95	0.66
1:A:4:ILE:HD12	1:A:4:ILE:H	1.61	0.65
2:B:299:THR:HG22	2:B:301:PHE:H	1.61	0.65
2:B:309:TYR:O	2:B:314:THR:HG21	1.97	0.65
1:A:268:ILE:HG12	2:B:62:VAL:HG22	1.80	0.63
2:B:310:LEU:HA	2:B:314:THR:CG2	2.29	0.61
1:A:268:ILE:CD1	2:B:62:VAL:HG13	2.32	0.59
3:C:4:DC:H2'	3:C:5:DC:C6	2.39	0.57
2:B:299:THR:CG2	2:B:301:PHE:H	2.17	0.56
2:B:72:VAL:O	2:B:345:ARG:HA	2.06	0.56
2:B:238:MET:HB2	3:C:1:DC:H5''	1.88	0.55
3:C:5:DC:H2'	3:C:6:DA:C8	2.41	0.55
1:A:97:ASP:OD1	1:A:100:ILE:HG12	2.07	0.55
2:B:282:SER:OG	2:B:284:LYS:HG2	2.07	0.54
1:A:122:TYR:OH	3:C:6:DA:OP1	2.18	0.54
2:B:95:GLU:O	2:B:112:ARG:HD3	2.08	0.53
3:C:6:DA:H8	3:C:6:DA:OP2	1.91	0.53
2:B:310:LEU:HA	2:B:314:THR:HG21	1.90	0.52
2:B:295:TYR:O	2:B:299:THR:HB	2.09	0.52
2:B:310:LEU:HA	2:B:314:THR:HG22	1.92	0.52
3:C:4:DC:H2'	3:C:5:DC:H6	1.74	0.52
2:B:2:GLN:HG2	2:B:400:GLU:OE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HG2	1:A:46:TYR:OH	2.10	0.51
1:A:233:HIS:NE2	1:A:250:TYR:OH	2.42	0.51
2:B:368:GLY:O	2:B:387:LYS:NZ	2.33	0.50
2:B:237:ARG:HB2	2:B:237:ARG:NH1	2.26	0.50
3:C:5:DC:H2'	3:C:6:DA:H5'	1.94	0.48
1:A:126:MET:HE1	1:A:141:TYR:CA	2.43	0.48
1:A:19:LEU:HD21	1:A:58:LEU:HD11	1.96	0.48
2:B:288:LYS:HE3	2:B:291:GLU:OE1	2.14	0.48
2:B:213:VAL:HB	2:B:226:VAL:HG22	1.95	0.47
2:B:121:LYS:O	2:B:125:THR:HG23	2.15	0.47
2:B:122:MET:O	2:B:126:LEU:HB2	2.15	0.47
2:B:18:TYR:OH	2:B:45:GLU:OE1	2.31	0.46
1:A:268:ILE:O	1:A:269:ASP:HB2	2.16	0.45
2:B:16:ASN:O	2:B:19:GLY:HA3	2.16	0.45
1:A:126:MET:HE1	1:A:141:TYR:CG	2.51	0.45
1:A:126:MET:HE1	1:A:141:TYR:HA	1.98	0.45
3:C:6:DA:OP2	3:C:6:DA:H3'	2.17	0.45
1:A:86:PHE:HB2	2:B:218:PHE:CE2	2.52	0.44
1:A:268:ILE:HD13	2:B:62:VAL:HG13	1.99	0.44
2:B:235:LYS:HE3	2:B:237:ARG:HE	1.81	0.44
2:B:239:LEU:HA	2:B:239:LEU:HD23	1.81	0.44
2:B:117:VAL:O	2:B:121:LYS:HG2	2.18	0.44
2:B:392:LEU:O	2:B:396:VAL:HG23	2.18	0.43
2:B:178:GLU:O	2:B:181:LYS:HB3	2.18	0.43
2:B:262:ASP:HB3	2:B:265:GLN:HB3	2.01	0.43
1:A:149:ILE:HD12	1:A:154:HIS:HA	2.01	0.42
1:A:238:ARG:NH1	2:B:245:HIS:ND1	2.67	0.42
1:A:126:MET:HE1	1:A:141:TYR:N	2.35	0.42
1:A:268:ILE:HD12	1:A:269:ASP:H	1.83	0.42
3:C:6:DA:H2'	3:C:7:DA:C8	2.55	0.42
1:A:151:LYS:HE3	3:C:4:DC:OP2	2.20	0.42
2:B:280:LYS:O	2:B:311:ASP:HB2	2.20	0.41
2:B:146:TYR:CD1	2:B:241:ALA:HA	2.55	0.41
2:B:237:ARG:HB2	2:B:237:ARG:HH11	1.85	0.41
2:B:119:TYR:HE1	2:B:132:ILE:HD13	1.84	0.41
2:B:126:LEU:HB3	2:B:130:ALA:HB2	2.02	0.41
1:A:268:ILE:HD12	1:A:268:ILE:N	2.36	0.40
3:C:5:DC:C2'	3:C:6:DA:H5'	2.51	0.40
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.92	0.40
2:B:136:ASP:HB3	2:B:155:VAL:HG13	2.04	0.40
2:B:18:TYR:O	2:B:46:ALA:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ALA:HB1	2:B:99:VAL:HB	2.04	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	245/269 (91%)	237 (97%)	8 (3%)	0	100	100
2	B	402/404 (100%)	391 (97%)	11 (3%)	0	100	100
All	All	647/673 (96%)	628 (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	217/243 (89%)	210 (97%)	7 (3%)	44	75
2	B	350/351 (100%)	339 (97%)	11 (3%)	45	75
All	All	567/594 (96%)	549 (97%)	18 (3%)	44	75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	51	ASP
1	A	101	ASP
1	A	174	ILE
1	A	211	TYR
1	A	216	HIS
1	A	268	ILE
2	B	92	ARG
2	B	106	SER
2	B	126	LEU
2	B	132	ILE
2	B	139	GLN
2	B	213	VAL
2	B	215	THR
2	B	238	MET
2	B	288	LYS
2	B	299	THR
2	B	314	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	2	U
4	D	3	G

There are no RNA pucker outliers to report.

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](#)

1 ligand is 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	B	1001	-	27,34,34	1.09	2 (7%)	27,54,54	2.01	7 (25%)

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
5	GTP	B	1001	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	GTP	C2-N1	2.76	1.40	1.35
5	B	1001	GTP	C6-N1	3.70	1.39	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	GTP	N3-C2-N1	-5.48	119.45	127.46
5	B	1001	GTP	C5-C6-N1	-3.37	118.68	123.48
5	B	1001	GTP	C4-C5-N7	-2.13	107.35	109.41
5	B	1001	GTP	C4'-O4'-C1'	2.85	112.80	109.77
5	B	1001	GTP	C6-N1-C2	3.35	120.89	116.06
5	B	1001	GTP	N2-C2-N1	3.64	123.06	117.24
5	B	1001	GTP	C2-N3-C4	4.66	120.60	115.16

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	249/269 (92%)	0.05	8 (3%)	48	48	52, 94, 142, 171	0
2	B	404/404 (100%)	0.03	10 (2%)	58	58	52, 89, 133, 166	0
3	C	11/48 (22%)	0.66	2 (18%)	1	1	100, 127, 192, 212	0
4	D	7/8 (87%)	1.63	2 (28%)	1	0	124, 142, 194, 198	0
All	All	671/729 (92%)	0.06	22 (3%)	47	46	52, 91, 142, 212	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	3	G	5.5
1	A	187	ALA	5.1
1	A	255	TRP	4.7
1	A	188	ASN	3.7
1	A	184	ASN	3.7
2	B	128	LYS	3.7
2	B	127	GLY	3.7
1	A	186	TRP	3.2
1	A	189	LEU	3.1
2	B	222	PRO	2.7
2	B	83	ILE	2.5
3	C	10	DA	2.5
1	A	182	VAL	2.4
4	D	4	G	2.4
2	B	215	THR	2.2
1	A	183	LYS	2.1
2	B	78	SER	2.1
3	C	6	DA	2.1
2	B	84	LEU	2.0
2	B	105	GLU	2.0
2	B	221	LYS	2.0
2	B	80	GLY	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 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	GTP	B	1001	32/32	0.73	0.28	0.94	96,164,229,231	0

6.5 Other polymers [i](#)

There are no such residues in this entry.