

wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 05:11 PM EDT

PDB ID	:	7RIQ
Title	:	RNA polymerase II elongation complex scaffold 1 without polyamide
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Deposited on	:	2021-07-20
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
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

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)	(# Entries, resolution range(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 cha	in			
1	R	9	33%		67%			
2	Т	30	7%	80%			7%	7%
3	А	1733	2% 60%		20%	•	19%	
4	В	1224	.% • 69%)		22%	•	8%

Continued on next page...



Mol | Chain | Length Quality of chain С 531865% 19% 16% 2% Е ••• 6 21574% 23% F 715545% 42% 13% • 5% Η 8 14667% 23% 9% • 9 Ι • 12269% 28% J 7010• 7% 61% 30% Κ 120 11 5% 78% 18% 4% 12L 7049% 13% 39% Ν 201330% 60% 10%





2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29255 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N 40	0 50	P	0	0	0
			195	88	40	59	ð			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Т	28	Total 560	C 270	N 90	0 173	Р 27	0	0	0

• Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
3	А	1397	Total 10933	C 6892	N 1913	O 2068	S 60	0	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues		Α	toms		ZeroOcc	AltConf	Trace	
4	В	1124	Total 8862	C 5609	N 1552	O 1648	S 53	0	0	0

• Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
5	С	267	Total 2101	C 1320	N 349	0 419	S 13	0	0	0

• Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
6	Е	212	Total 1731	C 1100	N 305	0 315	S 11	0	0	0



• Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	F	86	Total 684	C 437	N 115	0 129	${ m S} { m 3}$	0	0	0

• Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Н	133	Total 1064	C 670	N 179	0 211	${S \atop 4}$	0	0	0

• Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
9	Ι	118	Total 952	$\begin{array}{c} \mathrm{C} \\ 585 \end{array}$	N 173	0 184	S 10	0	0	0

• Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total 532	C 339	N 93	0 94	S 6	0	0	0

• Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total 919	C 590	N 156	0 171	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

• Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
12	L	43	Total 337	C 208	N 66	O 59	${S \over 4}$	0	0	0

• Molecule 13 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Ν	18	Total 376	C 177	N 78	O 103	Р 18	0	0	0

• Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	R	1	Total Mg 1 1	0	0

• Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	А	2	Total Zn 2 2	0	0
15	В	1	Total Zn 1 1	0	0
15	С	1	Total Zn 1 1	0	0
15	Ι	2	Total Zn 2 2	0	0
15	J	1	Total Zn 1 1	0	0
15	L	1	Total Zn 1 1	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 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: RNA









• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain C:	65%	19%	16%
MET 82 85 96 96 97 97 15 81 15 81 15 81 12 83 12 83 12 83 12 83 13 83 13 83 13 83 13 83 13 83 13 83 14 14 14 83 14 14 14 14 14 14 14 14 14 14 14 14 14	A39 E40 141 141 155 155 155 155 155 155 155 155	6105 E106 N112 S115 V146	D117 L118 L118 K137 R140 C145 C145 C145 K146 F147 R148
E152 A159 A164 H167 H167 F172 E177 F178 F178 F178 F178 F178 F178 F178 F	1227 N231 D241 D241 V245 R246 C247 1248 1248 1248 1248 1248 1248 1265 A255	M265 D268 LYS VAL	PHC ALA SER GIY GIY ASN ASN ASN ASN ASN ASN ASN ASN MET MET
LEU GLY SER ASP ASP ASP ASP ASP ALA GLU GLU GLU CLU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	MET GLY GLY THR GLY GLY TYR ASP ASP ASP ALA TRP		
• Molecule 6: DNA-directed	RNA polymerases I, II, and	d III sub	unit RPABC1
Chain E:	74%	2	3% ••
MET ASP GIN GIN B1 E1 N15 E2 F29 F29 F29 G33 F29 G33 F29 G33 F29 G33 F29 G33 F29 G33 F29 G33 F29 G33 F29 G32 F29 F29 G10 F37 F37 F37 F37 F37 F37 F37 F37 F37 F37	L37 F42 849 849 849 849 849 865 M55 M55 M55 M55 M55 764 764 765 F65 F65	E67 870 676 877	F82 C83 C83 M93 F105 F105 F110 G113
1117 1117 1117 1118 1118 1128 1128 1128	V150 8157 8157 8158 8159 8159 8159 8159 8199 8200 8200 8200 8201		

• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC2





• Molecule 13: Non-template strand DNA

Chain N:	30%	60%	10%
DG 15 66 73 68 69 69	410 411 412 413 414 415 415 618 618 618 619 00		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	167.85Å 223.47Å 193.03Å	Depositor
a, b, c, α , β , γ	90.00° 100.30° 90.00°	Depositor
Bosolution(A)	48.15 - 3.00	Depositor
Resolution (A)	48.15 - 3.00	EDS
% Data completeness	99.8 (48.15-3.00)	Depositor
(in resolution range)	99.8 (48.15-3.00)	EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.11 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13	Depositor
B B.	0.213 , 0.264	Depositor
II, II free	0.213 , 0.264	DCC
R_{free} test set	1919 reflections (1.38%)	wwPDB-VP
Wilson B-factor $(Å^2)$	79.5	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28 , 61.4	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29255	wwPDB-VP
Average B, all atoms $(Å^2)$	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities 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: MG, ZN

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	Bo	ond angles
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	R	0.25	0/219	0.82	0/341
2	Т	0.59	0/623	1.06	2/958~(0.2%)
3	А	0.24	0/11127	0.43	1/15053~(0.0%)
4	В	0.24	0/9033	0.43	0/12191
5	С	0.25	0/2139	0.44	0/2899
6	Е	0.24	0/1767	0.42	0/2378
7	F	0.23	0/696	0.42	0/943
8	Н	0.25	0/1082	0.48	0/1466
9	Ι	0.26	0/970	0.44	0/1308
10	J	0.27	0/541	0.47	0/727
11	K	0.24	0/937	0.42	0/1265
12	L	0.25	0/339	0.50	0/450
13	N	0.56	0/424	0.89	0/653
All	All	0.26	0/29897	0.47	3/40632~(0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	398	GLU	C-N-CA	6.62	138.24	121.70
2	Т	10	DT	N3-C4-O4	5.21	123.03	119.90
2	Т	13	DT	N3-C4-O4	5.12	122.97	119.90

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	R	195	0	99	6	0
2	Т	560	0	320	31	0
3	А	10933	0	10974	248	0
4	В	8862	0	8814	187	0
5	С	2101	0	2056	40	0
6	Е	1731	0	1758	32	0
7	F	684	0	692	15	0
8	Н	1064	0	1029	17	0
9	Ι	952	0	897	24	0
10	J	532	0	542	16	0
11	Κ	919	0	929	16	0
12	L	337	0	352	4	0
13	Ν	376	0	201	10	0
14	R	1	0	0	0	0
15	А	2	0	0	0	0
15	В	1	0	0	0	0
15	С	1	0	0	0	0
15	Ι	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	29255	0	28663	577	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 10.

The worst 5 of 577 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)
3:A:323:LYS:HZ1	3:A:328:ARG:NE	1.68	0.91
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.56	0.85
3:A:323:LYS:NZ	3:A:328:ARG:NE	2.26	0.83
13:N:10:DA:H2"	13:N:11:DG:H5"	1.62	0.81
3:A:1111:MET:HG3	3:A:1114:PRO:HG3	1.62	0.79

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	Perce	ntiles
3	А	1385/1733~(80%)	1327~(96%)	58 (4%)	0	100	100
4	В	1104/1224~(90%)	1067~(97%)	37~(3%)	0	100	100
5	С	265/318~(83%)	260~(98%)	5 (2%)	0	100	100
6	Ε	210/215~(98%)	201 (96%)	9~(4%)	0	100	100
7	F	84/155~(54%)	84 (100%)	0	0	100	100
8	Н	129/146~(88%)	113 (88%)	16 (12%)	0	100	100
9	Ι	116/122~(95%)	113~(97%)	3~(3%)	0	100	100
10	J	63/70~(90%)	62~(98%)	1 (2%)	0	100	100
11	Κ	112/120~(93%)	107~(96%)	5 (4%)	0	100	100
12	L	41/70~(59%)	40 (98%)	1 (2%)	0	100	100
All	All	3509/4173~(84%)	3374 (96%)	135 (4%)	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 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		
3	А	1206/1520~(79%)	1168~(97%)	38~(3%)	39	74	
4	В	955/1061~(90%)	928~(97%)	27 (3%)	43	77	
5	С	235/274~(86%)	234 (100%)	1 (0%)	91	97	
6	Е	193/197~(98%)	187 (97%)	6 (3%)	40	75	

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
7	F	73/137~(53%)	72 (99%)	1 (1%)	67	88
8	Н	116/128~(91%)	110 (95%)	6 (5%)	23	59
9	Ι	110/116~(95%)	108 (98%)	2 (2%)	59	85
10	J	60/65~(92%)	58 (97%)	2 (3%)	38	73
11	Κ	99/102~(97%)	98~(99%)	1 (1%)	76	91
12	L	37/57~(65%)	36~(97%)	1 (3%)	44	77
All	All	3084/3657~(84%)	2999 (97%)	85 (3%)	43	77

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5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	В	722	ASP
6	Е	157	SER
4	В	996	ARG
5	С	137	LYS
8	Н	38	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such side chains are listed below:

Mol	Chain	Res	Type
4	В	835	GLN
4	В	1205	GLN
6	Е	147	HIS
3	А	1390	ASN
3	А	1312	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9~(88%)	0	0

There are no RNA backbone outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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 (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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	R	9/9~(100%)	-0.59	0 100 100	83, 94, 157, 160	0
2	Т	28/30~(93%)	-0.28	0 100 100	75, 167, 234, 236	0
3	А	1397/1733~(80%)	-0.15	34 (2%) 59 30	45, 105, 184, 302	0
4	В	1124/1224 (91%)	-0.19	10 (0%) 84 63	44, 88, 156, 208	0
5	С	267/318~(83%)	-0.39	1 (0%) 92 79	53, 89, 145, 197	0
6	Е	212/215~(98%)	-0.10	4 (1%) 66 37	78, 134, 194, 239	0
7	F	86/155~(55%)	-0.31	0 100 100	73, 104, 141, 206	0
8	Н	133/146~(91%)	0.25	8 (6%) 21 7	96, 129, 194, 228	0
9	Ι	118/122~(96%)	-0.40	0 100 100	66, 109, 159, 217	0
10	J	65/70~(92%)	-0.28	0 100 100	63, 88, 128, 168	0
11	Κ	114/120~(95%)	-0.38	0 100 100	60, 96, 144, 161	0
12	L	43/70~(61%)	0.26	3 (6%) 16 5	76, 161, 223, 257	0
13	Ν	18/20~(90%)	0.01	0 100 100	144, 197, 246, 267	0
All	All	3614/4232~(85%)	-0.18	60 (1%) 70 41	44, 101, 180, 302	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	А	1252	THR	12.5
3	А	1254	ALA	9.3
3	А	1251	GLU	8.5
3	А	1250	ALA	6.2
3	А	1245	PRO	6.1

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 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^{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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
15	ZN	А	1801	1/1	0.79	0.10	330,330,330,330	0
15	ZN	С	401	1/1	0.90	0.34	240,240,240,240	0
15	ZN	L	101	1/1	0.92	0.11	388,388,388,388	0
15	ZN	В	1301	1/1	0.93	0.13	$155,\!155,\!155,\!155$	0
15	ZN	J	101	1/1	0.94	0.23	83,83,83,83	0
15	ZN	Ι	202	1/1	0.94	0.13	97,97,97,97	0
14	MG	R	2001	1/1	0.96	0.20	127,127,127,127	0
15	ZN	Ι	201	1/1	0.98	0.13	113,113,113,113	0
15	ZN	А	1802	1/1	0.99	0.09	113,113,113,113	0

6.5 Other polymers (i)

There are no such residues in this entry.

