



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

PDB ID : 3RZO
Title : RNA Polymerase II Initiation Complex with a 4-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-12
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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

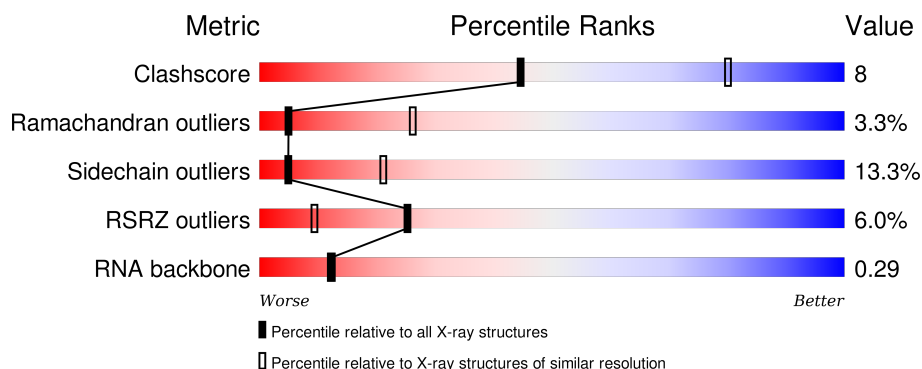
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	1733	<div> <div>8%</div> <div> <div></div> <div>58%</div> <div>20%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	1224	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>57%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
4	E	215	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>•</div> </div> </div>
5	F	155	<div> <div></div> <div> <div></div> <div>43%</div> <div>10%</div> <div>•</div> <div>45%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	4	
12	T	29	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28547 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	4	Total	C	N	O	P	0	0	0
			88	40	20	25	3			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	8	Total	C	N	O	P	0	0	0
			159	76	26	49	8			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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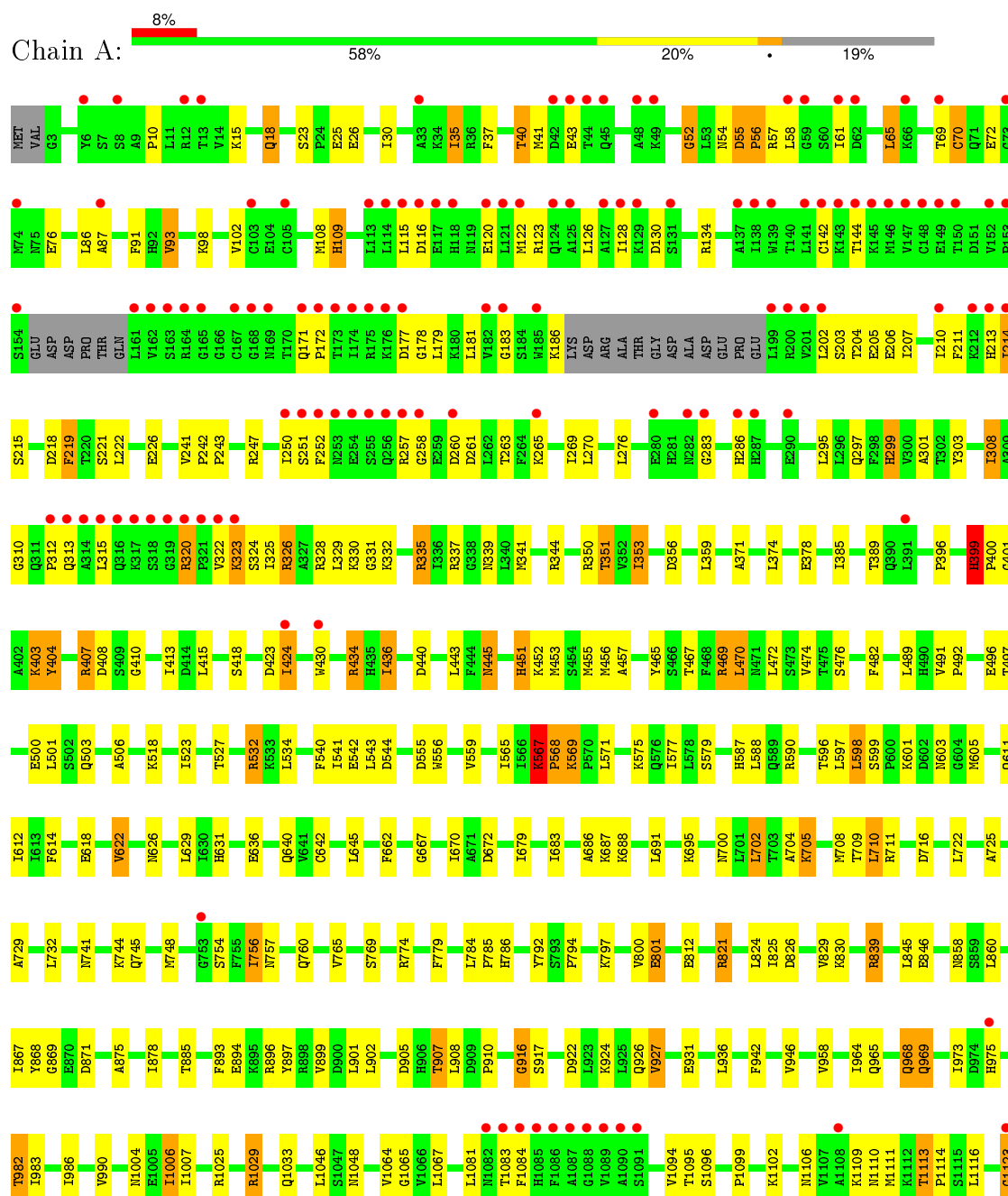
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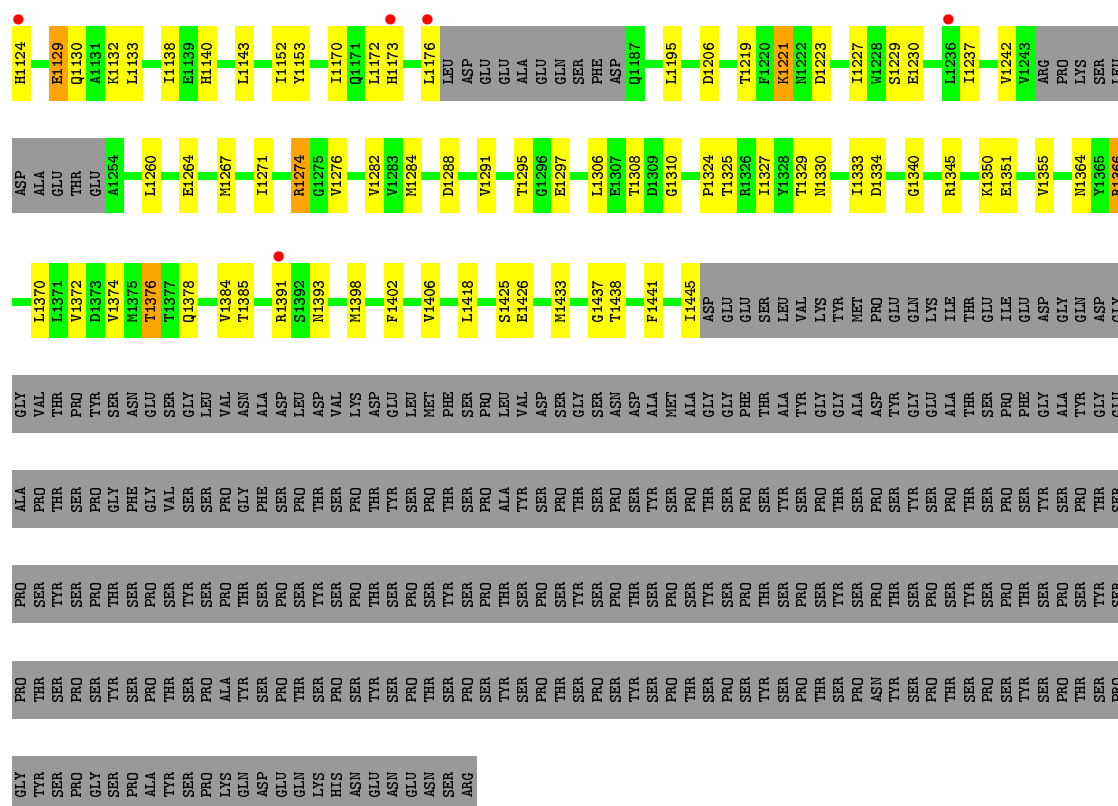
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

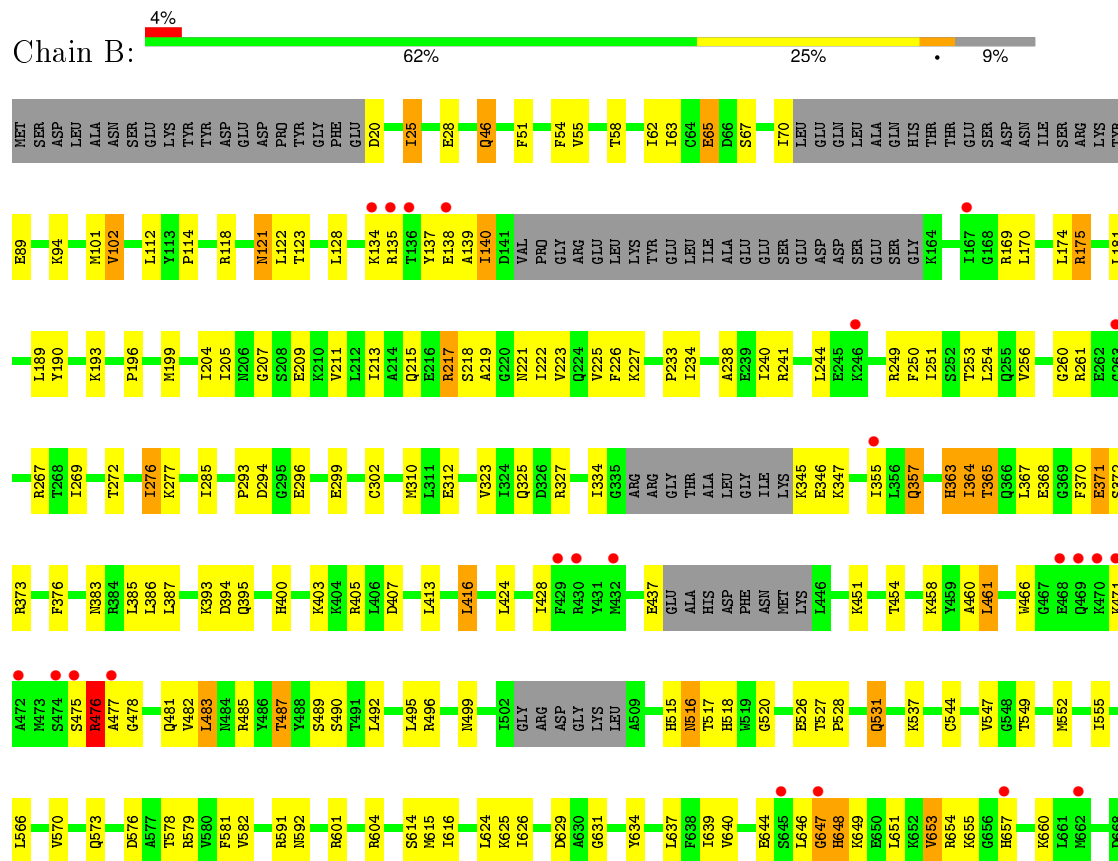
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

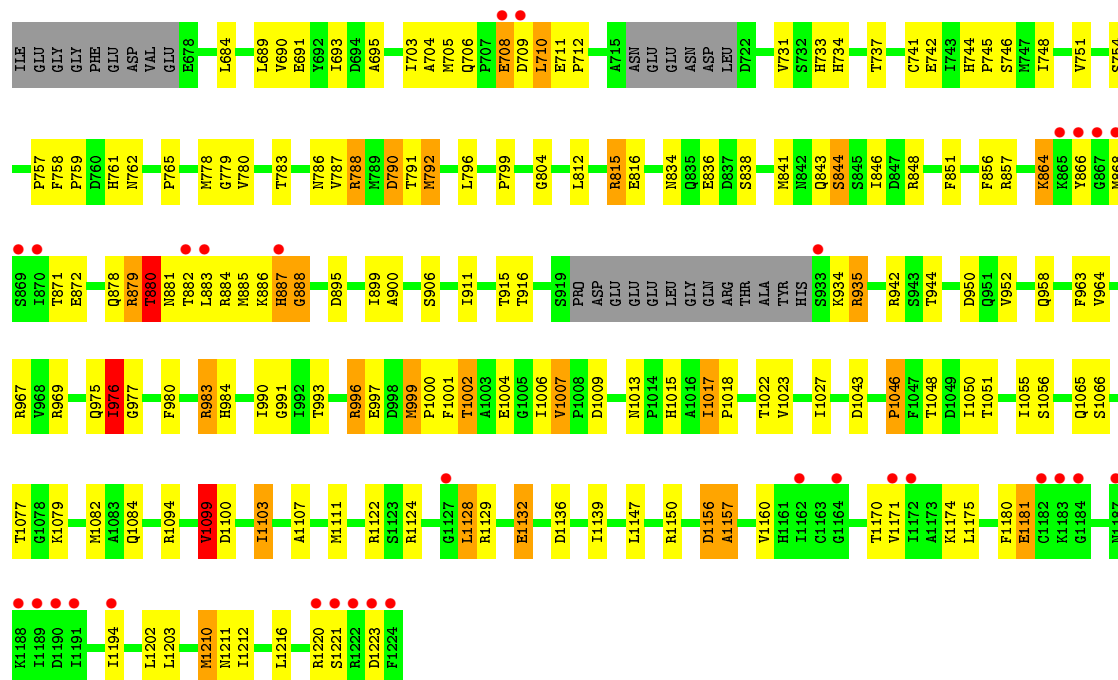
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



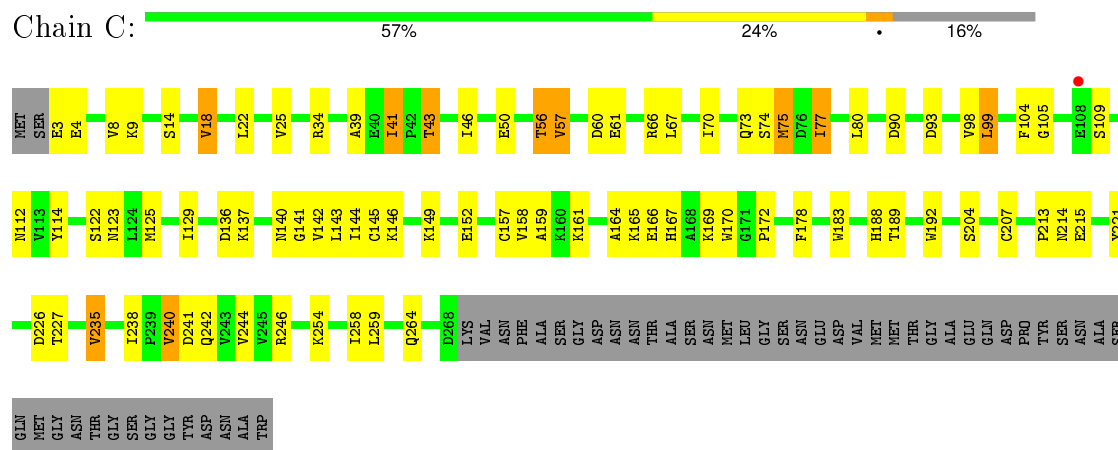


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

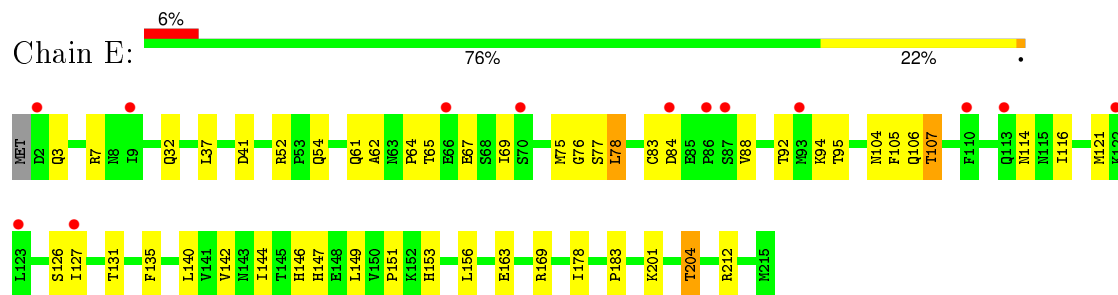




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



MET SER ASP TYR GLU ALA PHE ASN ASP GLY ASN GLU ASP PHE ASP VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU LYS LYS LYS THR THR GLY GLY GLY ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LYS E71 K72 K76 R79 T82 E89 R90 I93 F108 Y109 D110 L111 L118 K123 K129 PHE LYS I134 R135 R136 S142 T146 D154 L155

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 5% 61% 28% 9%

MET S2 R3 Q11 V12 S13 E14 V15 K22 V23 C24 R25 I26 Q35 F47 S61 S62 L63 ASN LEU GLU ASP THR PRO PRQ ALA ASN ASP SER SER SER ALA T76 R77 S78 Q83 A84 G85 D86 R87 S88 L89 A90 D91 D92 Y93 D94 Y95 Y96 N97 T100 S108 K109 D110

L111 T112 A113 G120 L121 L122 E126 R130 M131 L132 L135 K136 Q137 E138 M139 A140 R145 R146

- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 2% 77% 19% 2%

MET T2 N12 L26 E27 E28 V35 E36 V37 P41 Q60 D61 L63 F69 R70 C75 F76 K77 C78 N83 V84 Q87 Q90 D94 T95 S96 M97 L104 T111 K115 R118 T119 Q120 PHE SER

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 56% 29% 9% 7%

M1 I2 V3 R6 C7 G10 G11 K12 V13 V14 W18 E19 L22 Q26 E27 D28 D31 R43 R48 M49 I50 L51 T52 K59 F60 L61 R62 Y63 R64 P65 LEU GLU LYS ARG ASP

- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 76% 14% 5% 5%

W1 R6 F7 F10 L11 E14 G15 E16 A17 K18 L19 K20 I21 K26 V31 V32 I33 L51 V63 E64 H65 P66 F67 R74 L101 E108 W109 W110 L111 L114 ALA ASP ASP ALA PHE

- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 4% 29% 26% 10% 34%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR A25 T26 L27 K28 A32 F33 C34 S35 S36 K37 L38 S39 R42 T43 D44 A45 V46 R47 D50 C51 G52 H53 F54 I55 L56 K58 A59 R60 T61 A62 R63 L64

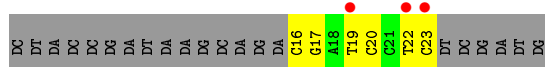
V65 Q66 F67 R70

- Molecule 11: RNA (5'-R(*GP*AP*GP*G)-3')

Chain R: 50% 100%



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*C
P*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.04Å 221.15Å 192.88Å 90.00° 98.34° 90.00°	Depositor
Resolution (Å)	40.01 – 3.00 40.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.01-3.00) 99.3 (40.01-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.188 , 0.236 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 112.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 132696 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28547	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/11241	0.76	2/15199 (0.0%)
2	B	0.52	0/9033	0.79	4/12181 (0.0%)
3	C	0.47	0/2133	0.80	0/2891
4	E	0.45	0/1788	0.71	0/2406
5	F	0.46	0/700	0.70	0/945
6	H	0.47	0/1086	0.82	1/1470 (0.1%)
7	I	0.48	0/989	0.79	0/1331
8	J	0.55	0/541	0.86	0/727
9	K	0.45	0/937	0.70	0/1265
10	L	0.54	0/365	0.93	1/485 (0.2%)
11	R	0.88	0/99	1.45	0/154
12	T	1.25	0/176	2.19	12/268 (4.5%)
All	All	0.50	0/29088	0.80	20/39322 (0.1%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	O4'-C1'-N1	8.75	114.12	108.00
2	B	647	GLY	C-N-CA	8.32	142.50	121.70
12	T	22	DT	P-O3'-C3'	7.60	128.82	119.70
12	T	16	DC	C2-N1-C1'	6.96	126.45	118.80
12	T	20	DC	O4'-C1'-N1	6.96	112.87	108.00

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	11043	0	11133	182	0
2	B	8861	0	8884	190	0
3	C	2095	0	2051	51	0
4	E	1752	0	1776	18	0
5	F	688	0	707	9	0
6	H	1068	0	1040	12	0
7	I	971	0	927	7	0
8	J	532	0	542	20	0
9	K	919	0	929	16	0
10	L	363	0	386	13	0
11	R	88	0	46	0	0
12	T	159	0	91	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	28547	0	28512	452	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.

The worst 5 of 452 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:756:ILE:CD1	1:A:756:ILE:CG1	1.77	1.56
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.90	1.06
1:A:869:GLY:O	4:E:204:THR:HG21	1.63	0.96
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.89	0.88
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.39	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1395/1733 (80%)	1239 (89%)	110 (8%)	46 (3%)	5	26
2	B	1096/1224 (90%)	962 (88%)	91 (8%)	43 (4%)	4	21
3	C	264/318 (83%)	238 (90%)	22 (8%)	4 (2%)	13	50
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	21	64
5	F	83/155 (54%)	77 (93%)	5 (6%)	1 (1%)	16	56
6	H	129/146 (88%)	101 (78%)	21 (16%)	7 (5%)	2	14
7	I	117/122 (96%)	102 (87%)	13 (11%)	2 (2%)	11	46
8	J	63/70 (90%)	58 (92%)	2 (3%)	3 (5%)	3	17
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	21	64
10	L	44/70 (63%)	31 (70%)	7 (16%)	6 (14%)	0	1
All	All	3515/4173 (84%)	3115 (89%)	285 (8%)	115 (3%)	5	26

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	ASP
1	A	56	PRO
1	A	109	HIS
1	A	260	ASP

5.3.2 Protein sidechains

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	1225/1520 (81%)	1066 (87%)	159 (13%)	5	22
2	B	967/1061 (91%)	842 (87%)	125 (13%)	5	23
3	C	234/274 (85%)	205 (88%)	29 (12%)	6	24
4	E	196/197 (100%)	170 (87%)	26 (13%)	5	21
5	F	75/137 (55%)	71 (95%)	4 (5%)	28	67
6	H	117/128 (91%)	94 (80%)	23 (20%)	1	9
7	I	113/116 (97%)	98 (87%)	15 (13%)	5	21
8	J	60/65 (92%)	49 (82%)	11 (18%)	2	11
9	K	99/102 (97%)	86 (87%)	13 (13%)	5	22
10	L	40/57 (70%)	29 (72%)	11 (28%)	0	2
All	All	3126/3657 (86%)	2710 (87%)	416 (13%)	5	21

5 of 416 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	276	ILE
2	B	690	VAL
8	J	13	VAL
2	B	323	VAL
2	B	476	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1258	HIS
2	B	363	HIS
4	E	147	HIS
1	A	1364	ASN
2	B	46	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/4 (75%)	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1405/1733 (81%)	0.28	130 (9%) 11 4	63, 111, 202, 234	0
2	B	1114/1224 (91%)	0.07	54 (4%) 34 14	62, 96, 166, 219	0
3	C	266/318 (83%)	-0.09	1 (0%) 93 80	67, 94, 132, 186	0
4	E	214/215 (99%)	0.21	13 (6%) 25 9	81, 139, 193, 210	0
5	F	85/155 (54%)	0.09	0 100 100	81, 115, 159, 172	0
6	H	133/146 (91%)	0.36	7 (5%) 30 12	109, 151, 177, 187	0
7	I	119/122 (97%)	0.01	2 (1%) 73 45	78, 114, 150, 167	0
8	J	65/70 (92%)	-0.08	0 100 100	65, 83, 114, 130	0
9	K	114/120 (95%)	-0.11	0 100 100	66, 102, 126, 149	0
10	L	46/70 (65%)	0.11	3 (6%) 22 8	82, 119, 152, 176	0
11	R	4/4 (100%)	2.15	2 (50%) 0 0	210, 216, 218, 219	0
12	T	8/29 (27%)	2.22	3 (37%) 0 0	200, 204, 210, 211	0
All	All	3573/4206 (84%)	0.16	215 (6%) 25 9	62, 106, 192, 234	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	9.3
1	A	1087	ALA	9.1
1	A	182	VAL	8.7
1	A	1090	ALA	6.6
2	B	647	GLY	6.5

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
13	ZN	L	105	1/1	0.94	0.11	-0.70	111,111,111,111	0
13	ZN	A	1734	1/1	0.22	0.26	-0.97	300,300,300,300	0
13	ZN	J	101	1/1	0.93	0.15	-1.25	88,88,88,88	0
13	ZN	B	1307	1/1	0.79	0.07	-1.95	206,206,206,206	0
13	ZN	A	1735	1/1	0.74	0.05	-2.14	177,177,177,177	0
13	ZN	I	204	1/1	0.95	0.05	-2.45	90,90,90,90	0
13	ZN	I	203	1/1	0.94	0.04	-2.68	113,113,113,113	0
13	ZN	C	319	1/1	0.92	0.05	-3.21	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.