



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:19 PM GMT

PDB ID : 4BXZ  
Title : RNA Polymerase II-Bye1 complex  
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.  
Deposited on : 2013-07-16  
Resolution : 4.80 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](mailto: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.

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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



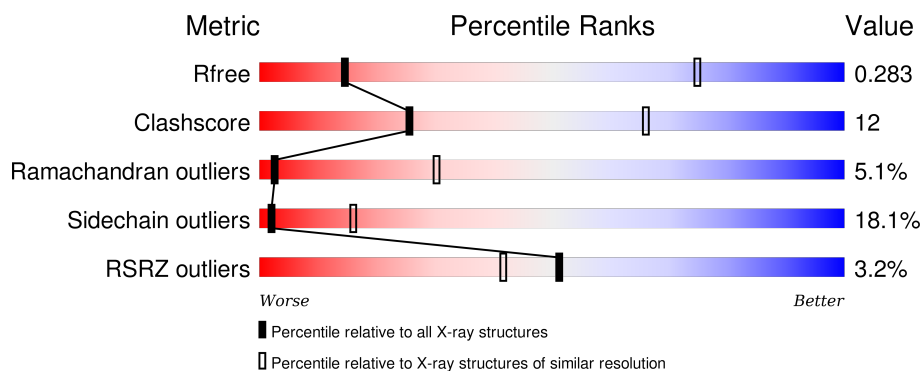
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 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))
$R_{free}$	91344	1117 (6.00-3.60)
Clashscore	102246	1017 (5.96-3.64)
Ramachandran outliers	100387	1156 (6.00-3.60)
Sidechain outliers	100360	1134 (6.00-3.60)
RSRZ outliers	91569	1120 (6.00-3.60)

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  $\geq 3$ , 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	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	

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Mol	Chain	Length	Quality of chain
6	F	155	<div><div></div><div>28%23%46%</div></div>
7	G	171	<div><div>4%</div><div>67%31%</div><div></div></div>
8	H	146	<div><div>6%</div><div>47%38%9%</div><div></div></div>
9	I	122	<div><div>11%</div><div>61%34%</div><div></div></div>
10	J	70	<div><div></div><div>47%37%6%7%</div><div></div></div>
11	K	120	<div><div>%</div><div>65%24%7%</div><div></div></div>
12	L	70	<div><div></div><div>37%20%7%34%</div><div></div></div>
13	X	594	<div><div>%</div><div>17%81%</div><div></div></div>



## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 31509 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	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- 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 POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- 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	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- 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	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a protein called TRANSCRIPTION FACTOR BYE1.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	X	113	Total	C	N	O	0	0	0
			564	338	113	113			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

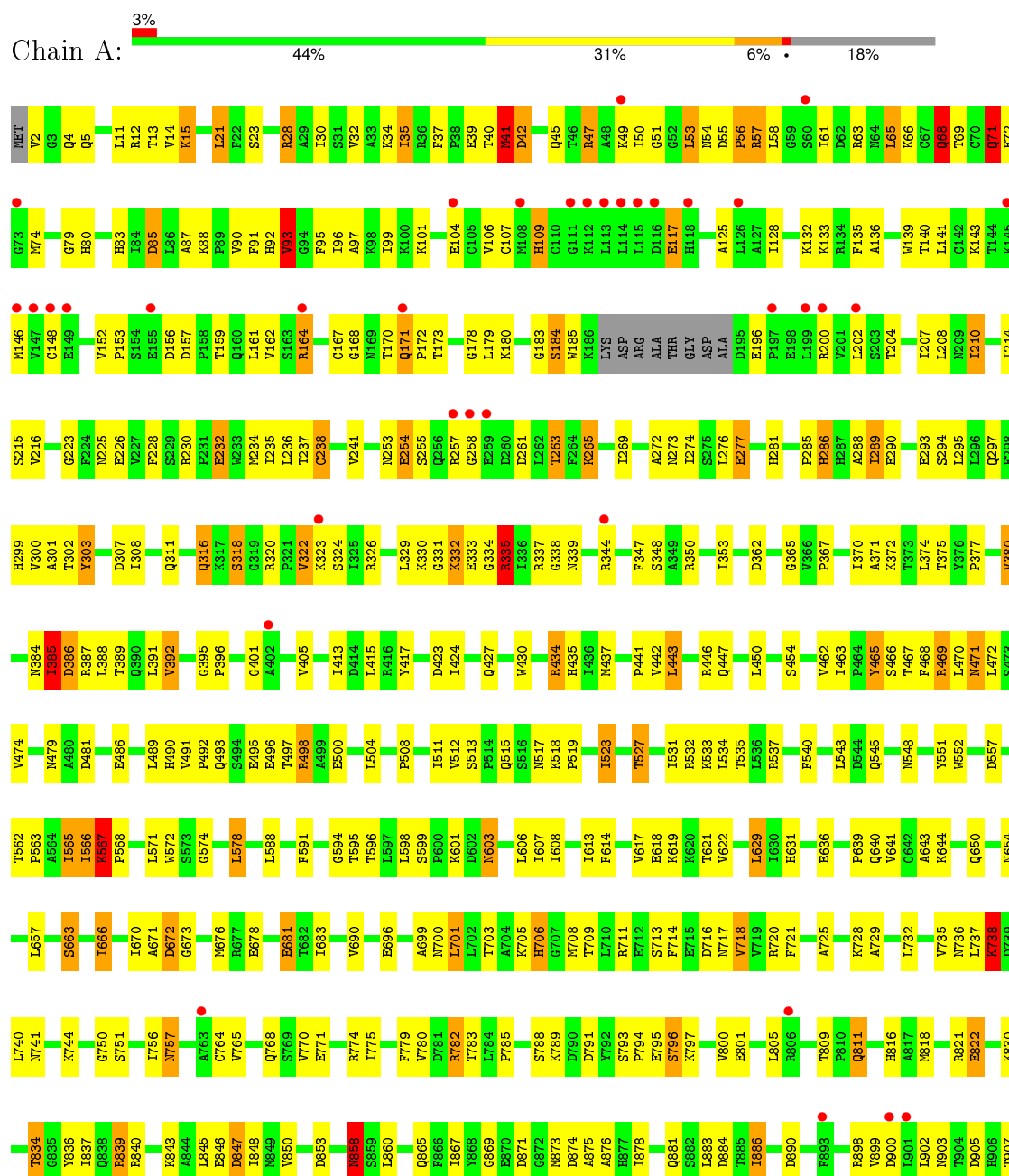
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		



### 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 ( $RSRZ > 2$ ). 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

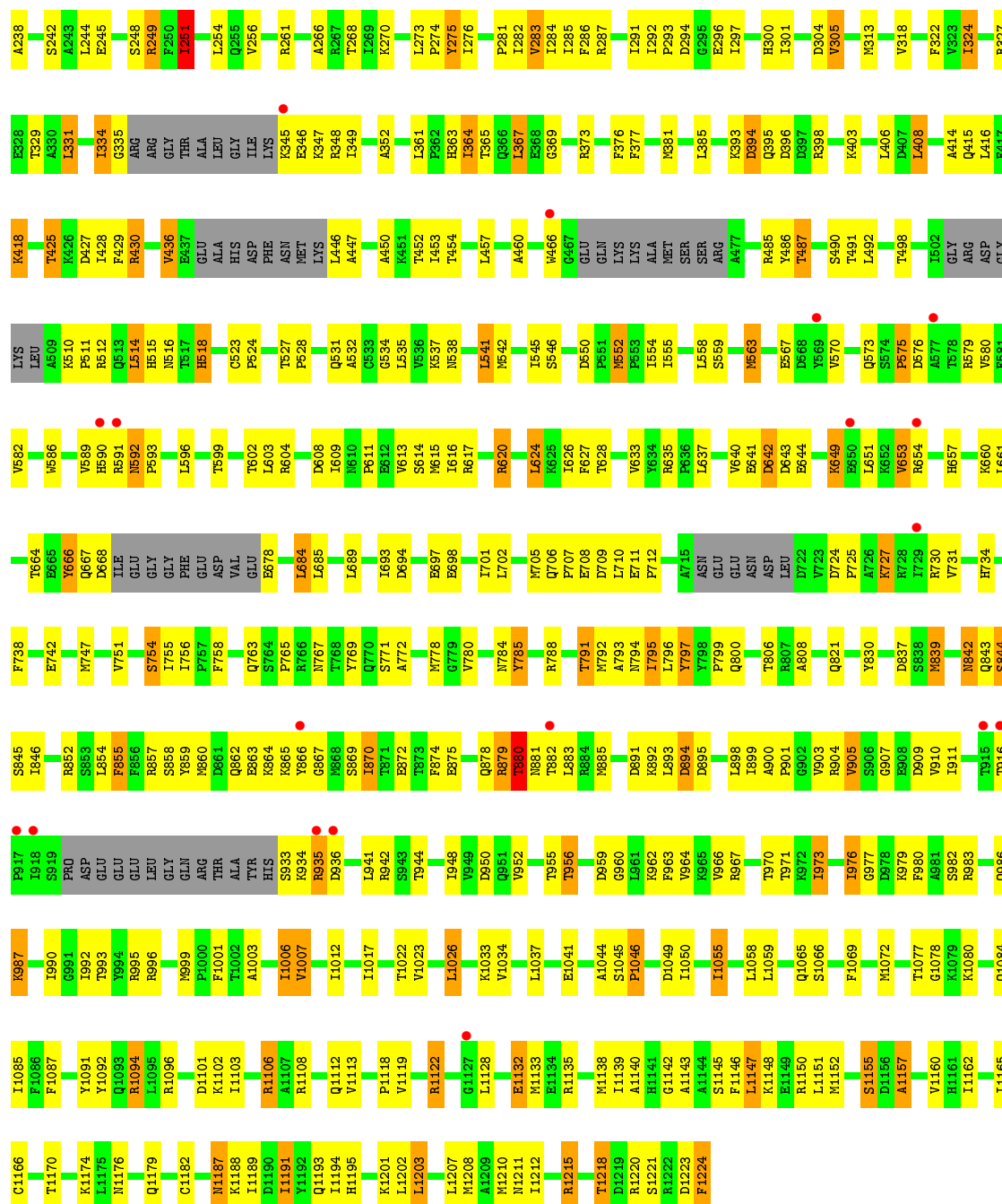




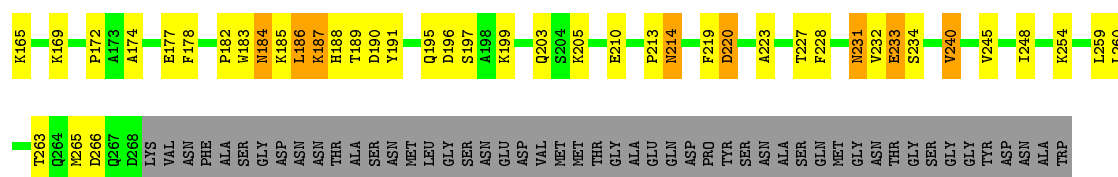


LEU	GLN	MET
LYS	HIS	SER
TYR	THR	ASP
GLU	THR	GLU
LEU	GLU	ALA
IIE	SER	ASN
ALA	ASP	SER
GLU	ASN	GLU
GLU	IIE	LVS
SER	SER	TYR
GLU	ARG	TYR
ASP	LVS	ASP
ASP	TYR	GLU
SER	GLU	ASP
GLU	I90	PRQ
GLY	S91	TYR
GLY	F92	GLY
K164	M101	PHE
G168	V102	DLQ
R169	N103	E21
L170		
P171	D106	I25
K177	G107	
	V108	V93
L181	L112	I34
D188	V113	S35
L189	P114	A36
	Q115	F97
L192	R118	F38
I204	L119	R39
I205	N121	E40
E206	L122	K41
G207	T123	
S208	I124	V44
E209	S125	S45
K210	I226	Q46
V211	G127	
	L128	S90
A214	F129	F31
Q215	V130	N32
E216	D131	V55
	V132	D56
N221	K133	Y57
I222	K134	T58
V223	ARG	L59
Q224	TYR	D61
Q225	TYR	I62
F226	GLU	I63
K227	ALA	
K228	IIE	S67
A229	ASP	
	VAL	T70
S232		LEU
E236	GLY	GLU
H237	PRQ	GLN
	ARG	LEU
	GLU	ALA

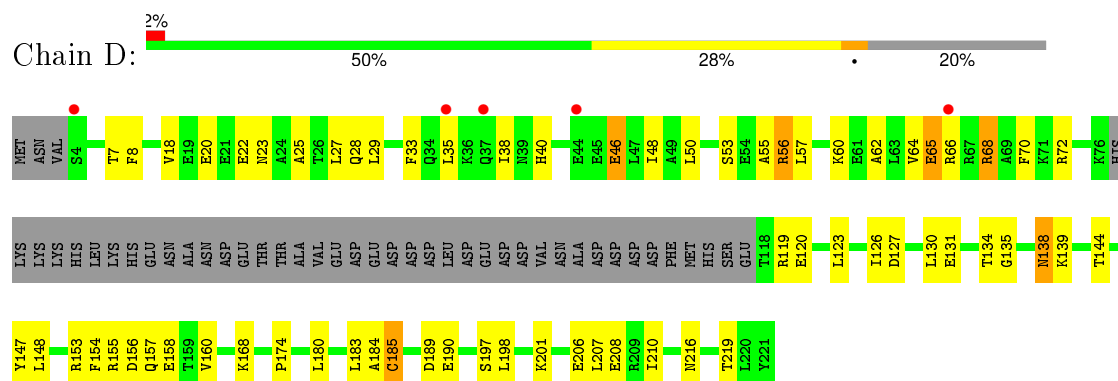




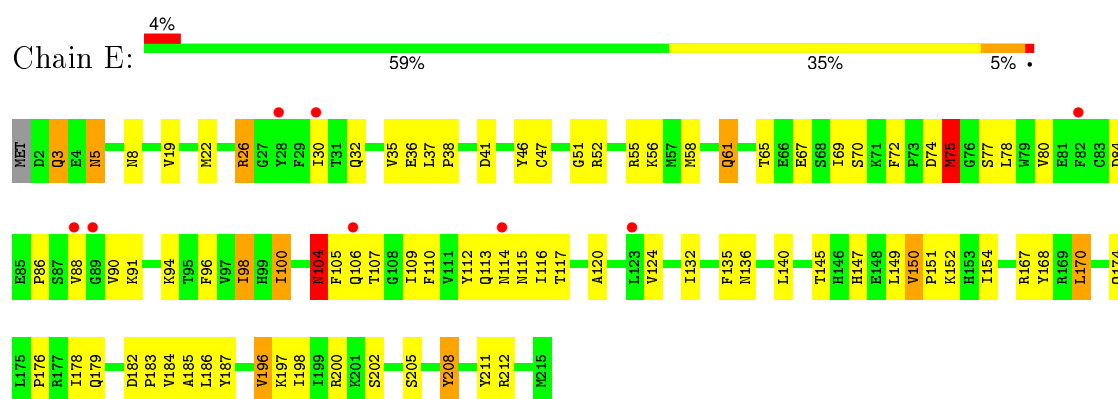




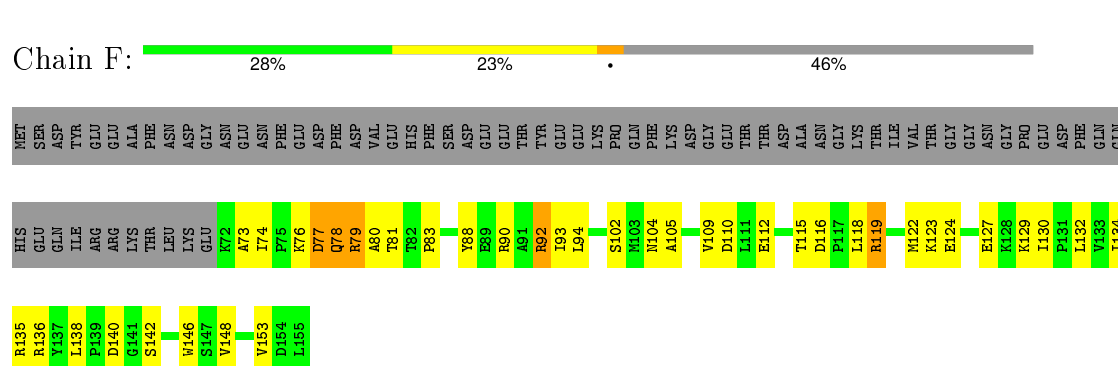
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1



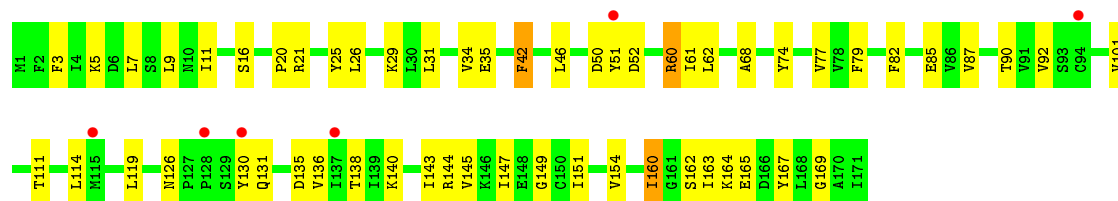
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



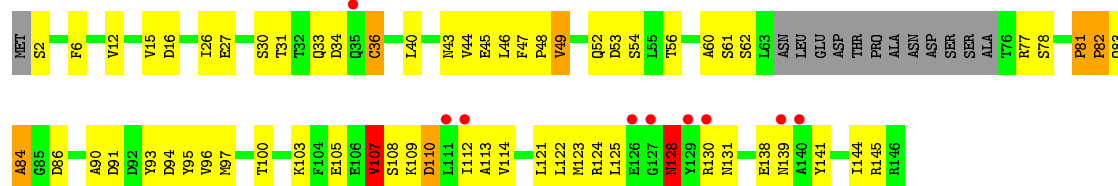
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



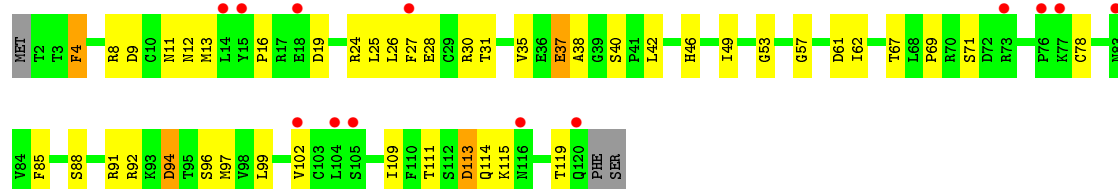




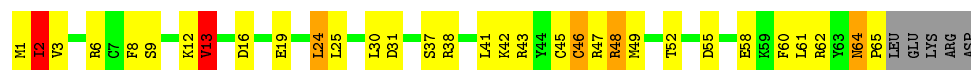
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3



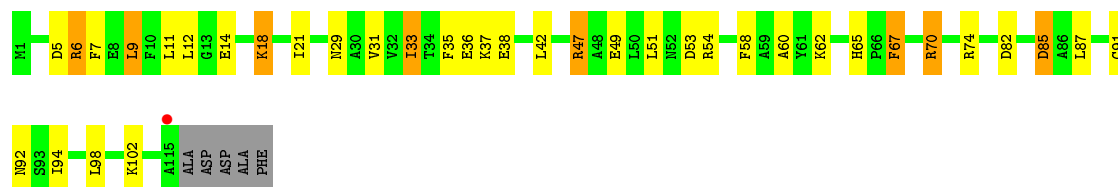
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

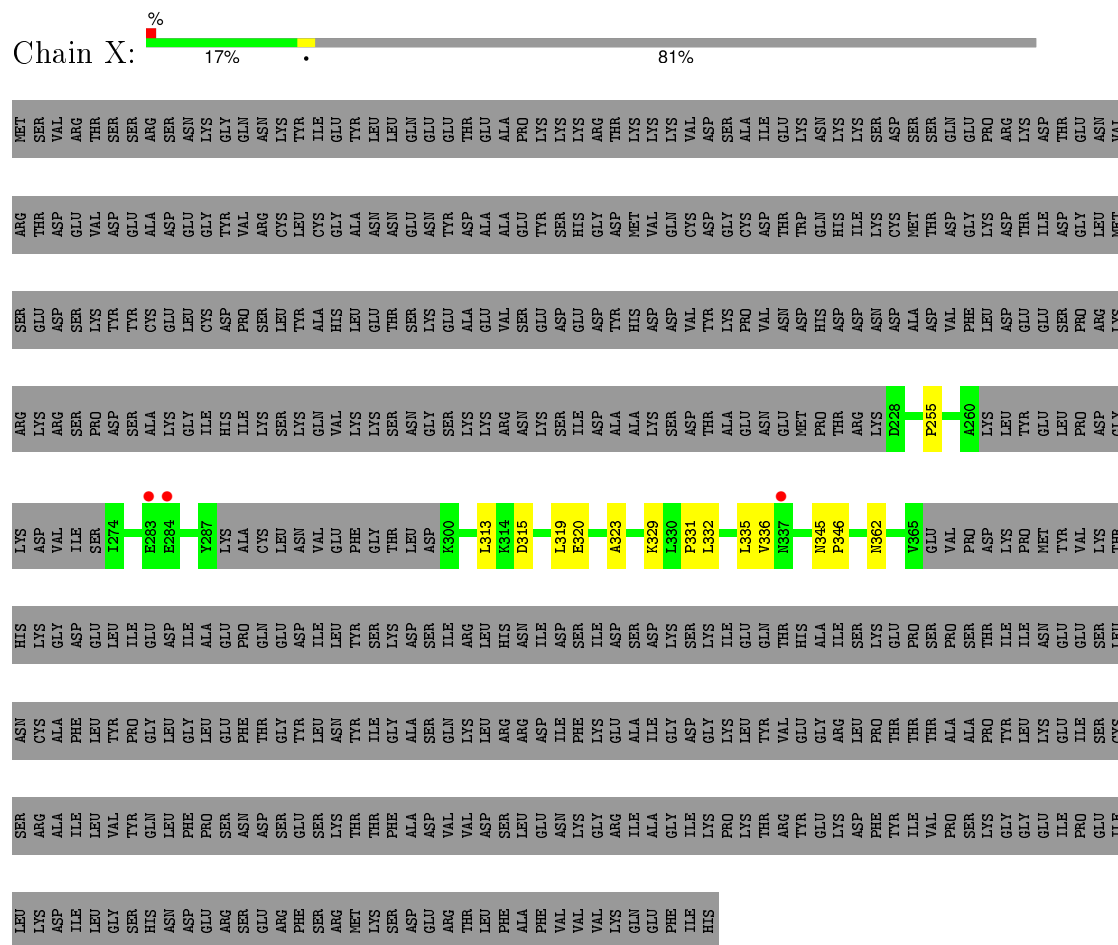


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4





- Molecule 13: TRANSCRIPTION FACTOR BYE1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.55Å 392.09Å 279.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 4.80 49.63 – 4.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.63-4.80) 100.0 (49.63-4.80)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 4.86Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.191 , 0.253 0.218 , 0.283	Depositor DCC
$R_{free}$ test set	1169 reflections (1.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	151.9	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 289.9	EDS
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.039 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 59394 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	31509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MG

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	0.53	0/11339	0.82	2/15334 (0.0%)
2	B	0.52	0/8889	0.80	2/11987 (0.0%)
3	C	0.48	0/2133	0.77	0/2891
4	D	0.51	0/1365	0.82	0/1837
5	E	0.48	0/1788	0.77	0/2406
6	F	0.54	0/691	0.82	0/933
7	G	0.47	0/1368	0.78	0/1844
8	H	0.53	0/1086	0.85	2/1470 (0.1%)
9	I	0.48	0/989	0.79	0/1331
10	J	0.52	0/541	0.77	0/727
11	K	0.49	0/938	0.75	0/1267
12	L	0.54	0/365	0.94	0/485
13	X	0.62	0/561	0.88	3/780 (0.4%)
All	All	0.52	0/32053	0.81	9/43292 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	56	PRO	C-N-CA	6.43	137.77	121.70
13	X	255	PRO	N-CA-CB	6.15	110.67	103.30
13	X	346	PRO	N-CA-CB	5.66	110.09	103.30
13	X	331	PRO	N-CA-CB	5.54	109.94	103.30
1	A	858	ASN	C-N-CA	5.39	135.18	121.70

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	11140	0	11218	359	0
2	B	8720	0	8745	225	0
3	C	2095	0	2051	71	0
4	D	1356	0	1319	31	0
5	E	1752	0	1776	46	0
6	F	679	0	701	21	0
7	G	1340	0	1357	26	0
8	H	1068	0	1040	29	0
9	I	971	0	930	25	0
10	J	532	0	543	16	0
11	K	920	0	929	27	0
12	L	363	0	386	12	0
13	X	564	0	239	4	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31509	0	31234	783	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 12.

The worst 5 of 783 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:C:83:SER:HA	3:C:95:CYS:HB2	1.36	1.05
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.38	1.04
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.46	0.97
1:A:821:ARG:HG2	2:B:514:LEU:H	1.31	0.95
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.53	0.89

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	1406/1733 (81%)	1111 (79%)	218 (16%)	77 (6%)	2	29
2	B	1075/1224 (88%)	861 (80%)	155 (14%)	59 (6%)	2	29
3	C	264/318 (83%)	208 (79%)	47 (18%)	9 (3%)	5	41
4	D	173/221 (78%)	144 (83%)	18 (10%)	11 (6%)	2	25
5	E	212/215 (99%)	176 (83%)	30 (14%)	6 (3%)	6	45
6	F	82/155 (53%)	69 (84%)	11 (13%)	2 (2%)	7	48
7	G	169/171 (99%)	143 (85%)	22 (13%)	4 (2%)	7	48
8	H	129/146 (88%)	96 (74%)	17 (13%)	16 (12%)	0	8
9	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	7	46
10	J	63/70 (90%)	46 (73%)	14 (22%)	3 (5%)	3	32
11	K	113/120 (94%)	94 (83%)	18 (16%)	1 (1%)	21	67
12	L	44/70 (63%)	25 (57%)	13 (30%)	6 (14%)	0	7
13	X	107/594 (18%)	83 (78%)	20 (19%)	4 (4%)	4	39
All	All	3954/5159 (77%)	3152 (80%)	601 (15%)	201 (5%)	2	30

5 of 201 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	47	ARG
1	A	57	ARG
1	A	65	LEU
1	A	71	GLN

### 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	1239/1520 (82%)	998 (80%)	241 (20%)	2	13
2	B	952/1061 (90%)	773 (81%)	179 (19%)	2	14
3	C	234/274 (85%)	197 (84%)	37 (16%)	3	22
4	D	140/200 (70%)	115 (82%)	25 (18%)	2	16
5	E	196/197 (100%)	164 (84%)	32 (16%)	3	21
6	F	74/137 (54%)	62 (84%)	12 (16%)	3	21
7	G	152/152 (100%)	130 (86%)	22 (14%)	4	26
8	H	117/128 (91%)	101 (86%)	16 (14%)	4	28
9	I	113/116 (97%)	98 (87%)	15 (13%)	5	29
10	J	60/65 (92%)	45 (75%)	15 (25%)	1	6
11	K	99/102 (97%)	82 (83%)	17 (17%)	2	18
12	L	40/57 (70%)	31 (78%)	9 (22%)	1	9
All	All	3416/4009 (85%)	2796 (82%)	620 (18%)	2	16

5 of 620 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	334	ILE
2	B	842	ASN
9	I	92	ARG
2	B	395	GLN
2	B	567	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	206	ASN
2	B	538	ASN
9	I	12	ASN
2	B	215	GLN
2	B	415	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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 ⓘ

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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1416/1733 (81%)	0.22	55 (3%) 43 36	118, 185, 242, 274	0
2	B	1097/1224 (89%)	0.19	21 (1%) 70 62	111, 200, 254, 282	0
3	C	266/318 (83%)	0.21	6 (2%) 64 55	139, 193, 237, 271	0
4	D	177/221 (80%)	0.19	5 (2%) 56 48	149, 199, 250, 261	0
5	E	214/215 (99%)	0.38	8 (3%) 45 37	153, 223, 267, 279	0
6	F	84/155 (54%)	0.17	0 100 100	113, 165, 217, 239	0
7	G	171/171 (100%)	0.26	6 (3%) 48 40	157, 188, 230, 261	0
8	H	133/146 (91%)	0.56	9 (6%) 20 16	185, 229, 254, 261	0
9	I	119/122 (97%)	0.62	13 (10%) 7 8	185, 233, 264, 271	0
10	J	65/70 (92%)	0.04	0 100 100	148, 173, 225, 245	0
11	K	115/120 (95%)	0.23	1 (0%) 85 80	140, 182, 230, 246	0
12	L	46/70 (65%)	0.30	0 100 100	153, 242, 260, 266	0
13	X	113/594 (19%)	0.33	3 (2%) 58 49	232, 271, 294, 295	0
All	All	4016/5159 (77%)	0.24	127 (3%) 51 42	111, 196, 260, 295	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	3.9
1	A	114	LEU	3.5
1	A	164	ARG	3.4
1	A	145	LYS	3.3
2	B	132	VAL	3.3

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
14	ZN	J	1066	1/1	0.99	0.30	0.03	192,192,192,192	0
14	ZN	B	2225	1/1	0.99	0.18	-1.35	96,96,96,96	0
14	ZN	I	1121	1/1	0.97	0.09	-1.68	230,230,230,230	0
14	ZN	A	2456	1/1	0.94	0.09	-1.91	181,181,181,181	0
14	ZN	L	1071	1/1	0.84	0.07	-1.96	266,266,266,266	0
14	ZN	I	1122	1/1	0.97	0.25	-2.05	245,245,245,245	0
14	ZN	A	2457	1/1	0.97	0.15	-2.07	105,105,105,105	0
14	ZN	C	1269	1/1	0.98	0.08	-2.07	140,140,140,140	0
15	MG	A	2458	1/1	-0.04	1.05	-	130,130,130,130	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.