



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:56 PM GMT

PDB ID : 1R5U  
Title : RNA POLYMERASE II TFIIB COMPLEX  
Authors : Bushnell, D.A.; Westover, K.D.; Davis, R.; Kornberg, R.D.  
Deposited on : 2003-10-13  
Resolution : 4.50 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

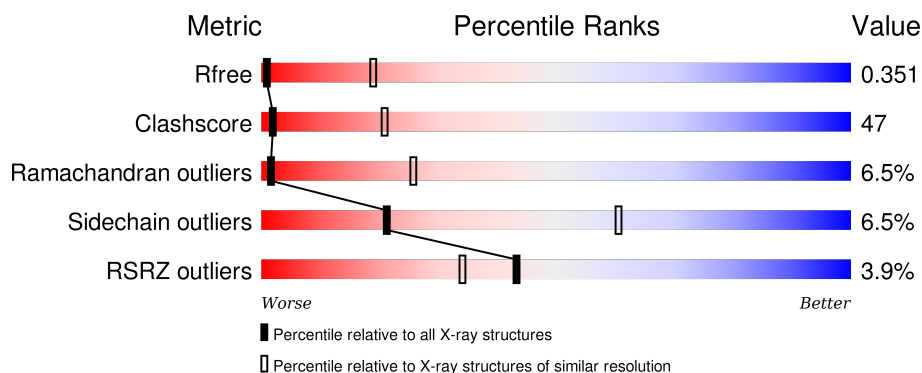
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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	E	215	
5	F	155	

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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	M	86	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	ZN	I	203	-	-	-	X
12	ZN	I	204	-	-	X	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28300 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 largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1380	Total	C	N	O	S	0	0	0
			10850	6847	1898	2044	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8721	5526	1523	1618	54			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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 27 kDa polypeptide.

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 23 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	118	Total	C	N	O	S	0	0	0
			967	594	178	185	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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 13.6 kDa polypeptide.

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 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is a protein called TRANSCRIPTION FACTOR II B (TFIIB).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	86	Total	C	N	O	0	0	0
			343	171	86	86			

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	2	Total 2	Zn 2	0	0
12	C	1	Total 1	Zn 1	0	0
12	A	2	Total 2	Zn 2	0	0
12	L	1	Total 1	Zn 1	0	0
12	M	1	Total 1	Zn 1	0	0

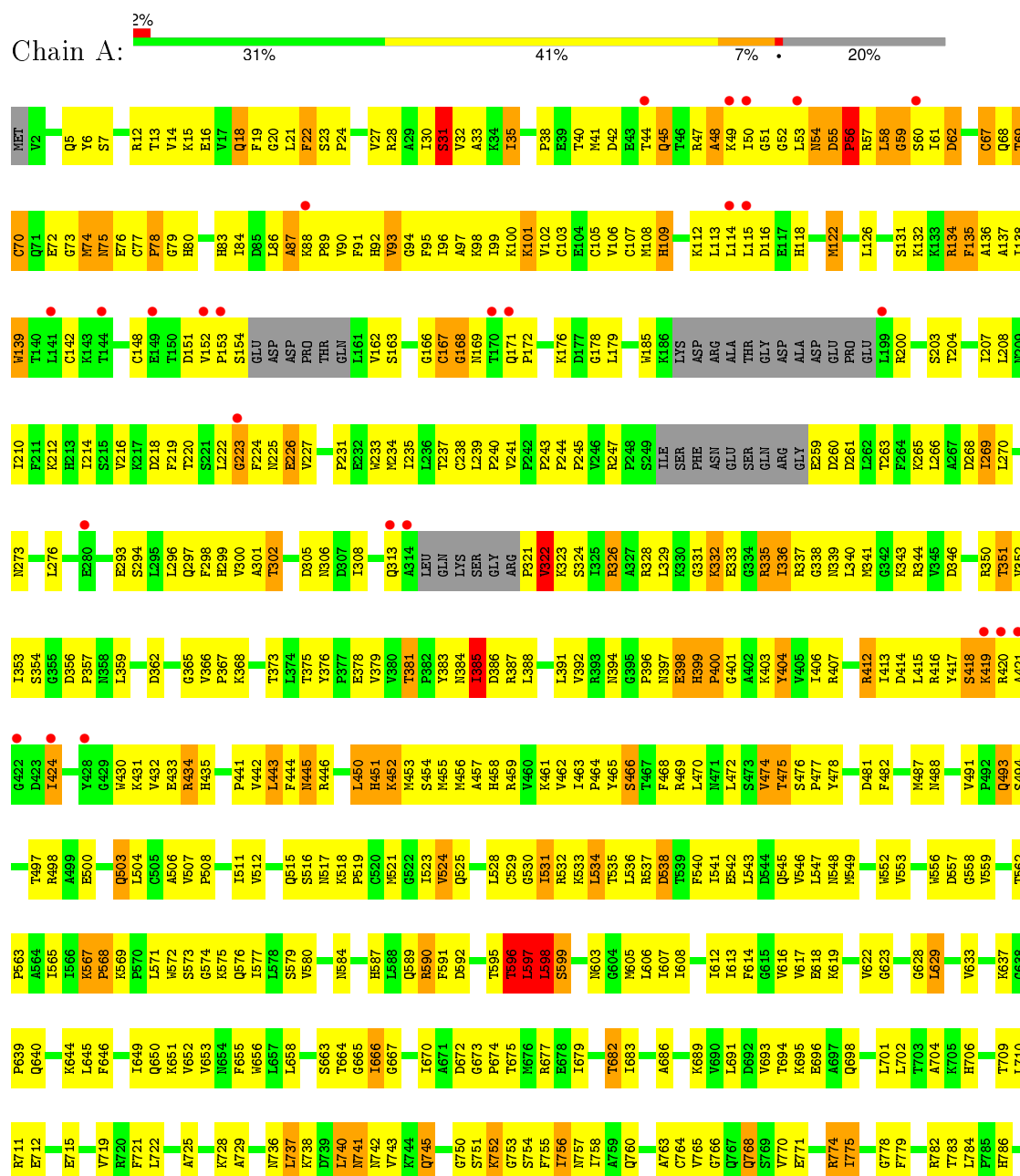
- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total 1	Mg 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 largest subunit

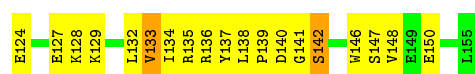




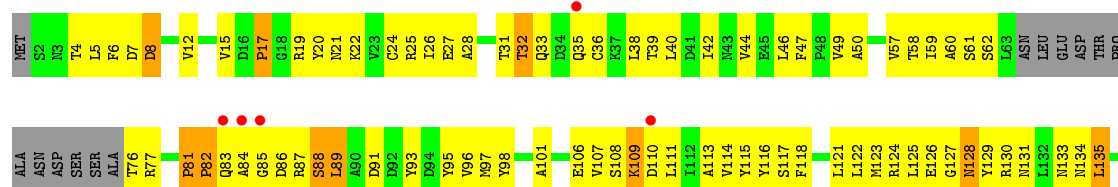


G980	L1030	G987	S831	P759	E699	A830	I555	R485	A409	ARG	T288	D198	V132	D66	MET
L961	L1033	L896	G832	D760	S700	G631	T556	Y486	G410	GLY	T289	M199	K133	L70	SER
A962	R1033	L899	Y833	E761	L701	R632	P557	T487	F417	THR	A271	G200	K134	LEU	ASP
F963	R1033	A900	N834	N762	L702	V633	L588	Y488	R418	ALA		G201	ARG	LEU	LEU
V964	V1034	P901	Q835	Q764	L703	G634	S559	S489	T419	LEU		F203	THR	GLN	ALA
K965	A1035		E836	P765	A704	R635	G562	L485	L420	ILE	P274	F204	TYR	LEU	ASN
V966			D837		N705	P636	N663	R496	F421	GLY		I204	GLY	LEU	SER
	S1038		S838		Q706	F638	L566		R423	ILE		I205	ALA	ALA	GLU
G969	G1039		N839		E708	V639	L566		K423	ILE	K277	N206	ILE	GLN	LYS
N1040	N1040		L840		E709	V640	L566		K423	THR	D279	S208	VAL	HIS	TYR
			N841		L710	E641	Y569		D427	PRO	T280	E209	PRO	THR	ASP
D1043	D1043		N842		E711	D642	V570		K427	GLY	T281	K210	GLY	GLU	GLU
A1044	A1044		Q843		E712	D643			I428	ARG	T282	V211	ARG	SER	ASP
Q975	S1045		S844		A713	E644	Q573		F429	ASP	V283	L212	GLU	ASP	PRO
P1046	P1046		S845		A714		S574		R430	GLY	T284	I213	LEU	ASN	TYR
			S846		A715		P575		Y431	GLY	T285	A214	ILE	ILE	GLY
D1049	D1049		D847		A716		D576		N432	LYS	F286	Q215	TYR	SER	PHE
K978	K978		T783		ASN		A577		N431	LEU	R287	E216	GLY	ARG	GLU
T1051	T1051		N784		GLY		T578		T435	LEU	A288	R217	LYS	LYS	D20
F980	F980		N785		GLU		R579		V436	GLY		N221	ILE	TYR	E21
A981	A981		L550		ASN		T579		E437	ALA			ALA	GLU	S22
V1052	V1052		L550		GLU		F580		GLU	ALA	T291		GLU	GLU	A23
E1053	E1053		L551		ASP		F581		ALA	ALA	T292		GLU	GLU	P24
G1054	G1054		R582		LEU		V511		ASP	ASP	T293		SER	F92	T25
S1055	S1055		R583		LEU		V512		ASP	ASP	T294		SER	F92	T26
S1056	S1056		R584		LEU		V513		ASP	ASP	T295		SER	F92	T26
K1057	K1057		R585		LEU		V514		ASP	ASP	T296		SER	F92	T26
L1058	L1058		R586		LEU		V515		ASP	ASP	T297		SER	F92	T26
L1059	L1059		R587		LEU		V516		ASP	ASP	T298		SER	F92	T26
R1060	R1060		R588		LEU		V517		ASP	ASP	T299		SER	F92	T26
E1061	E1061		R589		LEU		V518		ASP	ASP	T300		SER	F92	T26
L1062	L1062		R590		LEU		V519		ASP	ASP	T301		SER	F92	T26
G1063	G1063		R591		LEU		V520		ASP	ASP	T302		SER	F92	T26
T1064	T1064		R592		LEU		V521		ASP	ASP	T303		SER	F92	T26
Y1065	Y1065		R593		LEU		V522		ASP	ASP	T304		SER	F92	T26
Y1066	Y1066		R594		LEU		V523		ASP	ASP	T305		SER	F92	T26
Y1067	Y1067		R595		LEU		V524		ASP	ASP	T306		SER	F92	T26
Y1068	Y1068		R596		LEU		V525		ASP	ASP	T307		SER	F92	T26
Y1069	Y1069		R597		LEU		V526		ASP	ASP	T308		SER	F92	T26
Y1070	Y1070		R598		LEU		V527		ASP	ASP	T309		SER	F92	T26
Y1071	Y1071		R599		LEU		V528		ASP	ASP	T310		SER	F92	T26
Y1072	Y1072		R600		LEU		V529		ASP	ASP	T311		SER	F92	T26
Y1073	Y1073		R601		LEU		V530		ASP	ASP	T312		SER	F92	T26
T1077	T1077		R602		LEU		V531		ASP	ASP	T313		SER	F92	T26
G1078	G1078		R603		LEU		V532		ASP	ASP	T314		SER	F92	T26
K1079	K1079		R604		LEU		V533		ASP	ASP	T315		SER	F92	T26
K1080	K1080		R605		LEU		V534		ASP	ASP	T316		SER	F92	T26
L1081	L1081		R606		LEU		V535		ASP	ASP	T317		SER	F92	T26
Q1084	Q1084		R607		LEU		V536		ASP	ASP	T318		SER	F92	T26
L1085	L1085		R608		LEU		V537		ASP	ASP	T319		SER	F92	T26
F1086	F1086		R609		LEU		V538		ASP	ASP	T320		SER	F92	T26
F1087	F1087		R610		LEU		V539		ASP	ASP	T321		SER	F92	T26
Y1091	Y1091		R611		LEU		V540		ASP	ASP	T322		SER	F92	T26
R1094	R1094		R612		LEU		V541		ASP	ASP	T323		SER	F92	T26
L1095	L1095		R613		LEU		V542		ASP	ASP	T324		SER	F92	T26
L1096	L1096		R614		LEU		V543		ASP	ASP	T325		SER	F92	T26
R1097	R1097		R615		LEU		V544		ASP	ASP	T326		SER	F92	T26
M1098	M1098		R616		LEU		V545		ASP	ASP	T327		SER	F92	T26
			R617		LEU		V546		ASP	ASP	T328		SER	F92	T26
			R618		LEU		V547		ASP	ASP	T329		SER	F92	T26
			R619		LEU		V548		ASP	ASP	T330		SER	F92	T26
			R620		LEU		V549		ASP	ASP	T331		SER	F92	T26
			R621		LEU		V550		ASP	ASP	T332		SER	F92	T26
			R622		LEU		V551		ASP	ASP	T333		SER	F92	T26
			R623		LEU		V552		ASP	ASP	T334		SER	F92	T26
			R624		LEU		V553		ASP	ASP	T335		SER	F92	T26
			R625		LEU		V554		ASP	ASP	T336		SER	F92	T26
			R626		LEU		V555		ASP	ASP	T337		SER	F92	T26
			R627		LEU		V556		ASP	ASP	T338		SER	F92	T26
			R628		LEU		V557		ASP	ASP	T339		SER	F92	T26
			R629		LEU		V558		ASP	ASP	T340		SER	F92	T26
			R630		LEU		V559		ASP	ASP	T341		SER	F92	T26
			R631		LEU		V560		ASP	ASP	T342		SER	F92	T26
			R632		LEU		V561		ASP	ASP	T343		SER	F92	T26
			R633		LEU		V562		ASP	ASP	T344		SER	F92	T26
			R634		LEU		V563		ASP	ASP	T345		SER	F92	T26
			R635		LEU		V564		ASP	ASP	T346		SER	F92	T26
			R636		LEU		V565		ASP	ASP	T347		SER	F92	T26
			R637		LEU		V566		ASP	ASP	T348		SER	F92	T26
			R638		LEU		V567		ASP	ASP	T349		SER	F92	T26
			R639		LEU		V568		ASP	ASP	T350		SER	F92	T26
			R640		LEU		V569		ASP	ASP	T351		SER	F92	T26
			R641		LEU		V570		ASP	ASP	T352		SER	F92	T26
			R642		LEU		V571		ASP	ASP	T353		SER	F92	T26
			R643		LEU		V572		ASP	ASP	T354		SER	F92	T26
			R644		LEU		V573		ASP	ASP	T355		SER	F92	T26
			R645		LEU		V574		ASP	ASP	T356		SER	F92	T26
			R646		LEU		V575		ASP	ASP	T357		SER	F92	T26
			R647		LEU		V576		ASP	ASP	T358		SER	F92	T26
			R648		LEU		V577		ASP	ASP	T359		SER	F92	T26
			R649		LEU		V578		ASP	ASP	T360		SER	F92	T26
			R650		LEU		V579		ASP	ASP	T361		SER	F92	T26
			R651		LEU		V580		ASP	ASP	T362		SER	F92	T26
			R652		LEU		V581		ASP	ASP	T363		SER	F92	T26
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			R654		LEU		V583		ASP	ASP	T365		SER	F92	T26
			R655		LEU		V584		ASP	ASP	T366		SER	F92	T26
			R656		LEU		V585		ASP	ASP	T367		SER	F92	T26
			R657		LEU		V586		ASP	ASP	T368		SER	F92	T26
			R658		LEU		V587		ASP	ASP	T369		SER	F92	T26
			R659		LEU		V588		ASP	ASP	T370		SER	F92	T26
			R660		LEU		V589		ASP	ASP	T371		SER	F92	T26
			R661		LEU		V590		ASP	ASP	T372		SER	F92	T26
			R662		LEU		V591		ASP	ASP	T373		SER	F92	T26
			R663		LEU		V592		ASP	ASP	T374		SER	F92	T26
			R664		LEU		V593		ASP	ASP	T375		SER	F92	T26
			R665		LEU		V594		ASP	ASP	T376		SER	F92	T26
			R666		LEU		V595		ASP	ASP	T377		SER	F92	T26
			R667		LEU		V596		ASP	ASP	T378		SER	F92	T26
			R668		LEU		V597		ASP	ASP	T379		SER	F92	T26
			R669		LEU		V598		ASP	ASP	T380		SER	F92	T26
			R670		LEU		V599		ASP	ASP	T381		SER	F92	T26
			R671		LEU		V600		ASP	ASP	T382		SER	F92	T26
			R672		LEU		V601		ASP	ASP	T383		SER	F92	T26
			R673		LEU		V602		ASP	ASP	T384		SER	F92	T26
			R674		LEU		V603		ASP	ASP	T385		SER	F92	T26
			R675		LEU		V604		ASP	ASP	T386		SER	F92	T26
			R676		LEU		V605		ASP	ASP	T387		SER	F92	T26
			R677		LEU		V606		ASP	ASP	T388		SER	F92	T26

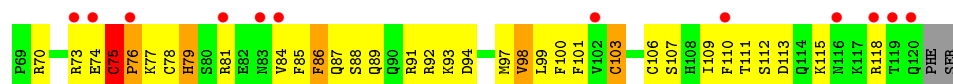
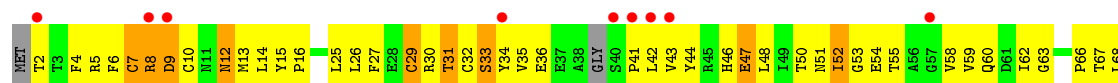




- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



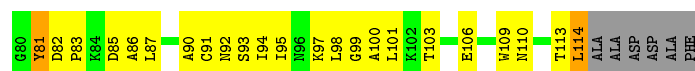
- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide



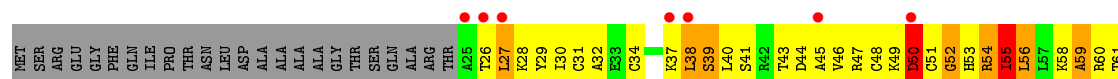
- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

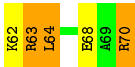


- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

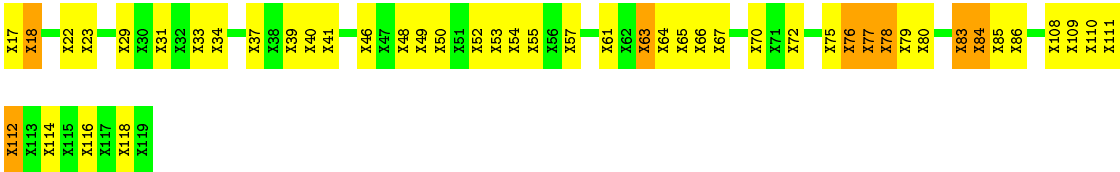


- Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide





● Molecule 11: TRANSCRIPTION FACTOR II B (TFIIB)



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.44Å 217.18Å 422.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.50 51.23 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-4.50) 99.2 (51.23-4.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 4.46Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.345 , 0.373 0.330 , 0.351	Depositor DCC
$R_{free}$ test set	1721 reflections (3.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	124.1	Xtriage
Anisotropy	1.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 177.8	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	6 of 111208 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	28300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.48	3/11040 (0.0%)	0.73	15/14922 (0.1%)
2	B	0.49	2/8891 (0.0%)	0.72	3/11990 (0.0%)
3	C	0.48	0/2133	0.76	2/2891 (0.1%)
4	E	0.36	0/1788	0.65	0/2406
5	F	0.40	0/691	0.64	0/933
6	H	0.40	0/1086	0.73	0/1470
7	I	0.48	0/984	0.76	1/1323 (0.1%)
8	J	0.53	0/541	0.78	0/727
9	K	0.46	0/937	0.68	0/1265
10	L	0.49	0/366	0.78	0/485
All	All	0.47	5/28457 (0.0%)	0.73	21/38412 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
11	M	0	33
All	All	0	35

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1274	ARG	C-N	21.02	1.70	1.33
2	B	217	ARG	C-N	-14.21	1.01	1.34
1	A	1141	THR	C-N	10.82	1.58	1.34
2	B	1150	ARG	C-N	9.61	1.56	1.34
1	A	346	ASP	C-N	8.96	1.54	1.34

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1141	THR	O-C-N	-12.22	103.15	122.70
1	A	1274	ARG	O-C-N	-8.93	108.02	123.20
2	B	217	ARG	O-C-N	-8.89	108.48	122.70
1	A	1141	THR	CA-C-N	8.53	135.97	117.20
1	A	1141	THR	C-N-CA	8.49	142.94	121.70

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	217	ARG	Mainchain
2	B	405	ARG	Mainchain
11	M	18	UNK	Mainchain,Peptide
11	M	29	UNK	Mainchain
11	M	54	UNK	Mainchain

## 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	10850	0	10952	1129	3
2	B	8721	0	8747	936	1
3	C	2095	0	2052	164	0
4	E	1752	0	1776	129	1
5	F	679	0	701	63	0
6	H	1068	0	1040	129	0
7	I	967	0	929	139	2
8	J	532	0	544	77	0
9	K	919	0	929	87	0
10	L	364	0	388	54	0
11	M	343	0	19	34	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	2	0
12	J	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1	0	0	0	0
12	M	1	0	0	0	0
13	A	1	0	0	0	0
All	All	28300	0	28077	2623	4

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 47.

The worst 5 of 2623 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:783:THR:HG21	1:A:815:PHE:CZ	1.39	1.57
1:A:783:THR:CG2	1:A:815:PHE:CZ	2.00	1.43
1:A:1274:ARG:C	1:A:1275:GLY:N	1.70	1.42
1:A:1147:THR:O	7:I:48:LEU:CD1	1.77	1.33
1:A:1151:GLU:CG	7:I:44:TYR:O	1.79	1.31

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ASN:OD1	7:I:33:SER:OG[7_554]	1.06	1.14
2:B:1223:ASP:O	2:B:1223:ASP:CB[2_565]	1.71	0.49
1:A:903:ASN:OD1	7:I:33:SER:CB[7_554]	2.14	0.06
1:A:163:SER:OG	4:E:74:ASP:OD1[2_565]	2.19	0.01

## 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	1362/1733 (79%)	1020 (75%)	252 (18%)	90 (7%)	<b>1</b> <b>25</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1077/1224 (88%)	836 (78%)	172 (16%)	69 (6%)	2	26
3	C	264/318 (83%)	208 (79%)	40 (15%)	16 (6%)	2	27
4	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	3	35
5	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	4	39
6	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	9
7	I	114/122 (93%)	90 (79%)	15 (13%)	9 (8%)	1	19
8	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	2	26
9	K	112/120 (93%)	96 (86%)	16 (14%)	0	100	100
10	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	1
All	All	3459/4173 (83%)	2647 (76%)	587 (17%)	225 (6%)	1	26

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO
1	A	74	MET

### 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	1205/1520 (79%)	1128 (94%)	77 (6%)	22	61
2	B	952/1061 (90%)	886 (93%)	66 (7%)	19	59
3	C	234/274 (85%)	222 (95%)	12 (5%)	29	67
4	E	196/197 (100%)	189 (96%)	7 (4%)	42	75
5	F	74/137 (54%)	68 (92%)	6 (8%)	15	52
6	H	117/128 (91%)	112 (96%)	5 (4%)	35	71
7	I	113/116 (97%)	104 (92%)	9 (8%)	15	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	60/65 (92%)	56 (93%)	4 (7%)	20	59
9	K	99/102 (97%)	90 (91%)	9 (9%)	12	46
10	L	40/57 (70%)	35 (88%)	5 (12%)	6	31
All	All	3090/3657 (84%)	2890 (94%)	200 (6%)	21	60

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	268	THR
2	B	644	GLU
8	J	47	ARG
2	B	313	MET
2	B	466	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	215	GLN
2	B	518	HIS
7	I	12	ASN
2	B	236	HIS
2	B	513	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 10 ligands modelled in this entry, 10 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	1380/1733 (79%)	0.05	37 (2%) 58 48	47, 179, 269, 300	0
2	B	1097/1224 (89%)	0.13	46 (4%) 40 31	26, 192, 280, 300	0
3	C	266/318 (83%)	-0.05	4 (1%) 76 67	45, 168, 245, 293	0
4	E	214/215 (99%)	0.14	13 (6%) 25 18	76, 206, 284, 300	0
5	F	84/155 (54%)	0.03	1 (1%) 81 73	61, 160, 231, 277	0
6	H	133/146 (91%)	0.43	6 (4%) 37 29	119, 207, 300, 300	0
7	I	118/122 (96%)	0.90	21 (17%) 2 3	133, 246, 300, 300	0
8	J	65/70 (92%)	-0.03	0 100 100	76, 169, 231, 270	0
9	K	114/120 (95%)	-0.12	1 (0%) 85 80	72, 155, 241, 274	0
10	L	46/70 (65%)	0.78	7 (15%) 3 4	129, 222, 288, 300	0
11	M	0/86	-	-	-	-
All	All	3517/4259 (82%)	0.12	136 (3%) 43 34	26, 186, 278, 300	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	26	THR	9.1
2	B	919	SER	8.3
10	L	25	ALA	8.0
2	B	881	ASN	6.7
7	I	41	PRO	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, 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
12	ZN	I	203	1/1	0.45	0.62	0.17	166,166,166,166	0
12	ZN	A	1735	1/1	0.89	0.12	-1.03	166,166,166,166	0
12	ZN	C	319	1/1	0.98	0.15	-1.05	166,166,166,166	0
12	ZN	A	1734	1/1	0.92	0.11	-1.72	166,166,166,166	0
12	ZN	J	101	1/1	0.99	0.14	-1.76	166,166,166,166	0
12	ZN	L	105	1/1	0.95	0.10	-2.00	175,175,175,175	0
12	ZN	I	204	1/1	0.84	0.09	-2.19	166,166,166,166	0
12	ZN	B	1307	1/1	0.93	0.13	-	166,166,166,166	0
12	ZN	M	209	1/1	0.36	0.27	-	156,156,156,156	0
13	MG	A	1736	1/1	0.88	0.39	-	47,47,47,47	0

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

There are no such residues in this entry.