



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:59 PM GMT

PDB ID : 1I50  
Title : RNA POLYMERASE II CRYSTAL FORM II AT 2.8 Å RESOLUTION  
Authors : Cramer, P.; Bushnell, D.A.; Kornberg, R.D.  
Deposited on : 2001-02-23  
Resolution : 2.80 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

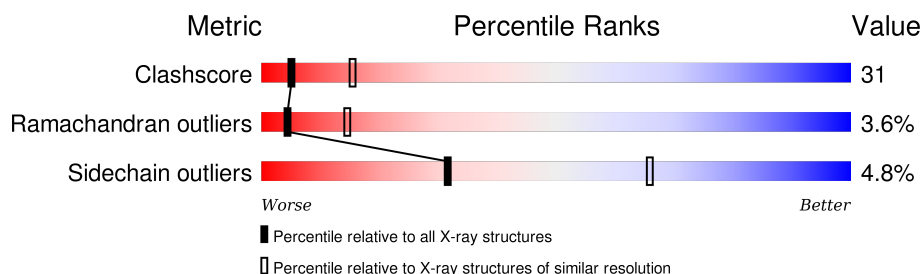
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	

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Mol	Chain	Length	Quality of chain
8	J	70	<div><div></div><div>50%40%7%</div></div>
9	K	120	<div><div></div><div>52%39%5%</div></div>
10	L	70	<div><div></div><div>16%37%11%34%</div></div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28366 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 SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11154	7023	1952	2118	61			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1094	Total	C	N	O	S	0	0	0
			8711	5525	1519	1614	53			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD 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 POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD 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 POLYMERASE II 14.5KD POLYPEPTIDE.

TIDE.

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 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD 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 13.6KD 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 POLYMERASE II 7.7KD 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 ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total 2	Zn 2	0	0
11	L	1	Total 1	Zn 1	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total 1	Mn 1	0	0

- Molecule 13 is water.

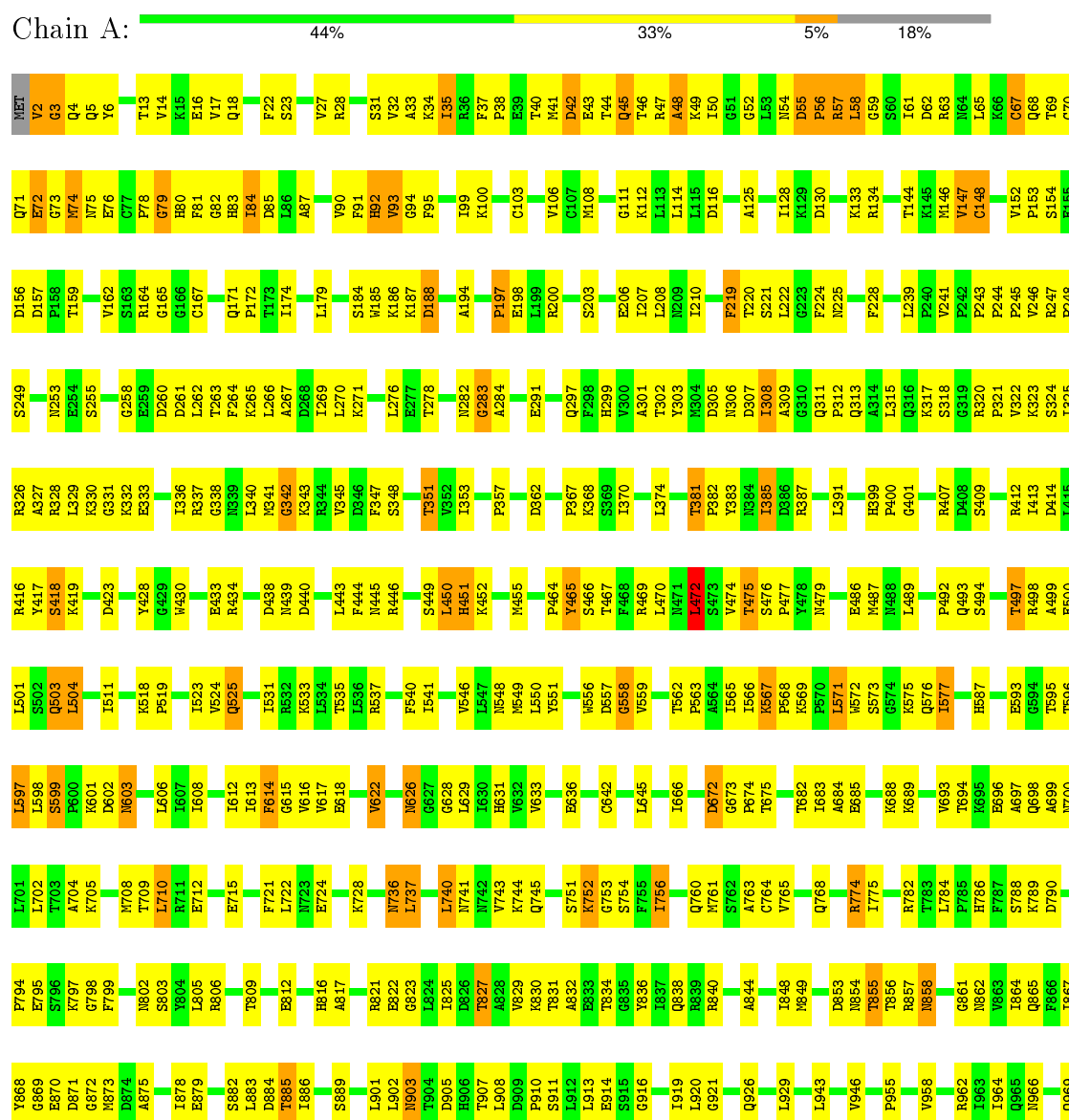
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	35	Total 35	O 35	0	0
13	B	23	Total 23	O 23	0	0
13	C	4	Total 4	O 4	0	0
13	E	7	Total 7	O 7	0	0
13	F	5	Total 5	O 5	0	0
13	I	2	Total 2	O 2	0	0
13	K	2	Total 2	O 2	0	0

### 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 ( $RSRZ > 2$ ). 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.


Note EDS was not executed.

#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT



T970	HIS	E1165	V1243	T1329		ASN	THR	TYR	GLN
F971	PHE	D1166	ARG	M1330	L1409	ALA	SER	SER	ASP
H972	ALA	E1167	PRO	M1331	F1410	ASP	PRO	PRO	GLU
I973	GLY	E1168	LYS	F1332	S1415	LEU	SER	THR	GLN
D974	VAL	I1169	LEU	I1333	A1416	ASP	THR	SER	LYS
H975	ALA	I1170	SER	M1336	E1417	VAL	PRO	SER	ASN
	SER	Q1171	ASP	E1337	L1418	ASP	THR	SER	ASN
P978	K1092	L1172	ALA	V1338	D1419	THR	THR	TYR	GLU
S979	K1093	H1173	GLU	L1339	D1420	LEU	PRO	PRO	ASN
D980	V1094		THR	G1340	C1421	THR	SER	THR	ASN
L981	T1095	L1176	GLU	L1341	R1422	PHE	THR	SER	SER
T982	S1096	LEU	A1254	I1342	S1425	SER	SER	PRO	ARG
I983	G1097	ASP	E1256	E1345	E1426	PRO	THR	SER	
K984	V1098	GLU	E1257	R1348	Q1432	VAL	THR	TYR	
D985	P1099	ALA	D1258	L1348	M1433	ASP	PRO	PRO	
L988	R1100	GLN	M1259	V1355	A1434	SER	TYR	SER	
L988	L1101	GLN	L1260	D1359	P1435	SER	PRO	PRO	
Q994	K1102	SER	K1261	M1364	G1437	ASP	THR	TYR	
		PHE	K1266	N1365	T1438	ALA	THR	THR	
L998	M1106	ASP	M1267	R1366	G1439	ALA	PRO	PRO	
V999	V1107	Q1187	L1268	E1370	D1446	GLY	TYR	THR	
L1000	M1111	Q1188	E1269	L1371	E1447	GLY	SER	SER	
R1001	K1112	L1192	L1269	V1372	S1449	PHE	PRO	TYR	
M1004	P1114	L1193	L1269	M1375	L1450	THR	PRO	THR	
V1015	S1115	L1194	E1269	T1376	VAL	GLY	TYR	THR	
C1019	T1117	L1197	R1274	M1375	L1450	GLY	PRO	THR	
	L1118	D1198	E1277	T1376	LYS	THR	TYR	THR	
R1023	E1121	R1199	M1278	G1379	LYS	GLY	TYR	THR	
	P1122	M1202	E1280	G1380	TYR	GLY	TYR	THR	
R1030	H1124	K1205	E1280	T1381	ASP	ALA	PRO	PRO	
Y1035	Q1128	D1206	V1283	L1382	TYR	GLY	TYR	TYR	
R1036	E1129	L1207	M1284	S1383	GLY	GLY	PRO	PRO	
A1041	Q1130	T1208	M1285	L1384	GLY	GLY	PRO	PRO	
F1042	A1131	M1209	S1293	T1385	ILE	THR	THR	THR	
D1043	K1132	G1210	P1294	R1386	THR	SER	SER	SER	
W1044	K1132	Q1211	T1295	H1387	ILE	PRO	PRO	PRO	
V1045	I1138	Q1211	G1296		GLY	PHE	SER	THR	
	E1139	R1215	E1297	M1390	ASP	GLY	PRO	TYR	
V1058	K1144	I1216	L1306	R1391	GLY	ALA	PRO	TYR	
V1064	S1145	Q1217	E1307	S1392	GLN	TYR	SER	PRO	
	S1146	Q1218	E1307	M1393	ASP	GLY	TYR	PRO	
L1067	V1146	T1219	T1308	T1394	GLY	GLY	PRO	PRO	
	T1147	F1220	D1309	G1395	GLY	ALA	PRO	PRO	
E1074	S1150	K1221	E1315	A1396	VAL	PRO	THR	THR	
	E1151	H1222		L1397	THR	THR	TYR	TYR	
T1077	I1152	D1223	T1318	M1398	PRO	PRO	PRO	PRO	
Q1078	D1155	D1233	P1323	C1400	TYR	GLY	TYR	TYR	
M1079	M1079		D1323	F1402	ASN	PHE	SER	SER	
T1080	T1161	L1236	P1324	E1403	GLY	GLY	PRO	PRO	
L1081	ASN	I1237	T1325	E1404	VAL	VAL	THR	THR	
THR	V1162	I1238	T1326	T1405	SER	SER	PRO	PRO	
PHE	P1164	R1239	I1327	L1406	GLY	GLY	PRO	PRO	
			Y1328		VAL	PRO	ALA	ALA	

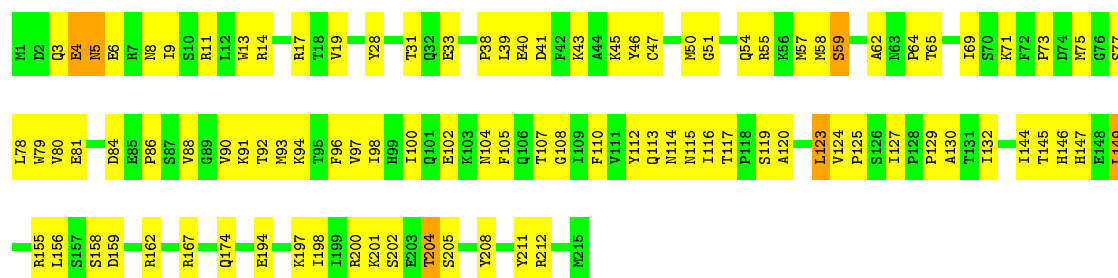
● Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE

Chain B:  49% 37% 11%

MET	ASP	GLU	E217	E296
SER	ASN	LEU	M217	E299
ASP	ILE	ILE	I222	H300
LEU	SER	ALA	V223	V305
ALA	ARG	GLU	Q224	Q309
ASN	LYS	GLU	K227	M310
SER	TYR	SER	E228	L311
GLU	E89	ASP	A229	E312
LYS	190	ASP	A230	M313
TYR	F92	GLU	P231	L314
SER	I95	SER	I234	K315
ASP		GLY	S235	C317
PRO	T98	K164	H236	
THR	K99	V165	E239	F322
GLY	F166	M101	T240	V323
F18	E19	M103	R241	L324
D20	E21	E104	S242	Q325
		S105	A243	D326
I25		D106	L244	
D29		G107	M173	D332
S35		V108	L174	F333
R39		T109	R175	L334
L43		H110	N178	G335
Q46		A111	C179	R336
Q47		L112	Y180	G337
Q53		Y113	L181	G338
F54		P114	S182	T339
T58		Q115	E183	I343
L59		R118	L185	K344
D60		L119	D188	E346
D61		M120	L189	K347
I62		N121	L192	R348
I63		S125	K193	Y351
O64		S126	E194	I355
L69		V130	C195	L356
I70		D131	G196	Q357
LEU		V132	F197	K358
GLU		R135	D198	E359
GLN		T136	M199	F360
GLY		Y137	G200	L361
LEU		E138	G201	T365
GLU		ALA	Y202	Q366
GLY		ILE	F203	E368
GLN		ASP	I204	G369
LEU		VAL	L205	F370
ALA		PRO	M206	
GLY		GLY	G207	
ARG		THR	K210	
HIS		GLU	Q215	
THR		LEU	E216	
THR		LYS		
GLU		TYR		
SER				

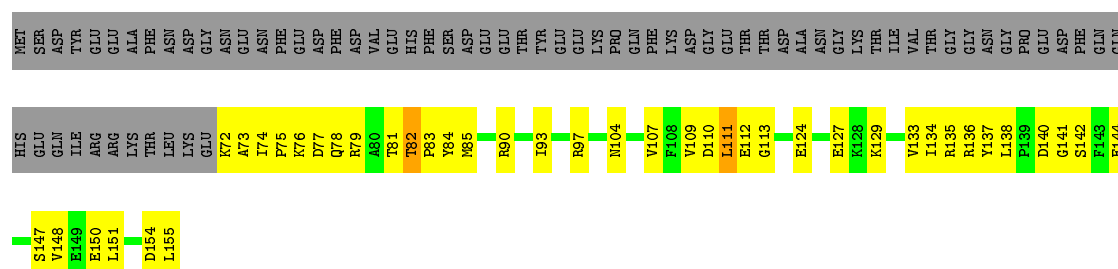






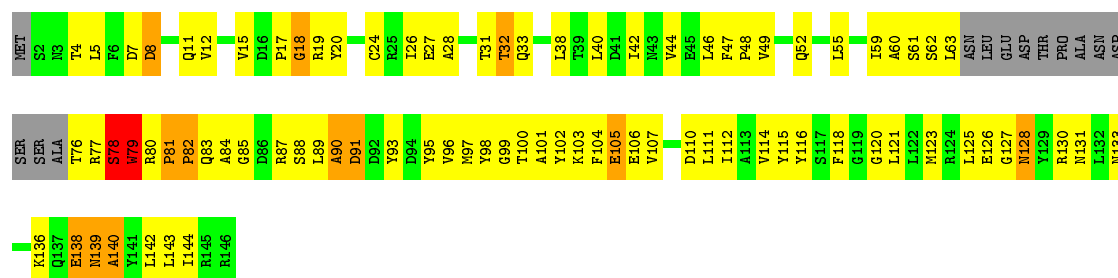
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F: 27% 26% 46%



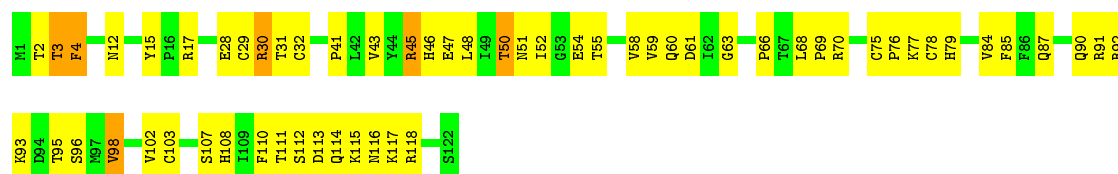
• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

Chain H: 32% 49% 8% 9%



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I: 52% 43% 5%

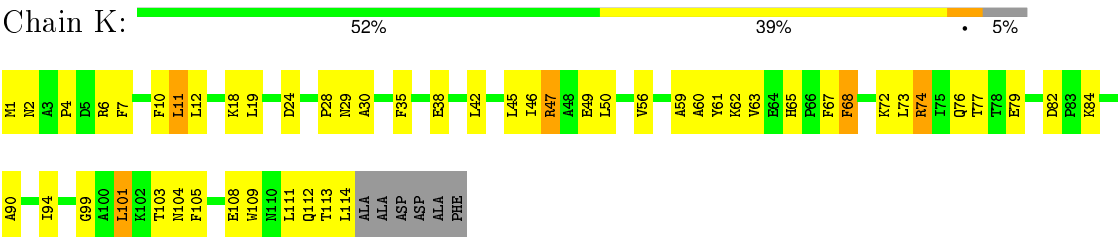


• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

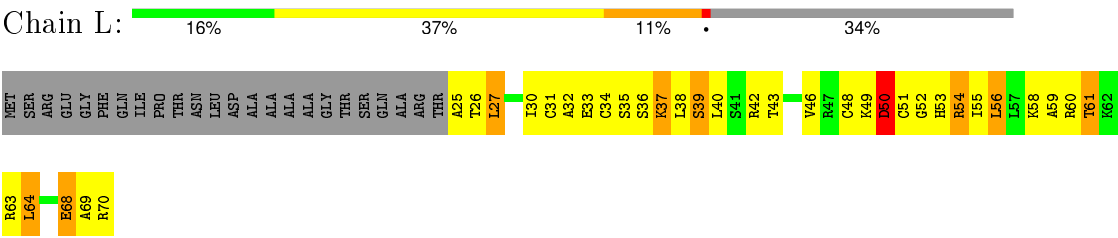
Chain J: 50% 40% 7%



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE



● Molecule 10: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.70Å 223.00Å 376.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.80)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.229 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

## 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, MN

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	0.39	1/11352 (0.0%)	0.68	2/15352 (0.0%)
2	B	0.42	2/8882 (0.0%)	0.70	5/11976 (0.0%)
3	C	0.37	0/2133	0.65	0/2891
4	E	0.37	0/1796	0.64	0/2416
5	F	0.40	0/691	0.63	0/933
6	H	0.88	1/1086 (0.1%)	1.23	3/1470 (0.2%)
7	I	0.40	0/1016	0.63	0/1365
8	J	0.41	0/541	0.70	0/727
9	K	0.38	0/937	0.60	0/1265
10	L	0.42	0/366	0.72	0/485
All	All	0.43	4/28800 (0.0%)	0.71	10/38880 (0.0%)

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
6	H	0	3
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	79	TRP	C-N	-26.78	0.72	1.34
2	B	707	PRO	C-N	-11.27	1.08	1.34
2	B	710	LEU	C-N	-7.44	1.17	1.34
1	A	3	GLY	C-N	-5.20	1.22	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	78	SER	O-C-N	-31.77	71.87	122.70
6	H	78	SER	CA-C-N	20.38	162.03	117.20
2	B	707	PRO	O-C-N	-13.53	101.05	122.70
6	H	78	SER	C-N-CA	12.14	152.06	121.70
1	A	472	LEU	CA-CB-CG	-6.84	99.57	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	707	PRO	Mainchain
2	B	710	LEU	Mainchain
6	H	78	SER	Mainchain,Peptide
6	H	79	TRP	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	11154	0	11222	754	0
2	B	8711	0	8734	539	0
3	C	2095	0	2051	141	0
4	E	1760	0	1788	87	0
5	F	679	0	701	50	0
6	H	1068	0	1038	121	0
7	I	997	0	956	64	0
8	J	532	0	542	47	0
9	K	919	0	929	65	0
10	L	364	0	387	68	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	1	0	0	0	0
13	A	35	0	0	2	0
13	B	23	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C	4	0	0	0	0
13	E	7	0	0	1	0
13	F	5	0	0	0	0
13	I	2	0	0	0	0
13	K	2	0	0	0	0
All	All	28366	0	28348	1743	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 31.

The worst 5 of 1743 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)
6:H:79:TRP:C	6:H:80:ARG:CA	1.90	1.41
2:B:708:GLU:O	2:B:711:GLU:HG3	1.20	1.34
6:H:79:TRP:CA	6:H:80:ARG:N	1.94	1.29
6:H:79:TRP:O	6:H:80:ARG:N	1.67	1.26
3:C:56:THR:HG23	3:C:58:LEU:H	1.14	1.13

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	1411/1733 (81%)	1203 (85%)	149 (11%)	59 (4%)	3	11
2	B	1074/1224 (88%)	953 (89%)	100 (9%)	21 (2%)	9	30
3	C	264/318 (83%)	228 (86%)	30 (11%)	6 (2%)	8	26
4	E	213/215 (99%)	184 (86%)	24 (11%)	5 (2%)	8	26
5	F	82/155 (53%)	74 (90%)	6 (7%)	2 (2%)	7	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	129/146 (88%)	83 (64%)	28 (22%)	18 (14%)	0	1
7	I	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	7	24
8	J	63/70 (90%)	58 (92%)	4 (6%)	1 (2%)	12	38
9	K	112/120 (93%)	101 (90%)	11 (10%)	0	100	100
10	L	44/70 (63%)	21 (48%)	13 (30%)	10 (23%)	0	0
All	All	3512/4173 (84%)	3008 (86%)	379 (11%)	125 (4%)	4	14

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	46	THR
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO

### 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	1239/1520 (82%)	1172 (95%)	67 (5%)	27	60
2	B	950/1061 (90%)	908 (96%)	42 (4%)	35	69
3	C	234/274 (85%)	222 (95%)	12 (5%)	29	63
4	E	197/197 (100%)	191 (97%)	6 (3%)	48	82
5	F	74/137 (54%)	72 (97%)	2 (3%)	52	85
6	H	117/128 (91%)	116 (99%)	1 (1%)	84	96
7	I	116/116 (100%)	109 (94%)	7 (6%)	24	56
8	J	60/65 (92%)	56 (93%)	4 (7%)	20	50
9	K	99/102 (97%)	93 (94%)	6 (6%)	23	55
10	L	40/57 (70%)	36 (90%)	4 (10%)	9	27
All	All	3126/3657 (86%)	2975 (95%)	151 (5%)	31	66



5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	20	ASP
2	B	485	ARG
8	J	28	ASP
2	B	120	ARG
2	B	217	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	300	HIS
2	B	648	HIS
7	I	12	ASN
2	B	366	GLN
2	B	516	ASN

### 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 [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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.