



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:25 pm BST

PDB ID : 1Y1V
Title : Refined RNA Polymerase II-TFIIS complex
Authors : Kettenberger, H.; Armache, K.-J.; Cramer, P.
Deposited on : 2004-11-19
Resolution : 3.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

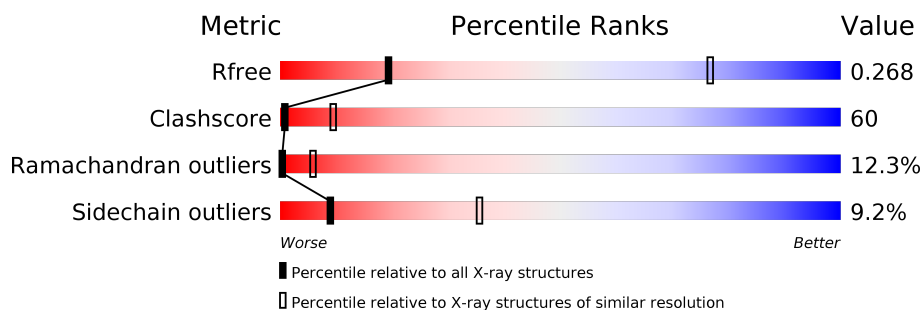
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1733	21% (green) 47% (yellow) 13% (orange) 18% (grey)
2	B	1224	24% (green) 52% (yellow) 13% (orange) 9% (grey)
3	C	318	22% (green) 48% (yellow) 12% (orange) 16% (grey)
4	D	221	33% (green) 40% (yellow) 6% (orange) 20% (grey)
5	E	215	34% (green) 55% (yellow) 11% (orange)
6	F	155	15% (green) 30% (yellow) 8% (orange) 46% (grey)
7	G	171	33% (green) 59% (yellow) 8% (orange)

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Mol	Chain	Length	Quality of chain
8	H	146	<div><div></div><div>30%53%8%9%</div></div>
9	I	122	<div><div></div><div>31%48%13%5%•</div></div>
10	J	70	<div><div></div><div>23%51%17%•7%</div></div>
11	K	120	<div><div></div><div>37%53%5%•5%</div></div>
12	L	70	<div><div></div><div>6%41%19%34%</div></div>
13	S	179	<div><div></div><div>62%28%•••</div></div>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 31803 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	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1112	Total	C	N	O	S	58	0	0
			8837	5594	1548	1640	55			

- 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 polymerase II 32 kDa polypeptide.

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 27 kDa polypeptide.

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 23 kDa polypeptide.

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 19 kDa polypeptide.

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 14.5 kDa polypeptide.

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 9.

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/III subunit 10.

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 13.6 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 13 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	S	174	Total	C	N	O	S	0	0	104
			666	454	99	108	5			

- 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		
14	S	1	Total	Zn	0	0
			1	1		

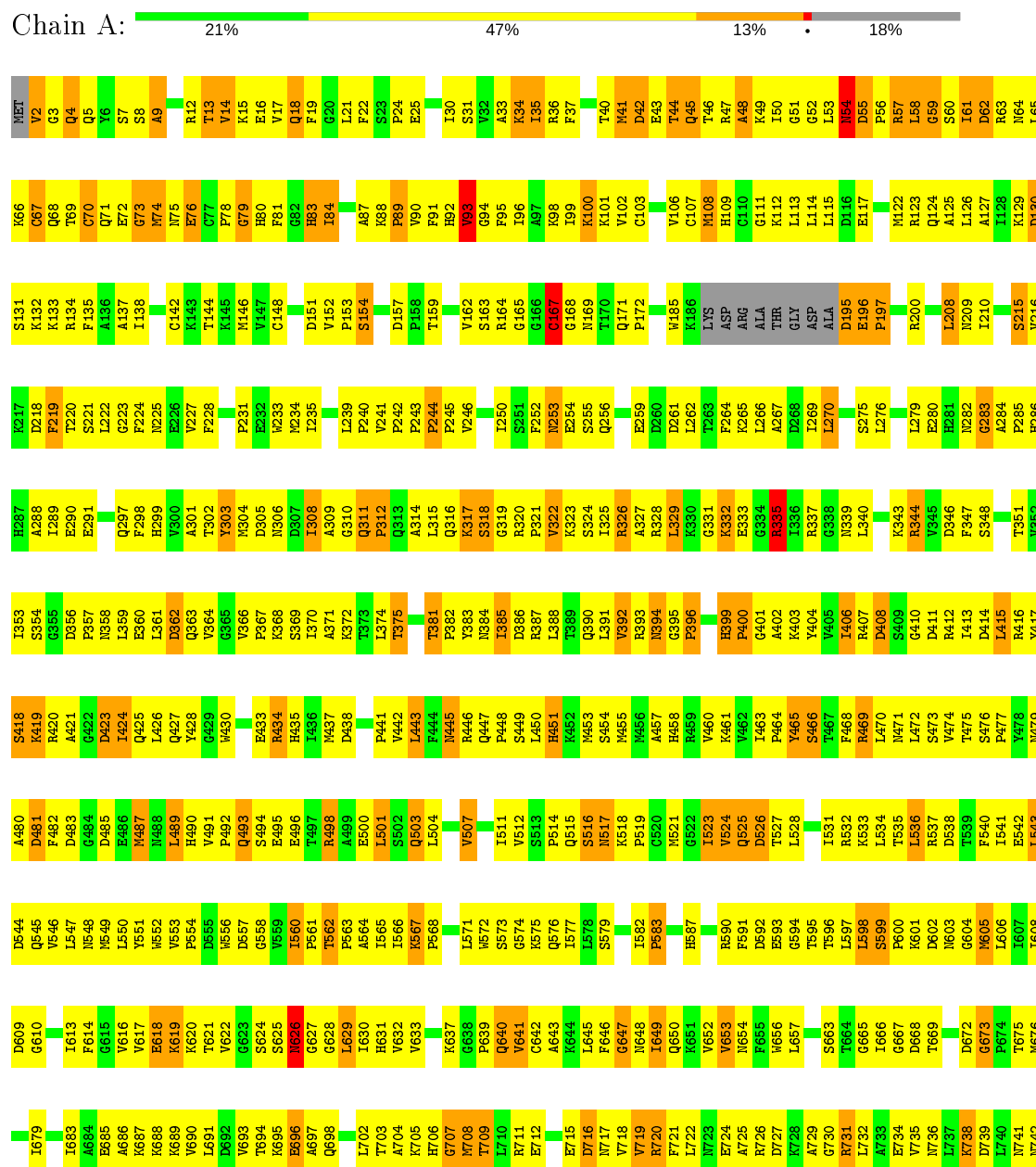
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

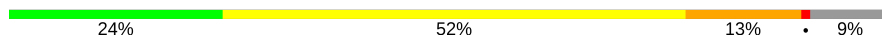
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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

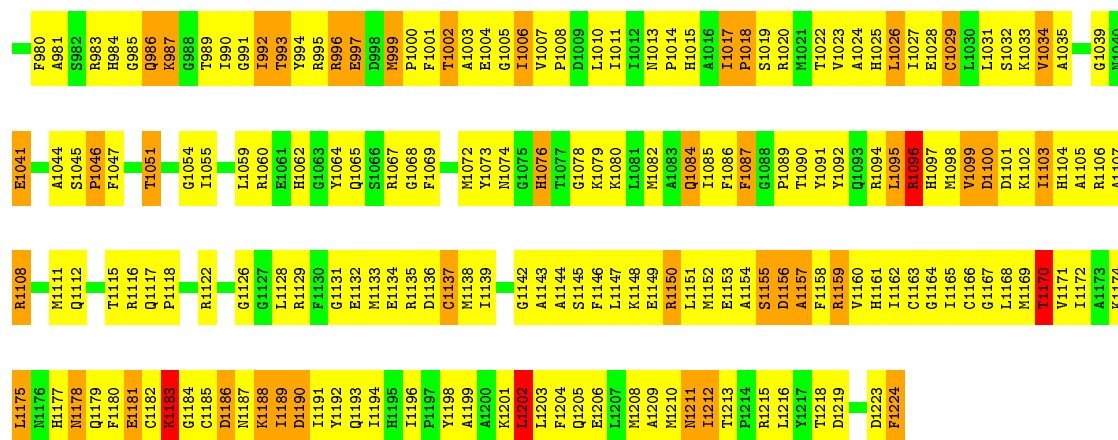


- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:

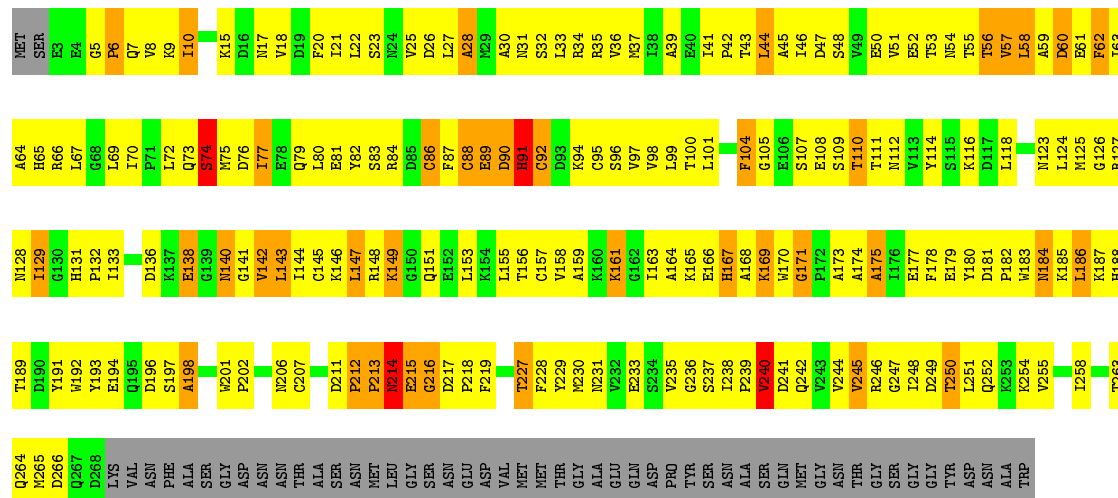


T846	T784	ASN	R654	R591	G530	T463	D391	R327	V256		L128	T62
D847	T785	ASP	H657	M592	Q531	G464	K392	E328	K257		F129	T63
R848	T786	LEU	H657	M592	A532	K465	K393	T329	L258		V130	C64
G849	T787	T722	I658	A594	C533	V466	D394	A330	Y259		E65	
L850	T788	D723	R659		G534	G467	Q395	L331	G260		D131	
R851	T789	D724	K660		M535	E468	Q396	D332	R361		K133	
S852		P725	L661	M597	V536	Q469		F333	R361		K133	
S853	T792	K726	M662	M598	K537	S474	F401	I334	S265		A170	
L854	T793	K727	A663	L600	M538	S475	G402	G335	A266		THR	
R855	T794		T664	R601	L539	S476	K403	R267	R267		TYR	
R857	T795	R730	E665	T602	S540	R476	K404	ARG	T268		GLU	
S858	T797	R731		L603	L541		R405	GLY	T269		GLN	
			D668	R604	M542	S480	L406	THR	R270		LEU	
			I1E	R605	S543	Q481	D407	ALA	T271		ASP	
			GLU	R606	C544	V482	L408	LEU	G272		VAL	
			GLY	G607	I545	M483	A409	GLY	L273		HIS	
			GLY	D608	I546	M484	G410	ILE	P274		GLY	
			PHE	I609	V547	R485	P411	LVS	Y275		THR	
			GLU	M610	G548	Y486	L412	K345	T276		ARG	
			ASP	R611	I554	T487	L413	E346	K277		GLU	
			VAL	E812	T549	R488	A414	R347	V211		LEU	
			GLU	M613	D550	Y489		K348	L212		LVS	
			V1U	V613	P551	S489	R347	D279	I213		TYR	
			E678	S614	M552	S490	F417	I349	I214		GLU	
			Y679	M615	P553	T491	K418	Q350	I280		LEU	
			T680	I616	I554	L492	T419	Y351	P281		SER	
			M681	R617	I555	H494	L420	I1E	T282		ARG	
			G682	E812	T556	H494	F421	I355	V283		LVS	
			S683	I619	F557	L495		L356	I285		GLU	
			T684	R620	L558	R496	L424	G220	F286		TYR	
			L685	E821	S559	R497		E359	T287		GLU	
			M686	E560	E561	T498	D427	F360	R287		S91	
			E687	E623	G622	N498	K428	L361	A288		ASP	
			G688	L624	M624	N498	F429	R362				
			R689	K625	G562	I502	R430	H363	I291		SER	
			V690	I626	M633	R502	F431	H363	I292		TYR	
			E691	F627	E564	G503	Y431	I364	V225		GLU	
			P692	F627	P665	R504	M432	T365	F226		SER	
			Y692	T628	L566			K164	K227		GLY	
			D693	R629	I566	K507	E437	Q366	K228		R399	
			G694	A630	Y569	L508	GLU	L367	E296		V165	
			A695	R631	V570	A509	ALA	E368	I297		H101	
				G632	G631	A509	ALA	R369	L298		P231	
				R632	P571	K510	HIS	F370	K41		V102	
				V633	H572	P511	ASP	E299	E299		G42	
				R634	Q573	R512	PHE	E371	H500		L43	
				E699	E634	Q573	THR	R372	I234		V108	
				S700	R635	Q513	ASN	R373	Y303		T109	
				T701	P636	L514	MET	K374	S235		S45	
				L702	L637	H515	LVS	A375	H236		S45	
				I703	F638	H516	L446	Q309	H308		L112	
				T704	I639	T517	A447	F377	V237		M173	
				M705	V640	R579		L378	L174		P114	
				E708	D641	V580	A450	R241	Q310		Q115	
				T709	E642	F581	G520	K379	E239		E116	
				D710	R643	G520	L314	N177	R241		S50	
				E644	D643	H582	L521	R380	R118		F51	
				E711	E644	H583	V522	M381	L119		Q53	
				E711	S645	G584	C523	I382	P316		F54	
				P712	L646	P524	L457	C317	R120		R120	
				T715	G647	A525	K458	F322	S248		M121	
				ASN	E715	R585	H586	R386	R249		L122	
				GLU	T715	H586	R386	F322			T123	
				GLU	ASN	H587	Y459	L387			E186	
				GLU	ASN	H587	Y459	L387			S252	
				GLU	ASN	H587	Y459	L387			S252	
				GLU	ASN	H587	Y459	L387			S252	
				GLU	ASN	H587	Y459	L387			S252	
				GLU	ASN	H587	Y459	L387			S252	
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				GLU	ASN	H587	Y459	L387			S252	
				GLU	ASN	H587	Y459	L387			S252	
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				GLU	ASN	H587	Y459	L387			S252	



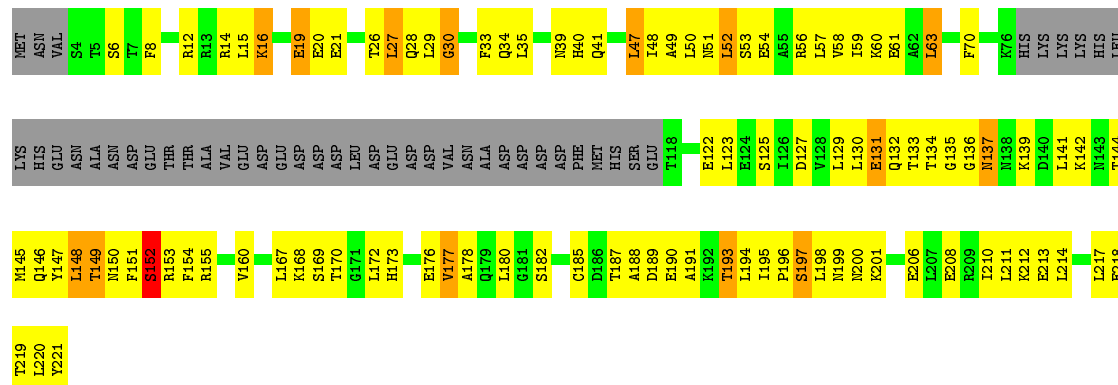
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 22% 48% 12% 16%



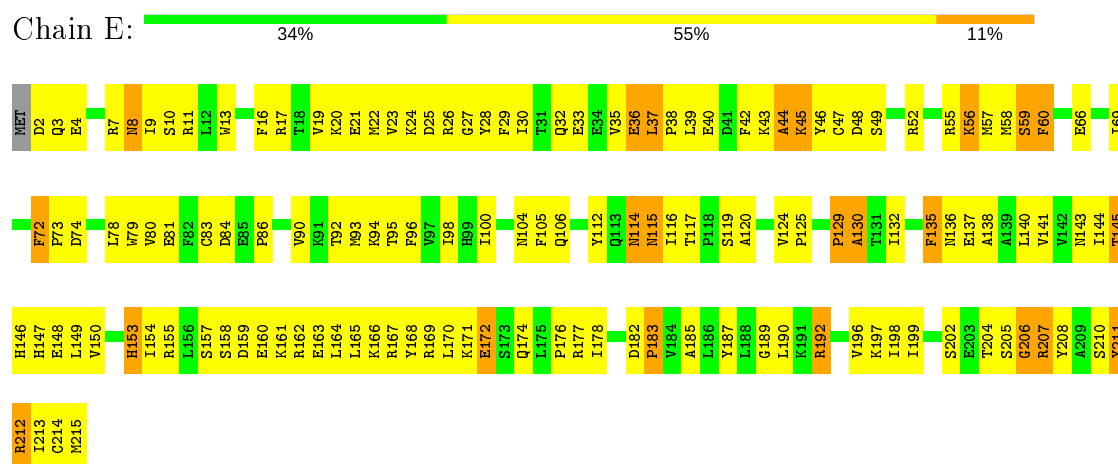
• Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D: 33% 40% 6% 20%



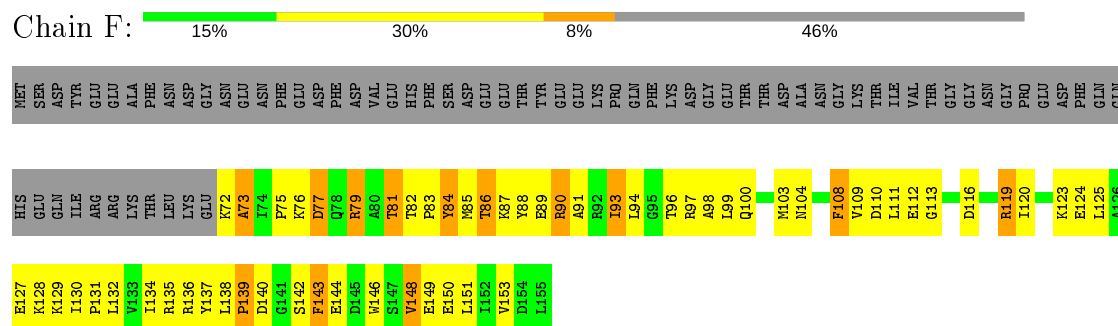
• Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:



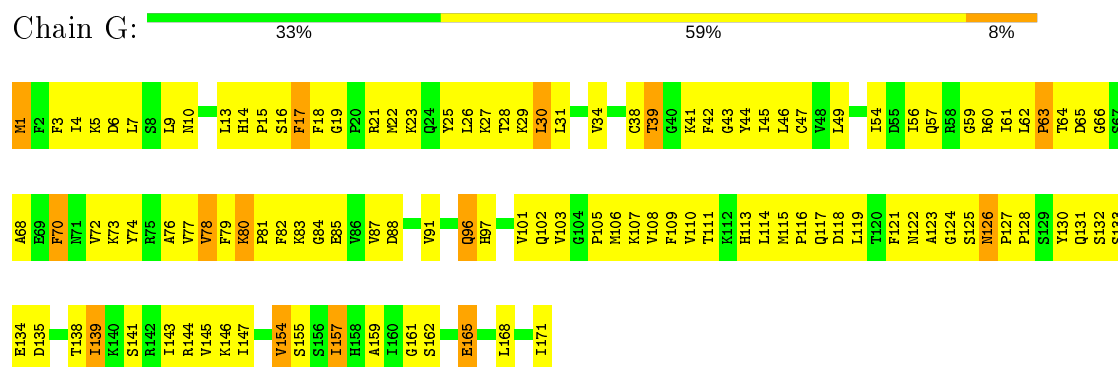
- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



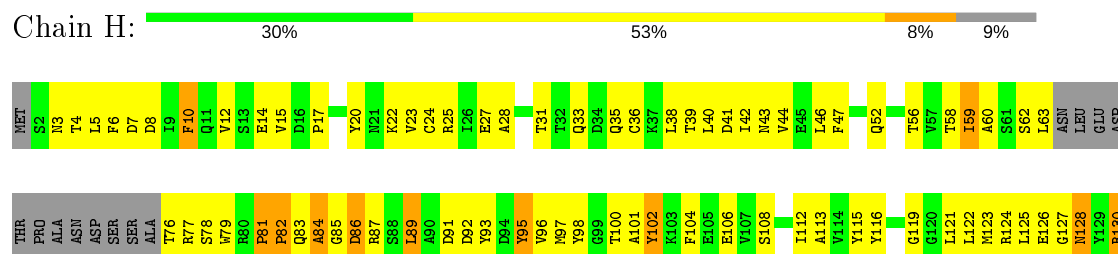
- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

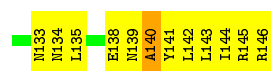
Chain G:



- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

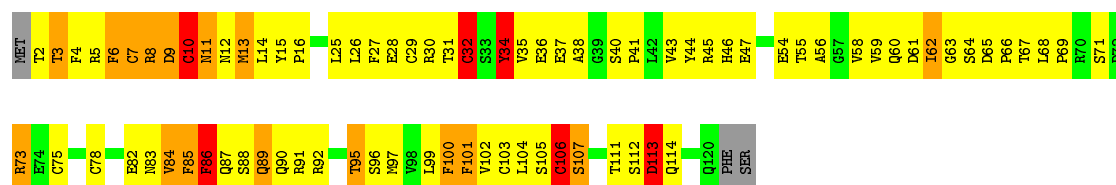
Chain H:





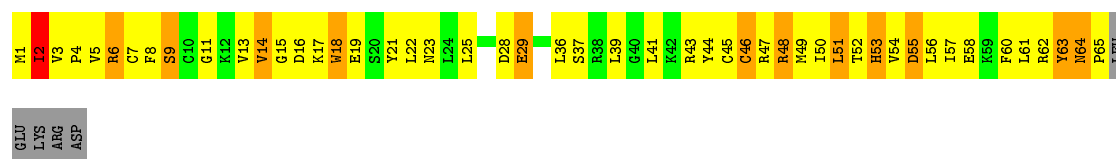
• Molecule 9: DNA-directed RNA polymerase II subunit 9

Chain I: 31% 48% 13% 5%



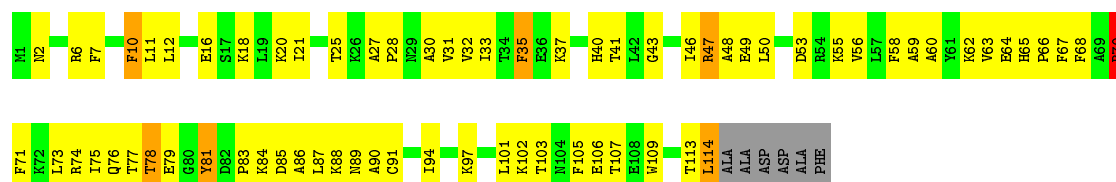
• Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10

Chain J: 23% 51% 17% 7%



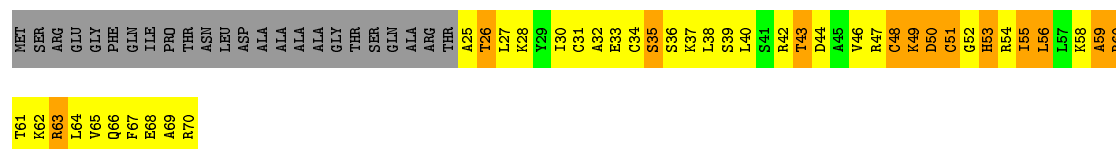
• Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 37% 53% 5% 5%



• Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L: 6% 41% 19% 34%



• Molecule 13: Transcription elongation factor S-II

Chain S: 62% 28%



Y282	Q283	L284	Q285	T286	R287	S288	A289	D290	E291	P292	L293	T294	T295	F296	C297	T298	C299	E300	A301	C302	G303	N304	R305	W306	K307	F308	S309
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	218.90Å 395.30Å 281.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.41 – 3.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 86.6 (49.41-3.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.294 0.257 , 0.268	Depositor DCC
R_{free} test set	2439 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.199 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.206 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	31803	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.50	2/11417 (0.0%)	0.78	4/15442 (0.0%)
2	B	0.51	4/9009 (0.0%)	0.76	8/12146 (0.1%)
3	C	0.48	0/2133	0.77	1/2891 (0.0%)
4	D	0.41	0/1365	0.64	0/1837
5	E	0.43	0/1788	0.66	0/2406
6	F	0.52	0/691	0.77	0/933
7	G	0.49	0/1368	0.72	0/1844
8	H	0.38	0/1086	0.65	1/1470 (0.1%)
9	I	0.46	0/989	0.77	1/1331 (0.1%)
10	J	0.48	0/541	0.75	0/727
11	K	0.45	0/937	0.67	0/1265
12	L	0.54	0/366	0.79	0/485
13	S	1.31	4/571 (0.7%)	1.64	7/765 (0.9%)
All	All	0.51	10/32261 (0.0%)	0.77	22/43542 (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	3
13	S	0	2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	269	PHE	C-N	-16.91	0.95	1.34
2	B	467	GLY	C-O	-11.91	1.04	1.23
13	S	260	THR	CA-CB	10.48	1.80	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	468	GLU	CB-CG	8.39	1.68	1.52
13	S	268	ARG	CG-CD	6.05	1.67	1.51

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	269	PHE	O-C-N	-19.02	92.27	122.70
13	S	269	PHE	C-N-CA	16.73	163.51	121.70
13	S	269	PHE	CA-C-N	16.08	152.57	117.20
1	A	195	ASP	N-CA-C	9.35	136.25	111.00
2	B	510	LYS	CB-CA-C	-7.63	95.14	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	510	LYS	Mainchain
2	B	785	TYR	Sidechain
2	B	833	TYR	Sidechain
13	S	269	PHE	Sidechain,Peptide

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	11214	0	11281	1514	0
2	B	8837	0	8871	1206	0
3	C	2095	0	2052	260	0
4	D	1356	0	1319	101	0
5	E	1752	0	1776	200	0
6	F	679	0	701	82	0
7	G	1340	0	1357	159	0
8	H	1068	0	1040	115	0
9	I	971	0	929	110	0
10	J	532	0	542	103	0
11	K	919	0	929	96	0
12	L	364	0	387	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	S	666	0	553	105	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
14	S	1	0	0	0	0
15	S	1	0	0	0	0
All	All	31803	0	31737	3774	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 60.

The worst 5 of 3774 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)
13:S:260:THR:CA	13:S:260:THR:CB	1.80	1.53
13:S:269:PHE:CZ	13:S:297:CYS:SG	2.04	1.50
13:S:269:PHE:CE2	13:S:297:CYS:SG	2.14	1.39
1:A:1230:GLU:OE2	13:S:201:ILE:CA	1.75	1.32
1:A:1283:VAL:CG1	13:S:256:ALA:O	1.78	1.31

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	1418/1733 (82%)	914 (64%)	316 (22%)	188 (13%)	0 4
2	B	1096/1224 (90%)	726 (66%)	223 (20%)	147 (13%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	264/318 (83%)	169 (64%)	62 (24%)	33 (12%)	0	6
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	0	10
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	0	10
6	F	82/155 (53%)	60 (73%)	15 (18%)	7 (8%)	1	12
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	1	17
8	H	129/146 (88%)	93 (72%)	26 (20%)	10 (8%)	1	15
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0	5
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0	2
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	2	25
12	L	44/70 (63%)	18 (41%)	14 (32%)	12 (27%)	0	0
13	S	68/179 (38%)	51 (75%)	10 (15%)	7 (10%)	0	9
All	All	3947/4744 (83%)	2622 (66%)	838 (21%)	487 (12%)	0	6

5 of 487 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	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	1246/1520 (82%)	1133 (91%)	113 (9%)	9	36
2	B	964/1061 (91%)	880 (91%)	84 (9%)	10	38
3	C	234/274 (85%)	205 (88%)	29 (12%)	4	24
4	D	140/200 (70%)	126 (90%)	14 (10%)	7	32
5	E	196/197 (100%)	184 (94%)	12 (6%)	18	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	74/137 (54%)	63 (85%)	11 (15%)	3	18
7	G	152/152 (100%)	143 (94%)	9 (6%)	19	51
8	H	117/128 (91%)	110 (94%)	7 (6%)	19	50
9	I	113/116 (97%)	97 (86%)	16 (14%)	3	21
10	J	60/65 (92%)	55 (92%)	5 (8%)	11	40
11	K	99/102 (97%)	91 (92%)	8 (8%)	11	41
12	L	40/57 (70%)	33 (82%)	7 (18%)	2	13
13	S	62/156 (40%)	55 (89%)	7 (11%)	6	28
All	All	3497/4165 (84%)	3175 (91%)	322 (9%)	9	35

5 of 322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	629	ASP
2	B	1047	PHE
10	J	46	CYS
2	B	658	ILE
2	B	856	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	465	ASN
2	B	957	ASN
9	I	89	GLN
2	B	515	HIS
2	B	657	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	269:PHE	C	270:THR	N	0.95

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.