



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:50 PM GMT

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 validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

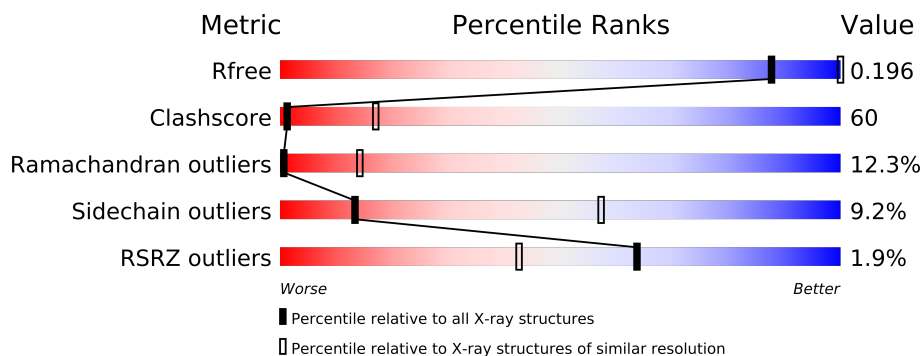
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	S	179	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
14	MG	S	1	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31803 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

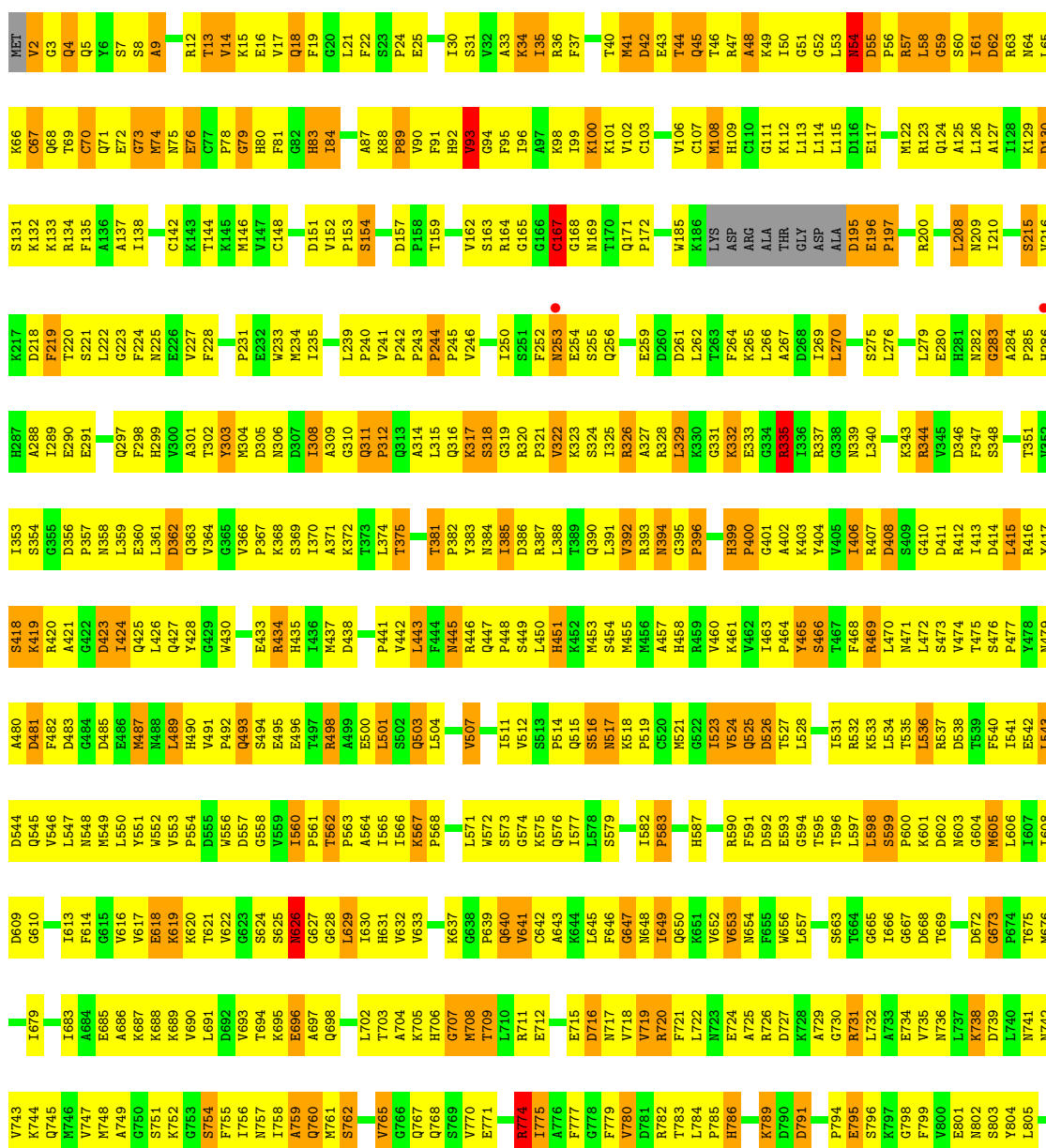
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	1	Total	Zn	0	0
			1	1		
15	B	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	C	1	Total	Zn	0	0
			1	1		
15	A	2	Total	Zn	0	0
			2	2		
15	L	1	Total	Zn	0	0
			1	1		
15	S	1	Total	Zn	0	0
			1	1		

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 largest subunit

Chain A:



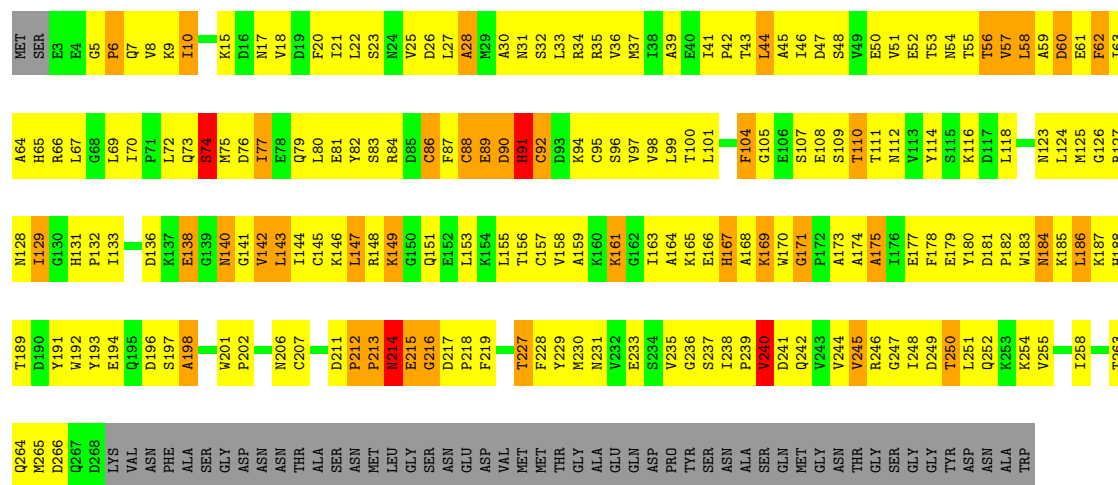


1973	P974	Q975	Q976	Q977	F880	A981	P917	I918	G919	PRO	H984	G985	G986	K987	G988	G989	F990	G991	G992	T993	Y994	R995	R996	E997	D998	M999	P1000	F1001	T1002	A1003	E1004	G1005	I1006	V1007	P1008	E945	N946	G947	I948	V949	D950	G951	V952	L953	V954	T955	S1019	R1020	Q958	T1021	V1022	G1023	A1024	H1025	L1026	I1027	G1028	L1030	L1031	S1032	K1033
M841	N842	Q843	S844	S845	I846	D847	R848	G849	L850	F851	R852	G853	L854	F855	F856	R857	S858	Y859	M860	Q861	Q862	E863	K864	R865	R866	G867	M868	S869	M870	E871	L872	S873	F874	P875	G876	R877	R878	T880	N881	T882	L883	L884	D885	D891	D895	L898	T899	A900	P901	G902	V903	R904	V905	S906	G907	E908	T909	K972			
V910	I911	I912	G913	K914	P917	I918	G919	PRO	ASP	GLU	GLU	GLU	GLU	LEU	GLY	GLN	ARG	THR	ALA	TYR	HIS	S933	K934	R935	D936	A937	S938	T939	P940	I941	R942	S943	T944	E945	N946	G947	I948	V949	D950	G951	V952	L953	V954	T955	S956	N957	Q958	T959	G960	L961	G962	F963	V964	K965	V966	S906	G907	E908	T909	K972	
Q779	V780	F781	L782	T783	M784	Y785	M786	V787	M788	M789	M792	A793	M794	I795	L796	Y797	Y798	F799	Q800	H801	E802	S803	K804	T805	T806	R807	A808	M809	E810	I811	L812	K813	F814	R815	E816	L817	P818	A819	G820	Q821	N822	A823	I824	V825	A826	I827	A828	C829	Y830	S831	G832	Y833	N834	Q835	E836	D837	S838	M839	I840		
M841	N842	Q843	S844	S845	I846	D847	R848	G849	L850	F851	R852	G853	L854	F855	F856	R857	S858	Y859	M860	Q861	Q862	E863	K864	R865	R866	G867	M868	S869	M870	E871	L872	S873	F874	P875	G876	R877	R878	T880	N881	T882	L883	L884	D885	D891	D895	L898	T899	A900	P901	G902	V903	R904	V905	S906	G907	E908	T909	K972			
ASN	GLU	GLU	ASN	ASP	LEU	P722	V723	V724	F725	A726	K727	R730	V731	H734	T737	F738	V739	H740	C741	E742	I743	T744	T805	T806	R807	A808	M809	E810	I811	L812	K813	F814	R815	E816	L817	P818	A819	G820	Q821	N822	A823	I824	V825	A826	I827	A828	C829	Y830	S831	G832	Y833	N834	Q835	E836	D837	S838	M839	I840			
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V589	H590	R591	N592	P593	A594	M597	E598	L599	M600	T601	G602	L603	R604	R605	S606	G607	D608	I609	M610	P611	E612	V613	S614	M615	R616	L617	D618	E619	R620	E621	K622	E623	L624	K625	I626	F627	T628	D629	A630	G631	R632	V633	Y634	R635	S636	L637	F638	I639	V640	E641	D642	D643	E644	S645	L646	G647	H648	K649			
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V589	H590	R591	N592	P593	A594	M597	E598	L599	M600	T601	G602	L603	R604	R605	S606	G607	D608	I609	M610	P611	E612	V613	S614	M615	R616	L617	D618	E619	R620	E621	K622	E623	L624	K625	I626	F627	T628	D629	A630	G631	R632	V633	Y634	R635	S636	L637	F638	I639	V640	E641	D642	D643	E644	S645	L646	G647	H648	K649			
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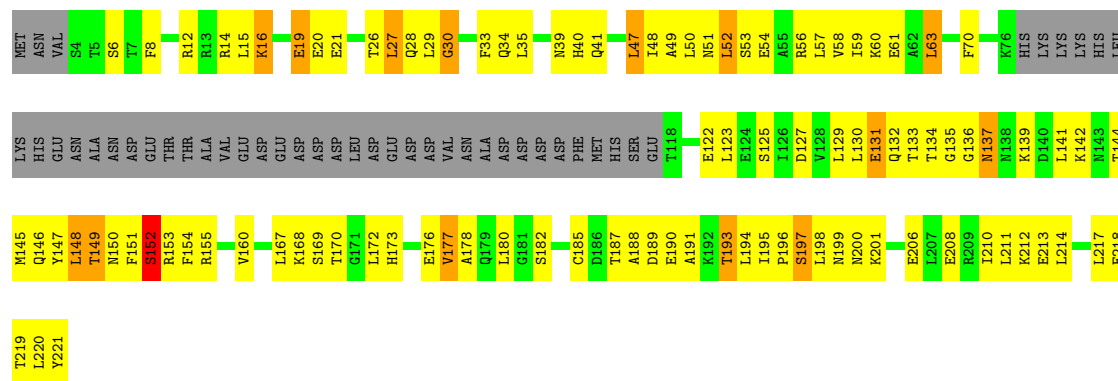
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:



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

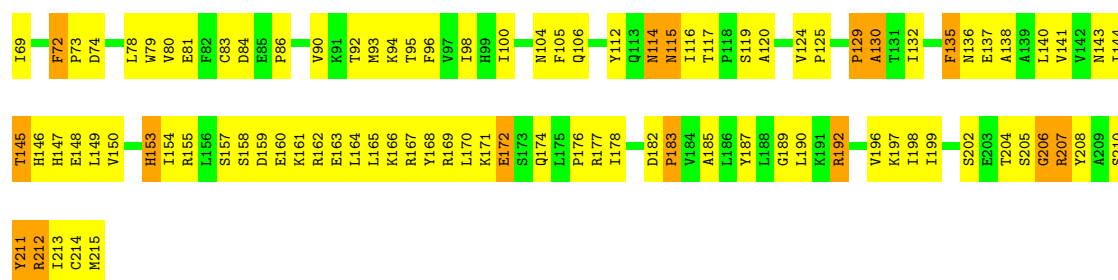
Chain D:



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

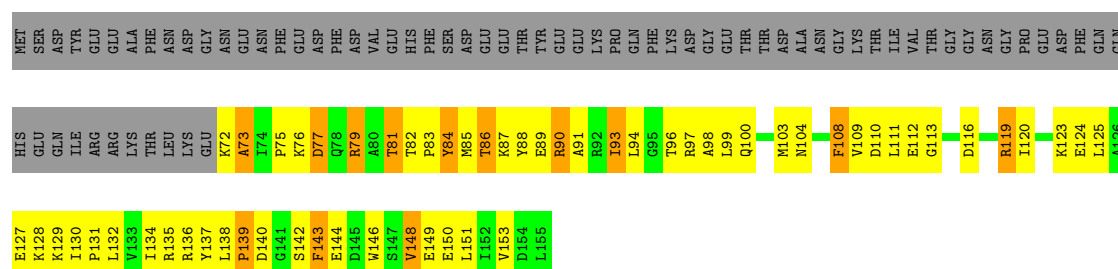
Chain E:





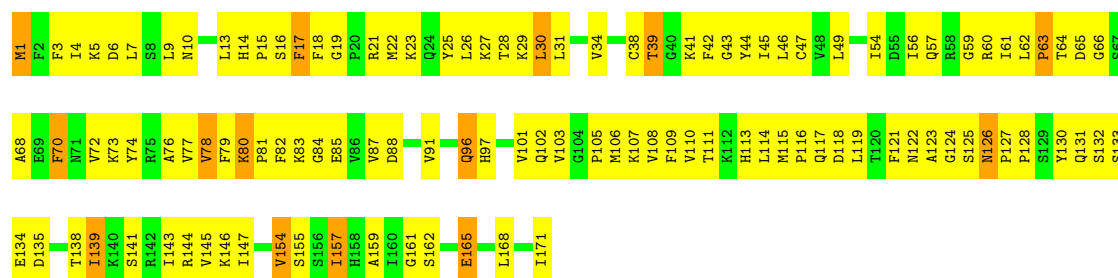
- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



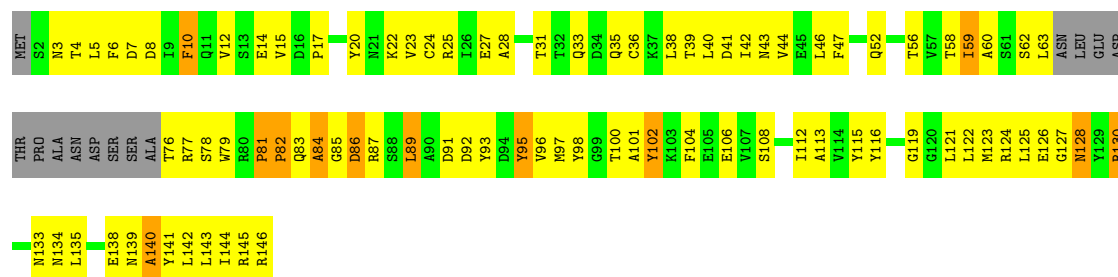
- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

Chain G:



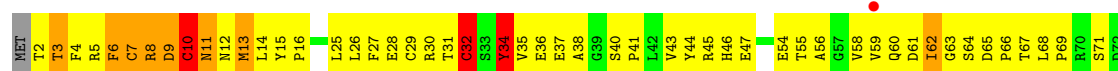
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



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

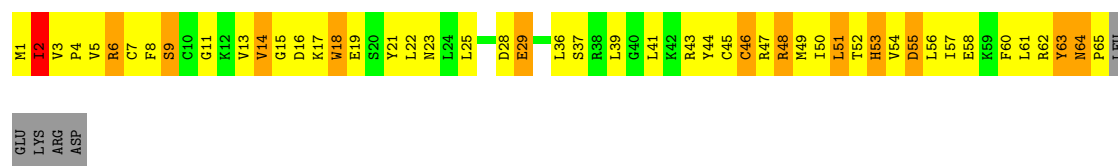
Chain I:





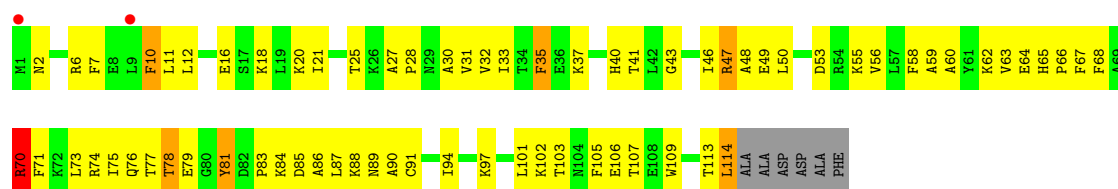
- Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



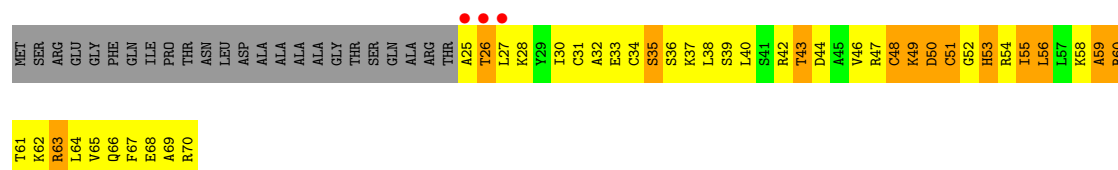
- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



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

Chain L:



- Molecule 13: Transcription elongation factor S-II

Chain S:



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	4.75 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.294 0.196 , 0.196	Depositor DCC
R_{free} test set	2288 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.4	EDS
Estimated twinning fraction	0.208 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.216 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.12$	Xtriage
Outliers	0 of 115462 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	259	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	919	0	929	96	0
12	L	364	0	387	68	0
13	S	666	0	553	103	0
14	S	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
15	S	1	0	0	0	0
All	All	31803	0	31737	3771	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 60.

The worst 5 of 3771 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	1418/1733 (82%)	914 (64%)	316 (22%)	188 (13%)	0	12
2	B	1096/1224 (90%)	726 (66%)	223 (20%)	147 (13%)	0	12
3	C	264/318 (83%)	169 (64%)	62 (24%)	33 (12%)	1	14
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	1	21
6	F	82/155 (53%)	60 (73%)	15 (18%)	7 (8%)	1	27
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	2	33
8	H	129/146 (88%)	93 (72%)	26 (20%)	10 (8%)	1	30
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0	13
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0	4
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	4	47
12	L	44/70 (63%)	18 (41%)	14 (32%)	12 (27%)	0	1
13	S	68/179 (38%)	51 (75%)	10 (15%)	7 (10%)	1	19
All	All	3947/4744 (83%)	2622 (66%)	838 (21%)	487 (12%)	1	14

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%)	14	58
2	B	964/1061 (91%)	880 (91%)	84 (9%)	15	60
3	C	234/274 (85%)	205 (88%)	29 (12%)	7	41
4	D	140/200 (70%)	126 (90%)	14 (10%)	11	53
5	E	196/197 (100%)	184 (94%)	12 (6%)	26	75
6	F	74/137 (54%)	63 (85%)	11 (15%)	4	31
7	G	152/152 (100%)	143 (94%)	9 (6%)	28	76
8	H	117/128 (91%)	110 (94%)	7 (6%)	27	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	113/116 (97%)	97 (86%)	16 (14%)	5	34
10	J	60/65 (92%)	55 (92%)	5 (8%)	16	63
11	K	99/102 (97%)	91 (92%)	8 (8%)	17	64
12	L	40/57 (70%)	33 (82%)	7 (18%)	3	21
13	S	62/156 (40%)	55 (89%)	7 (11%)	9	45
All	All	3497/4165 (84%)	3175 (91%)	322 (9%)	13	57

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 chains 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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1426/1733 (82%)	0.18	3 (0%) 93 86	1, 54, 131, 183	0
2	B	1104/1224 (90%)	0.29	13 (1%) 75 54	4, 67, 147, 180	0
3	C	266/318 (83%)	0.18	0 100 100	17, 61, 118, 143	0
4	D	177/221 (80%)	0.17	0 100 100	23, 78, 141, 157	0
5	E	214/215 (99%)	0.24	1 (0%) 88 74	10, 93, 155, 173	0
6	F	84/155 (54%)	0.07	0 100 100	1, 40, 79, 101	0
7	G	171/171 (100%)	0.23	0 100 100	25, 56, 96, 113	0
8	H	133/146 (91%)	0.48	0 100 100	60, 115, 156, 175	0
9	I	119/122 (97%)	0.50	6 (5%) 28 19	45, 109, 153, 196	0
10	J	65/70 (92%)	0.17	0 100 100	30, 56, 107, 124	0
11	K	114/120 (95%)	0.26	2 (1%) 65 44	21, 67, 121, 129	0
12	L	46/70 (65%)	0.54	3 (6%) 18 14	51, 117, 149, 169	0
13	S	174/179 (97%)	1.74	50 (28%) 1 2	50, 50, 110, 125	0
All	All	4093/4744 (86%)	0.30	78 (1%) 64 42	1, 64, 141, 196	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	S	162	LYS	12.6
13	S	141	THR	11.2
13	S	145	HIS	10.6
13	S	142	ALA	8.3
13	S	161	ALA	7.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	MG	S	1	1/1	0.71	14.41	91,91,91,91	0
15	ZN	B	1307	1/1	0.19	-0.59	15,15,15,15	0
15	ZN	S	310	1/1	0.16	-1.01	94,94,94,94	0
15	ZN	L	105	1/1	0.13	-1.43	68,68,68,68	0
15	ZN	A	1735	1/1	0.19	-1.47	15,15,15,15	0
15	ZN	C	319	1/1	0.17	-1.52	20,20,20,20	0
15	ZN	I	204	1/1	0.14	-1.94	97,97,97,97	0
15	ZN	I	203	1/1	0.13	-1.97	63,63,63,63	0
15	ZN	J	101	1/1	0.14	-2.03	16,16,16,16	0
15	ZN	A	1734	1/1	0.13	-2.77	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.