



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 01:26 PM EDT

PDB ID : 5U0S  
EMDB ID: : EMD-8480  
Title : Cryo-EM structure of the Mediator-RNAPII complex  
Authors : Tsai, K.-L.; Yu, X.; Gopalan, S.; Chao, T.-C.; Zhang, Y.; Florens, L.; Washburn, M.P.; Murakami, K.; Conaway, R.C.; Conaway, J.W.; Asturias, F.  
Deposited on : unknown  
Resolution : 7.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

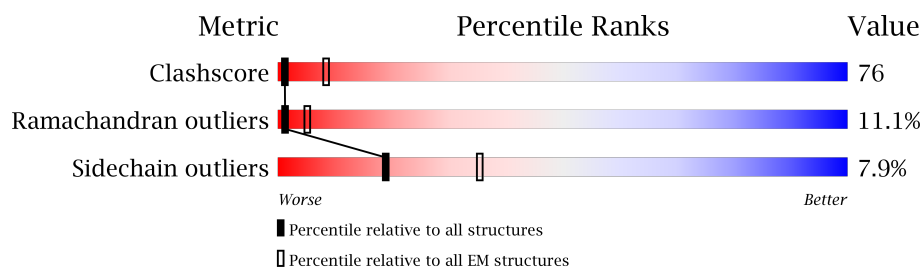
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.80 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.











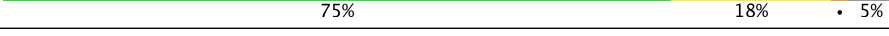


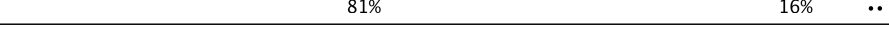

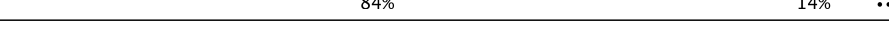


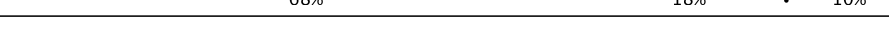

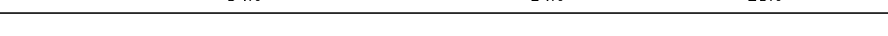
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	F	216	37% 49% 13%
2	H	200	41% 50% 9%
3	Q	545	45% 45% 8%
4	R	207	35% 64%
5	T	193	22% 65% 9%
6	K	116	35% 49% 16%
7	V	136	40% 46% 13%
8	N	931	25% 29% 44%
9	D	239	38% 60%

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Mol	Chain	Length	Quality of chain
10	G	376	
11	U	138	
12	3	139	
13	2	273	
14	I	121	
15	S	139	
16	J	132	
17	a	1752	
18	b	1210	
19	c	297	
20	d	135	
21	e	210	
22	f	142	
23	g	172	
24	h	125	
25	i	113	
26	j	71	
27	k	123	
28	l	63	

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 51548 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Mediator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	188	Total	C	N	O	S	0	0
			1534	979	258	288	9		

- Molecule 2 is a protein called Mediator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	182	Total	C	N	O	S	0	0
			1493	941	257	292	3		

- Molecule 3 is a protein called Mediator complex subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	500	Total	C	N	O	S	0	0
			3787	2393	651	725	18		

- Molecule 4 is a protein called Mediator complex subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	207	Total	C	N	O	S	0	0
			1694	1082	288	316	8		

- Molecule 5 is a protein called Mediator complex subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	176	Total	C	N	O	S	0	0
			1435	938	234	258	5		

- Molecule 6 is a protein called Mediator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	98	Total	C	N	O	S	0	0
			769	486	128	154	1		

- Molecule 7 is a protein called Mediator complex subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	118	Total	C	N	O	S	0	0
			949	599	161	187	2		

- Molecule 8 is a protein called Mediator complex subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	520	Total	C	N	O	S	0	0
			3887	2498	683	698	8		

- Molecule 9 is a protein called Mediator complex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	D	96	Total	C	N	O	0	0
			480	288	96	96		

- Molecule 10 is a protein called Mediator complex subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	G	194	Total	C	N	O	0	0
			965	577	194	194		

- Molecule 11 is a protein called Mediator complex subunit 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	U	122	Total	C	N	O	0	0
			608	364	122	122		

- Molecule 12 is a protein called Mediator complex subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	3	103	Total	C	N	O	0	0
			515	309	103	103		

- Molecule 13 is a protein called Mediator complex subunit 27.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	2	78	Total	C	N	O	0	0
			388	232	78	78		

- Molecule 14 is a protein called Mediator complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	I	75	Total	C	N	O	0	0
			374	224	75	75		

- Molecule 15 is a protein called Mediator complex subunit 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	S	122	Total	C	N	O	0	0
			610	366	122	122		

- Molecule 16 is a protein called Mediator complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	J	131	Total	C	N	O	0	0
			655	393	131	131		

- Molecule 17 is a protein called RNA polymerase II subunit Rpb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	1490	Total	C	N	O	S	0	0
			11761	7388	2065	2238	70		

- Molecule 18 is a protein called RNA polymerase II subunit Rpb2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	1150	Total	C	N	O	S	0	0
			9180	5772	1630	1716	62		

- Molecule 19 is a protein called RNA polymerase II subunit Rpb3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	263	Total	C	N	O	S	0	0
			2088	1315	355	406	12		

- Molecule 20 is a protein called RNA polymerase II subunit Rpb4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	125	Total	C	N	O	S	0	0
			988	619	166	197	6		

- Molecule 21 is a protein called RNA polymerase II subunit Rpb5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	207	Total	C	N	O	S	0	0
			1663	1050	301	306	6		

- Molecule 22 is a protein called RNA polymerase II subunit Rpb6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	f	83	Total	C	N	O	S	0	0
			656	416	112	125	3		

- Molecule 23 is a protein called RNA polymerase II subunit Rpb7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	170	Total	C	N	O	S	0	0
			1330	860	217	247	6		

- Molecule 24 is a protein called RNA polymerase II subunit Rpb8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	h	124	Total	C	N	O	S	0	0
			996	631	167	195	3		

- Molecule 25 is a protein called RNA polymerase II subunit Rpb9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	i	111	Total	C	N	O	S	0	0
			902	551	164	176	11		

- Molecule 26 is a protein called RNA polymerase II subunit Rpb10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	64	Total	C	N	O	S	0	0
			518	330	87	94	7		

- Molecule 27 is a protein called RNA polymerase II subunit Rpb11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	k	119	Total	C	N	O	S	0	0
			955	608	159	182	6		

- Molecule 28 is a protein called RNA polymerase II subunit Rpb12.

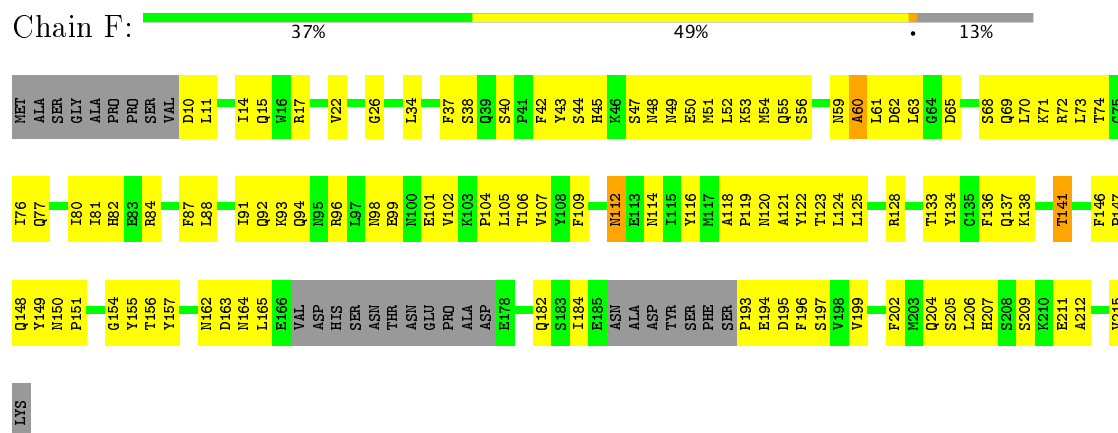
Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	45	Total	C	N	O	S	0	0
			368	225	74	61	8		



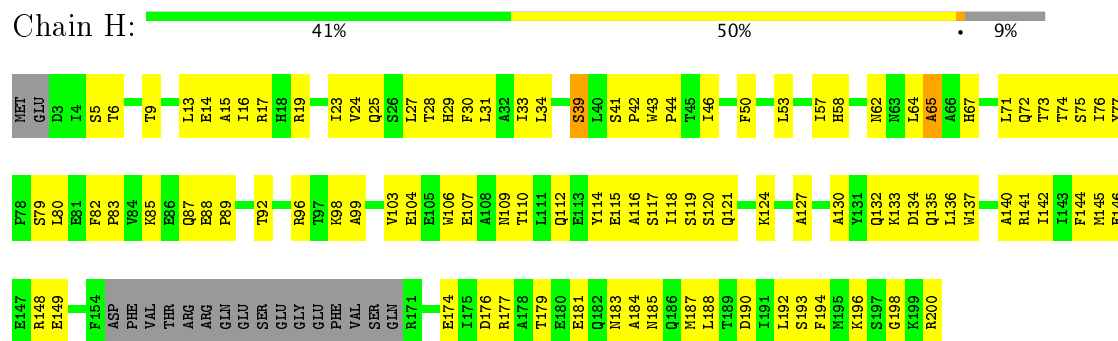
### 3 Residue-property plots

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.

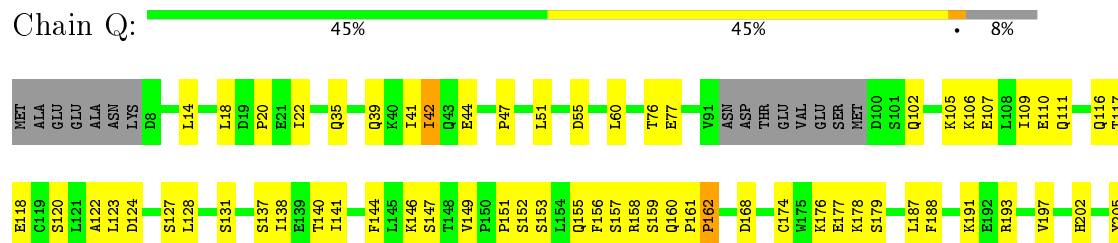
#### • Molecule 1: Mediator complex subunit 6

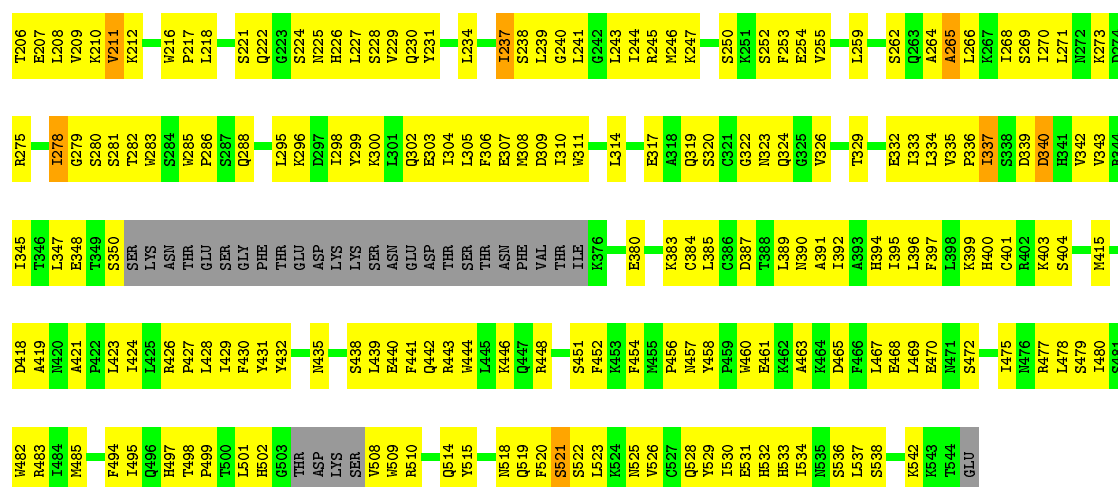


#### • Molecule 2: Mediator complex subunit 8



#### • Molecule 3: Mediator complex subunit 17

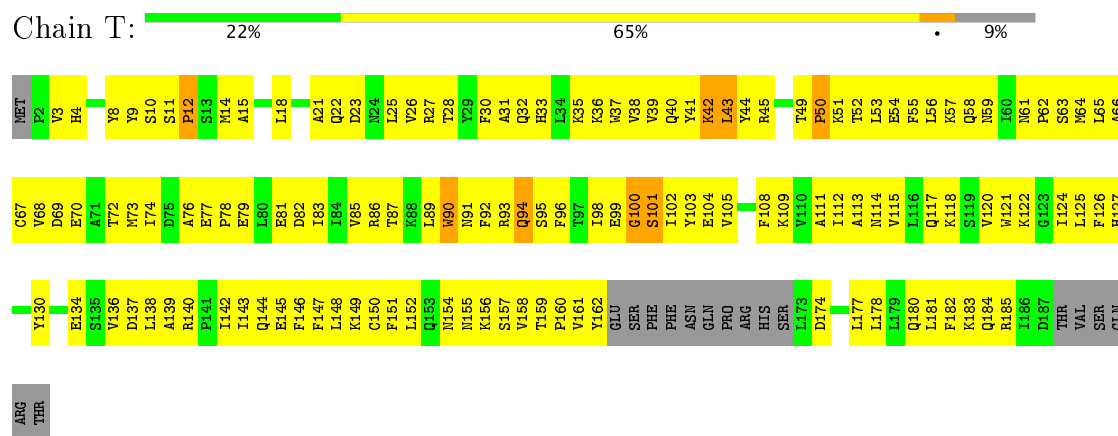




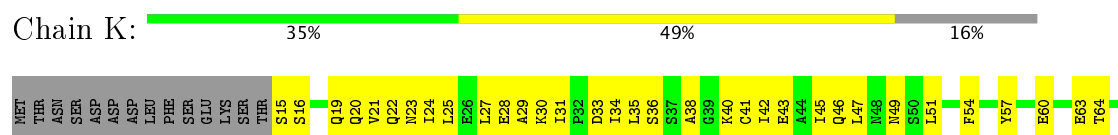
### • Molecule 4: Mediator complex subunit 18



### • Molecule 5: Mediator complex subunit 20



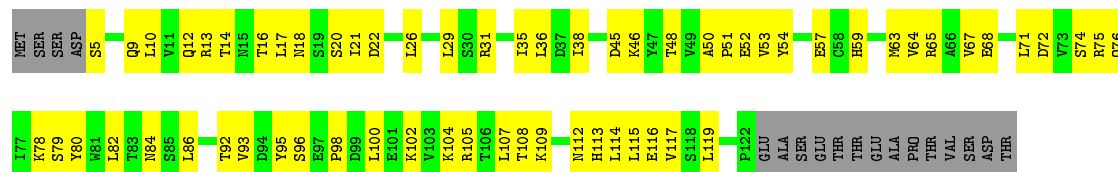
### • Molecule 6: Mediator complex subunit 11





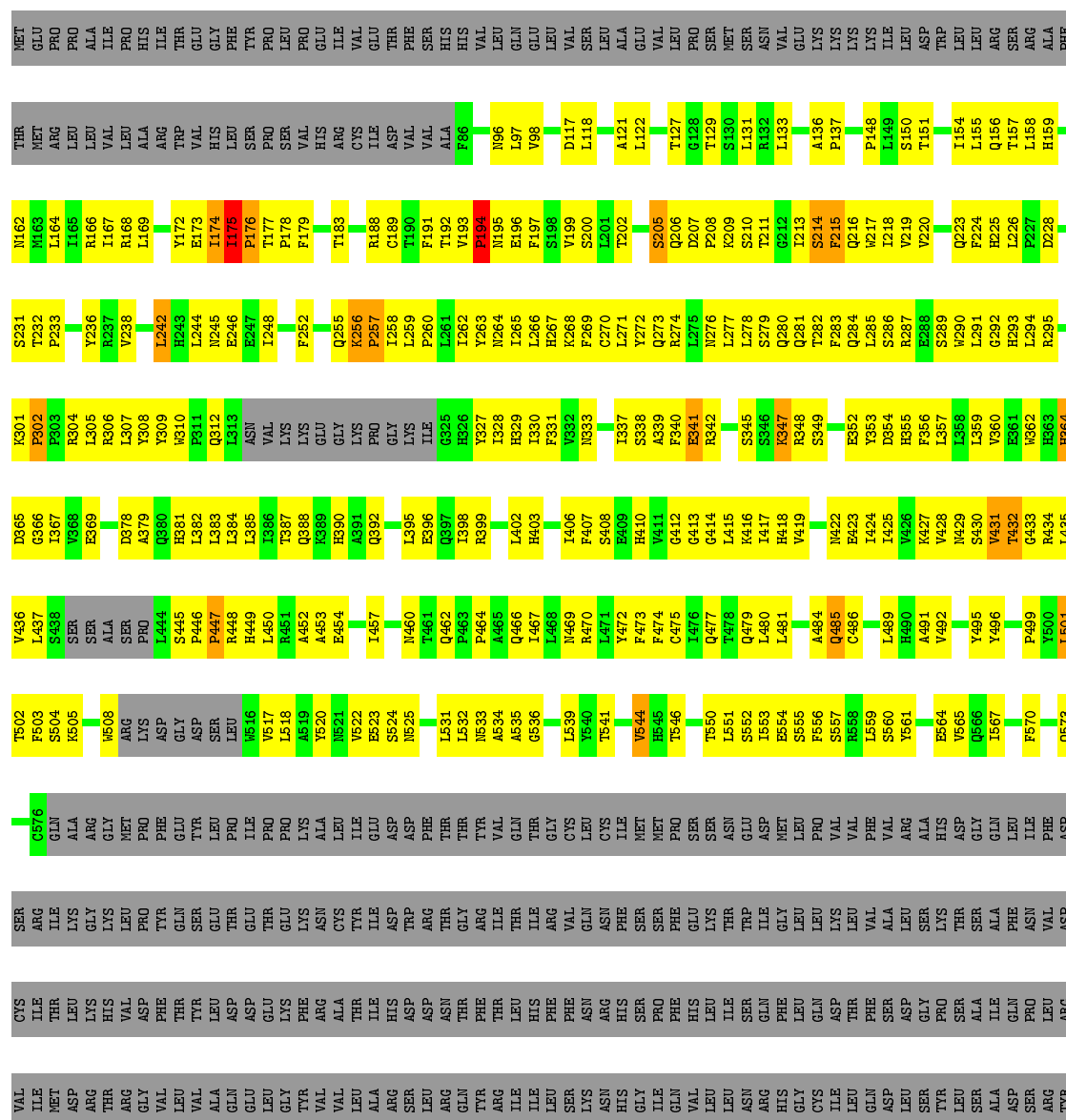
• Molecule 7: Mediator complex subunit 22

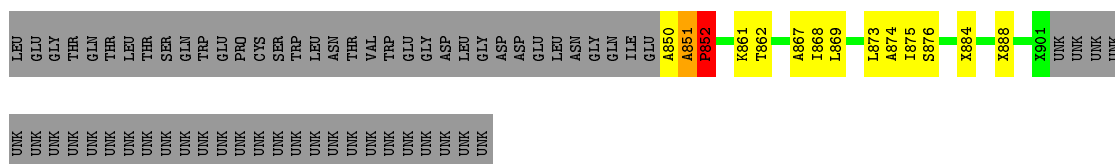
Chain V: 40% 46% 13%



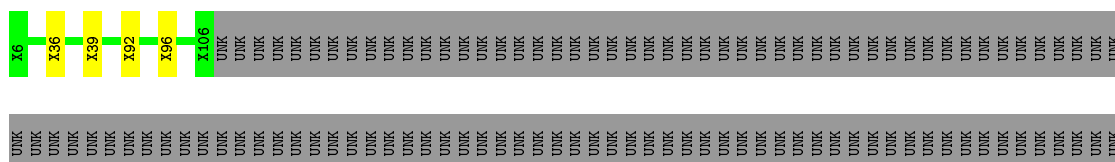
• Molecule 8: Mediator complex subunit 14

Chain N: 25% 29% 44%

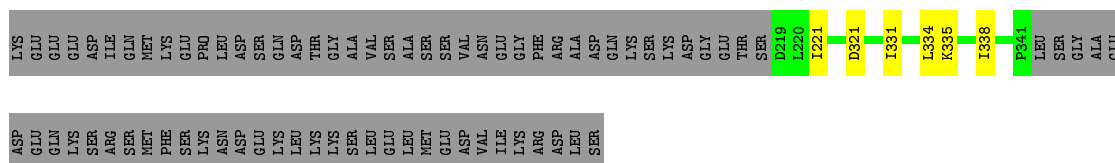
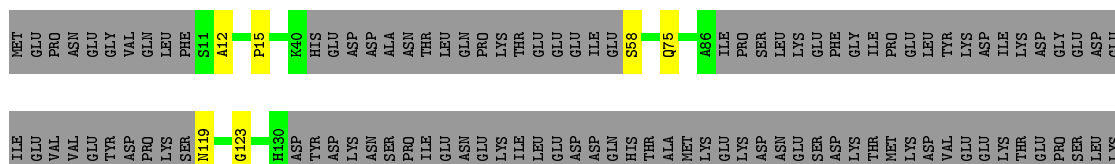




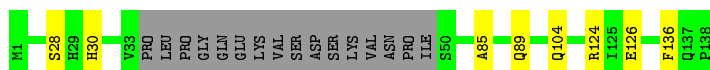
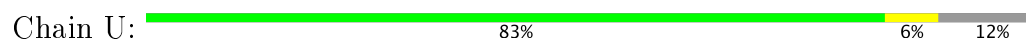
- Molecule 9: Mediator complex subunit 4



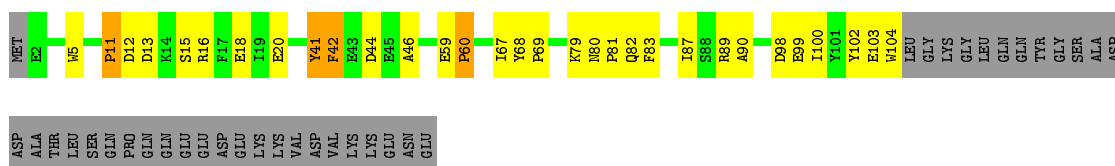
- Molecule 10: Mediator complex subunit 7



- Molecule 11: Mediator complex subunit 21



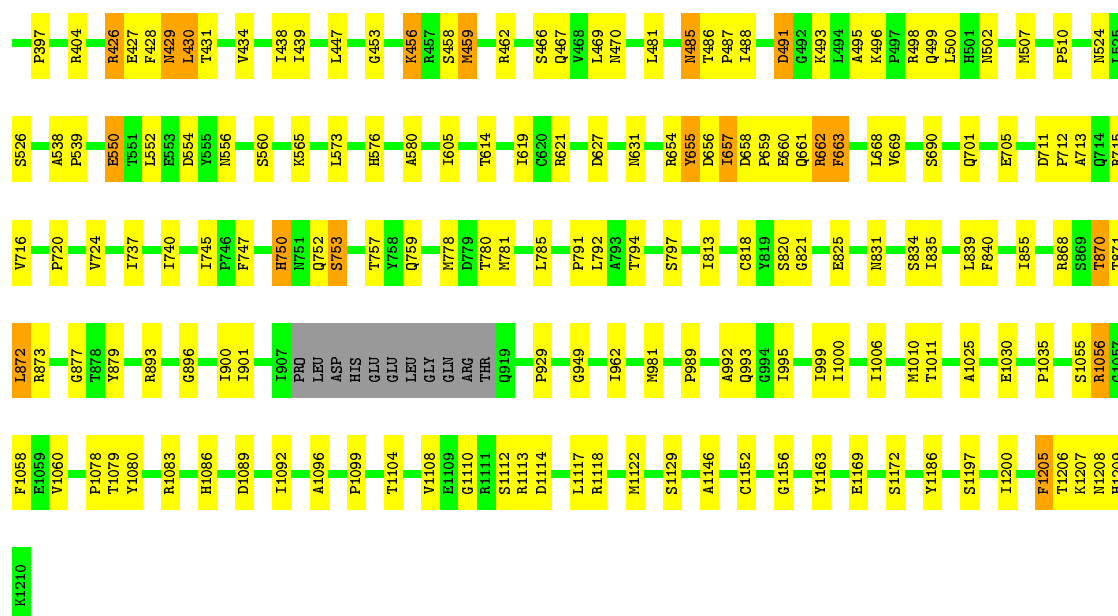
- Molecule 12: Mediator complex subunit 31



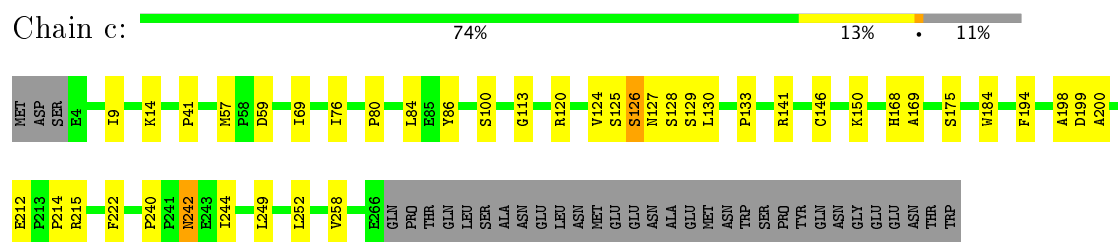
- Molecule 13: Mediator complex subunit 27



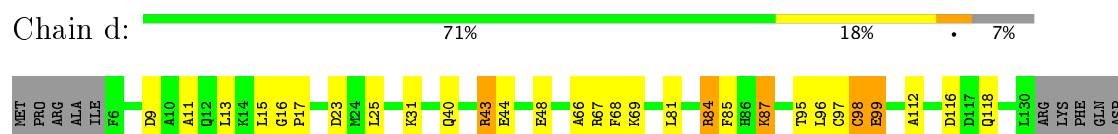




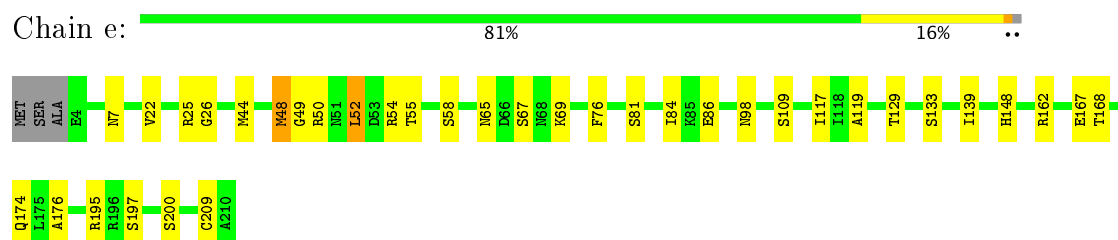
- Molecule 19: RNA polymerase II subunit Rpb3



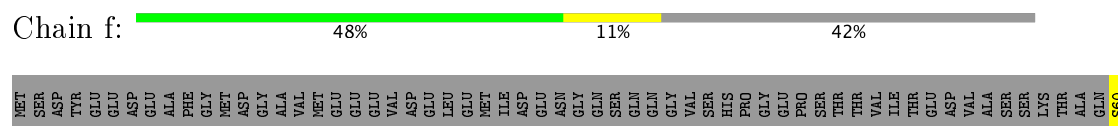
- Molecule 20: RNA polymerase II subunit Rpb4



- Molecule 21: RNA polymerase II subunit Rpb5



- Molecule 22: RNA polymerase II subunit Rpb6





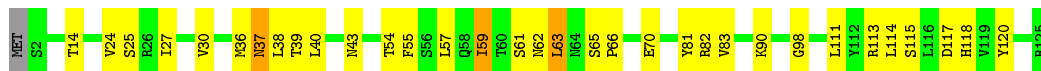
- Molecule 23: RNA polymerase II subunit Rpb7

Chain g: 84% 14% ..



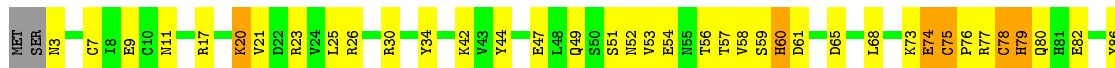
- Molecule 24: RNA polymerase II subunit Rpb8

Chain h: 73% 24% ..



- Molecule 25: RNA polymerase II subunit Rpb9

Chain i: 52% 40% 6% .



- Molecule 26: RNA polymerase II subunit Rpb10

Chain j: 68% 18% 10% .



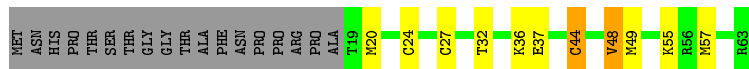
- Molecule 27: RNA polymerase II subunit Rpb11

Chain k: 82% 15% .



- Molecule 28: RNA polymerase II subunit Rpb12

Chain l: 54% 14% 29%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	9.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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  >2	RMSZ	# Z  >2
1	F	0.28	0/1570	0.49	0/2126
10	G	0.30	0/961	0.50	0/1336
11	U	0.27	0/606	0.47	0/844
12	3	0.26	0/514	0.52	1/718 (0.1%)
13	2	0.23	0/382	0.40	0/524
14	I	0.25	0/373	0.45	0/520
17	a	0.42	0/11983	0.57	1/16197 (0.0%)
18	b	0.44	0/9360	0.60	5/12643 (0.0%)
19	c	0.45	0/2135	0.60	0/2904
2	H	0.27	0/1523	0.48	0/2063
20	d	0.25	0/1000	0.38	0/1348
21	e	0.39	0/1695	0.60	0/2287
22	f	0.50	0/666	0.67	0/901
23	g	0.27	0/1361	0.57	3/1847 (0.2%)
24	h	0.42	0/1010	0.65	0/1363
25	i	0.23	0/921	0.37	0/1246
26	j	0.57	0/526	0.77	0/709
27	k	0.47	0/972	0.62	0/1317
28	l	0.37	0/371	0.57	0/491
3	Q	0.29	0/3856	0.49	2/5223 (0.0%)
4	R	0.28	0/1739	0.51	0/2362
5	T	0.31	0/1469	0.74	5/1992 (0.3%)
6	K	0.30	0/778	0.50	0/1049
7	V	0.27	0/963	0.46	0/1309
8	N	0.30	0/3865	0.61	6/5275 (0.1%)
All	All	0.37	0/50599	0.57	23/68594 (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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
8	N	0	2

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	100	GLY	C-N-CA	12.78	153.64	121.70
5	T	101	SER	O-C-N	-9.55	107.42	122.70
8	N	175	ILE	C-N-CD	-9.20	100.37	120.60
8	N	194	PRO	CA-N-CD	-8.83	99.14	111.50
5	T	100	GLY	CA-C-N	7.08	132.76	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	N	256	LYS	Peptide
8	N	302	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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	F	1534	0	1484	111	0
2	H	1493	0	1467	105	0
3	Q	3787	0	3544	229	0
4	R	1694	0	1670	144	0
5	T	1435	0	1447	146	0
6	K	769	0	783	70	0
7	V	949	0	961	67	0
8	N	3887	0	3543	317	0
9	D	480	0	101	8	0
10	G	965	0	402	6	0
11	U	608	0	265	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	3	515	0	209	15	0
13	2	388	0	155	14	0
14	I	374	0	163	5	0
15	S	610	0	138	2	0
16	J	655	0	144	12	0
17	a	11761	0	11738	0	0
18	b	9180	0	9164	0	0
19	c	2088	0	2044	0	0
20	d	988	0	977	0	0
21	e	1663	0	1684	0	0
22	f	656	0	679	0	0
23	g	1330	0	1329	0	0
24	h	996	0	1006	0	0
25	i	902	0	843	0	0
26	j	518	0	532	0	0
27	k	955	0	968	0	0
28	l	368	0	381	0	0
All	All	51548	0	47821	1120	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 76.

The worst 5 of 1120 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)
8:N:192:THR:C	8:N:194:PRO:HD3	1.19	1.54
8:N:199:VAL:HG12	8:N:217:TRP:CE3	1.42	1.52
8:N:851:ALA:HA	8:N:852:PRO:CB	1.35	1.39
8:N:199:VAL:CG1	8:N:217:TRP:CE3	2.12	1.31
8:N:199:VAL:CG1	8:N:217:TRP:CD2	2.12	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 PDB entries followed by that with respect to all EM entries.

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	F	182/216 (84%)	154 (85%)	24 (13%)	4 (2%)	8	44
2	H	178/200 (89%)	161 (90%)	15 (8%)	2 (1%)	17	60
3	Q	492/545 (90%)	424 (86%)	55 (11%)	13 (3%)	6	40
4	R	205/207 (99%)	177 (86%)	23 (11%)	5 (2%)	7	42
5	T	172/193 (89%)	141 (82%)	21 (12%)	10 (6%)	2	24
6	K	96/116 (83%)	88 (92%)	7 (7%)	1 (1%)	18	61
7	V	116/136 (85%)	107 (92%)	8 (7%)	1 (1%)	20	63
8	N	489/931 (52%)	382 (78%)	72 (15%)	35 (7%)	1	19
10	G	186/376 (50%)	166 (89%)	18 (10%)	2 (1%)	17	60
11	U	118/138 (86%)	110 (93%)	5 (4%)	3 (2%)	6	41
12	3	101/139 (73%)	76 (75%)	9 (9%)	16 (16%)	0	4
13	2	66/273 (24%)	62 (94%)	3 (4%)	1 (2%)	12	53
14	I	73/121 (60%)	67 (92%)	3 (4%)	3 (4%)	3	30
17	a	1486/1752 (85%)	937 (63%)	276 (19%)	273 (18%)	0	3
18	b	1142/1210 (94%)	735 (64%)	244 (21%)	163 (14%)	0	5
19	c	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	0	11
20	d	123/135 (91%)	85 (69%)	20 (16%)	18 (15%)	0	5
21	e	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	0	7
22	f	81/142 (57%)	57 (70%)	16 (20%)	8 (10%)	1	12
23	g	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	1	14
24	h	122/125 (98%)	73 (60%)	27 (22%)	22 (18%)	0	3
25	i	109/113 (96%)	46 (42%)	27 (25%)	36 (33%)	0	0
26	j	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	1	13
27	k	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	0	9
28	l	43/63 (68%)	23 (54%)	12 (28%)	8 (19%)	0	3
All	All	6393/8004 (80%)	4635 (72%)	1047 (16%)	711 (11%)	1	9

5 of 711 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	319	GLN
4	R	50	ARG

*Continued on next page...*

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Mol	Chain	Res	Type
5	T	101	SER
8	N	175	ILE
8	N	194	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 PDB entries followed by that with respect to all EM entries.

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	F	171/198 (86%)	171 (100%)	0	100	100
2	H	168/185 (91%)	168 (100%)	0	100	100
3	Q	389/509 (76%)	389 (100%)	0	100	100
4	R	191/191 (100%)	191 (100%)	0	100	100
5	T	161/178 (90%)	161 (100%)	0	100	100
6	K	88/108 (82%)	88 (100%)	0	100	100
7	V	112/129 (87%)	112 (100%)	0	100	100
8	N	369/799 (46%)	369 (100%)	0	100	100
17	a	1296/1536 (84%)	1109 (86%)	187 (14%)	4	22
18	b	1012/1064 (95%)	912 (90%)	100 (10%)	9	34
19	c	236/267 (88%)	219 (93%)	17 (7%)	17	49
20	d	106/115 (92%)	90 (85%)	16 (15%)	3	20
21	e	182/184 (99%)	169 (93%)	13 (7%)	17	49
22	f	71/121 (59%)	64 (90%)	7 (10%)	9	34
23	g	146/148 (99%)	139 (95%)	7 (5%)	30	61
24	h	113/114 (99%)	99 (88%)	14 (12%)	5	26
25	i	103/105 (98%)	80 (78%)	23 (22%)	1	7
26	j	59/66 (89%)	46 (78%)	13 (22%)	1	7
27	k	109/113 (96%)	104 (95%)	5 (5%)	31	62
28	l	39/53 (74%)	34 (87%)	5 (13%)	5	25
All	All	5121/6183 (83%)	4714 (92%)	407 (8%)	19	45

5 of 407 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	a	1449	ILE
18	b	565	LYS
25	i	77	ARG
18	b	89	MET
18	b	352	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
17	a	887	GLN
18	b	339	HIS
24	h	108	HIS
17	a	919	ASN
17	a	1156	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	S	6
16	J	3
9	D	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	56:UNK	C	160:UNK	N	39.54
1	J	204:UNK	C	310:UNK	N	28.97
1	S	265:UNK	C	271:UNK	N	28.24
1	S	366:UNK	C	381:UNK	N	25.63
1	S	287:UNK	C	301:UNK	N	18.84