



## wwPDB EM Map/Model Validation Report ⓘ

Jun 14, 2016 – 12:26 PM EDT

PDB ID : 5IYA  
EMDB ID: : EMD-8135  
Title : Human core-PIC in the closed state  
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.  
Deposited on : 2016-03-24  
Resolution : 5.40 Å(reported)  
Based on PDB ID : ?

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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>

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MolProbity : 4.02b-467  
Mogul : unknown  
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) : rb-20027790

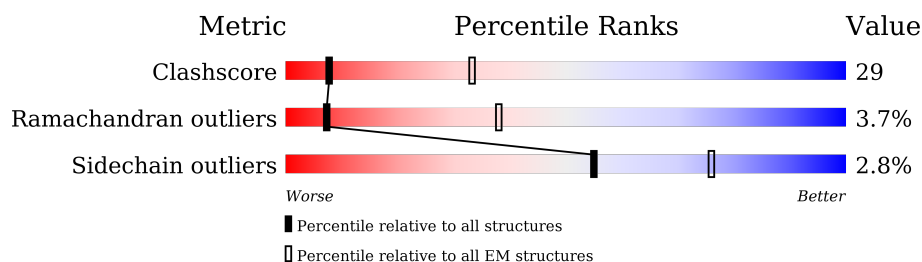
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.40 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	A	1970	41% 30% .. 26%
2	B	1174	50% 46% . .
3	C	275	47% 50% .
4	D	142	65% 25% 9%
5	E	210	52% 46% .
6	F	127	35% 31% . 32%
7	G	172	65% 32% ..
8	H	150	44% 47% 7% .
9	I	125	39% 53% 8%

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Mol	Chain	Length	Quality of chain
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	U	301	
22	X	59	
23	Y	59	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 46697 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1454	Total	C	N	O	S	0	0
			11515	7234	2058	2150	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1165	Total	C	N	O	S	0	0
			9317	5878	1637	1738	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	275	Total	C	N	O	S	0	0
			2213	1386	380	440	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	129	Total	C	N	O	S	0	0
			1062	665	179	214	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	86	Total	C	N	O	S	0	0
			689	437	120	127	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	260	Total	C	N	O	S	0	0
			2018	1265	360	376	17		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1137	719	207	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	59	Total	C	N	O	P	0	0
			1218	575	235	350	58		

- Molecule 23 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	59	Total	C	N	O	P	0	0
			1195	568	215	354	58		

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	B	1	Total	Mg	0
			1	1	
24	A	1	Total	Mg	0
			1	1	

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	J	1	Total	Zn	0
			1	1	
25	Q	1	Total	Zn	0
			1	1	
25	B	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	C	1	Total	Zn	0
			1	1	
25	A	2	Total	Zn	0
			2	2	
25	U	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
25	M	1	1	1	0





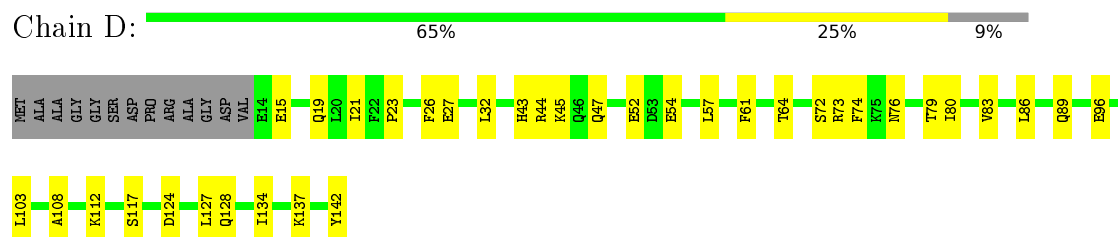


I152	E79	Met
P153	E80	Tyr
I154	P81	Asp
M155	P82	Ala
L156	R83	Asp
R157	P84	Glu
	L85	Asp
Y160	L86	Met
C161	K87	Gln
M164	F88	Y10
G165	E89	D11
L166	Q90	E12
	I91	
R169	Y92	L21
D170	L93	W22
L171	S94	Q23
C172		E24
E173	T97	A25
L174	H98	C26
M175	W99	W27
E176	M100	L28
	R101	V29
	D102	I30
P161		
G182	P107	E36
G183	M108	K37
Y184	M109	
		V40
G189	E112	R41
		Q42
K192	R116	
V193	N117	S46
L194		
E198	Y120	F50
	S121	I51
A201	A122	Q52
	P123	M53
	L124	S54
V205	Y125	V55
	V126	Q56
A209	D127	R57
K210	I128	
R211	T129	E60
	K130	D61
A216	T131	A62
R222	V132	P63
S223	I133	P64
C224	K134	I65
L225	E135	D66
E226	L136	L67
N227	E137	Q68
D228	E138	A69
S229	T127	E70
R230	Q139	A71
T231	L140	Q72
	Q141	H73
T232	Q145	A74
W236	F143	E77
		H76

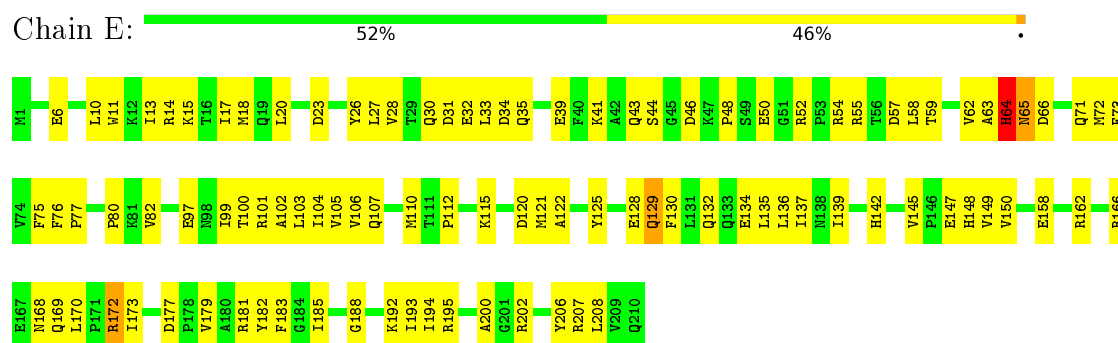


N223	Y151	I74	M1
R228	K152	S75	P2
Y231	K155	D76	Y3
N232	E158	D77	A5
V233	L159	I78	Q8
E234	R160	D80	P7
S235	L161	K81	T8
S238	R162	L82	R9
L239	A163	T89	R10
R240	A165	C90	I11
P241	K166	E91	E13
I244	K167	G94	L14
A248	G170	S98	T15
K253	K171	V99	D16
D258	E172	E100	V19
Q262	H173	F101	R20
E266	H176	V105	I22
D270	M177	R106	E24
N275	P178	C107	I25
	T179	M108	T26
	A183	E109	D27
	F184	D110	V30
	E185	R113	S33
	I186	H114	I34
	D189	V115	R35
	M190	T116	R36
	R193	S117	V37
	H194	L120	F38
	T195	I121	I39
	V196	S124	A40
	P198	P125	P43
	K199	R126	I44
	P200	V127	I45
	E201	I128	A46
	E202	P129	D48
	P204	V130	I47
	K205	M134	I49
	S209	R135	V50
	E210	D136	D83
	L211	M137	A54
	D212	D138	S56
	E213	V143	D61
	D214	E144	E82
	E215	Q145	F63
	S216	D146	
	Q217	D147	R67
	A218	I148	L68
		I149	
		I150	T71

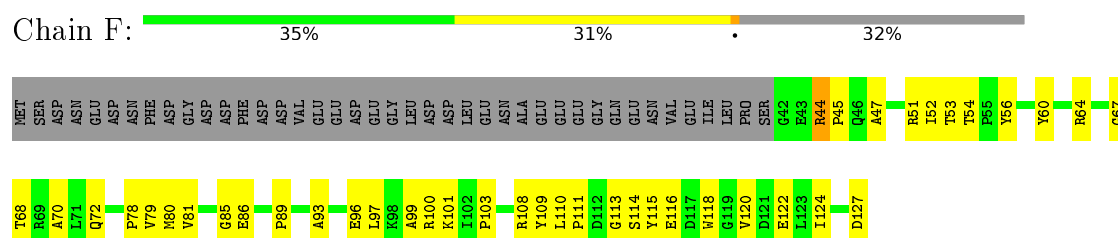
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



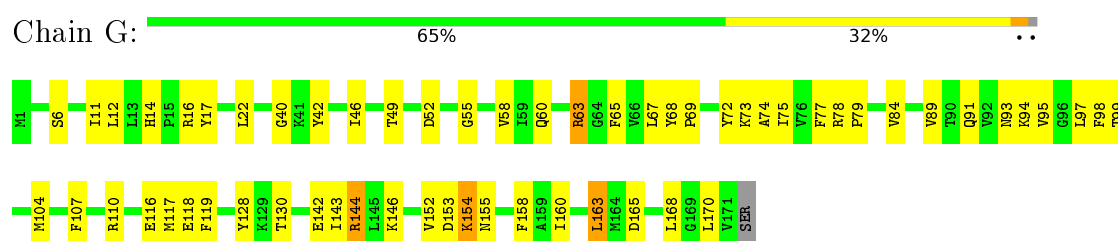
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



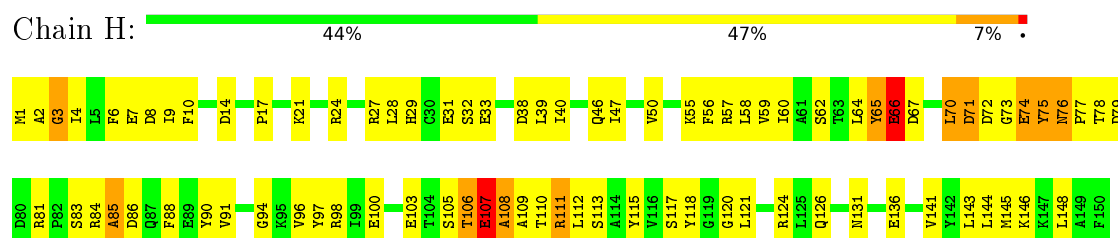
- Molecule 6: DNA-directed RNA polymerase II subunit RPB6



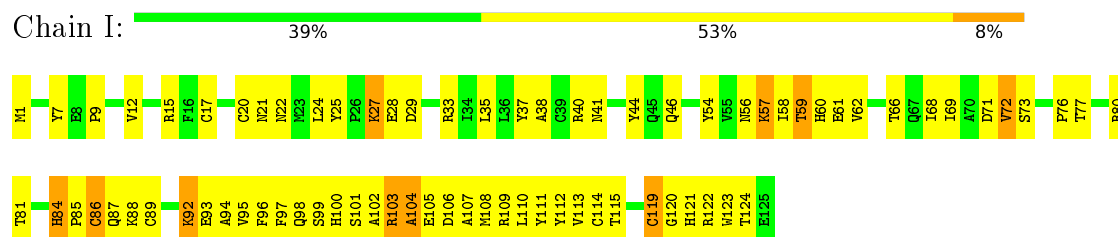
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



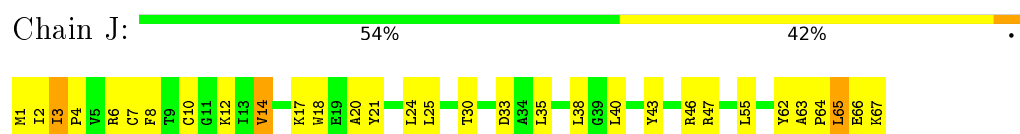
- Molecule 8: DNA-directed RNA polymerase II subunit RPB8



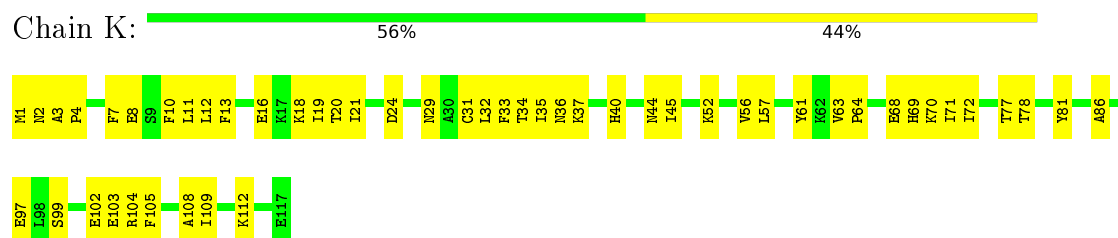
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



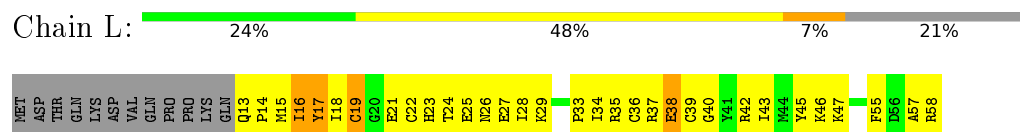
- Molecule 10: DNA-directed RNA polymerase II subunit RPB10



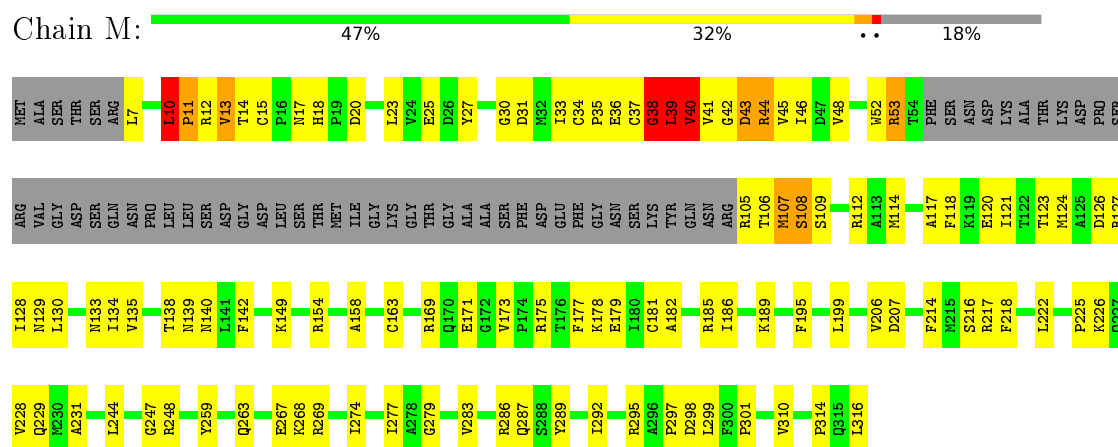
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 12: DNA-directed RNA polymerase II subunit RPB12

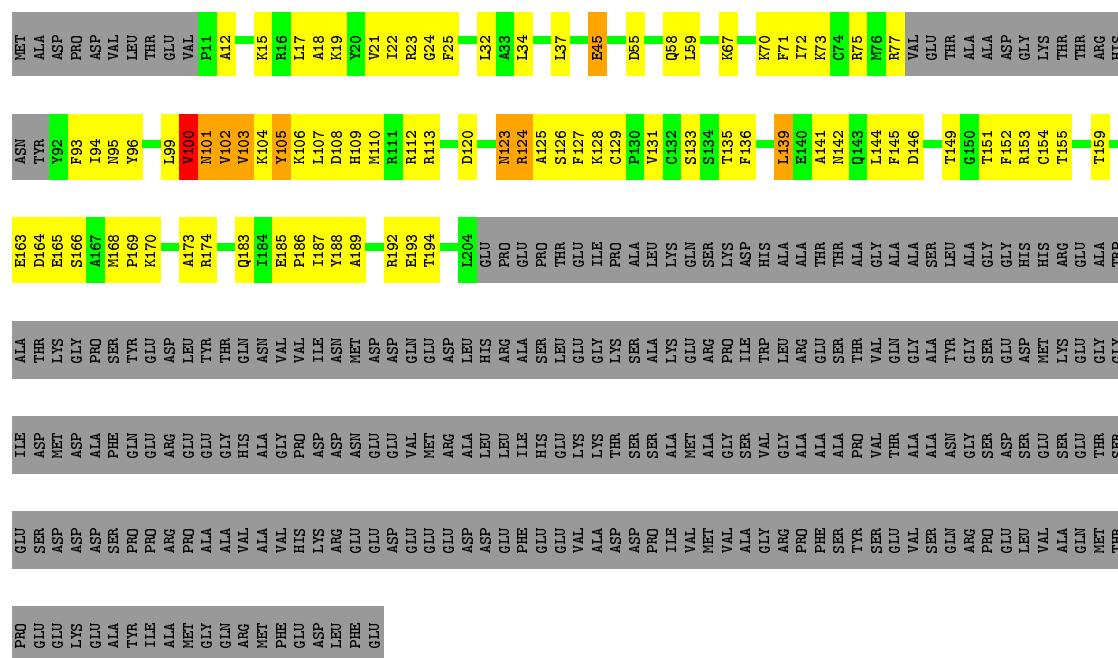


- Molecule 13: Transcription initiation factor IIB

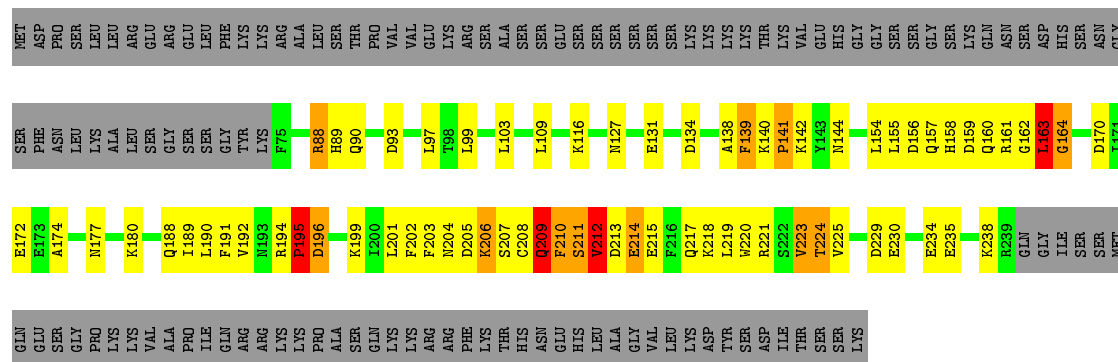
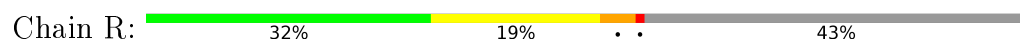


- Molecule 14: Transcription initiation factor IIA subunit 1

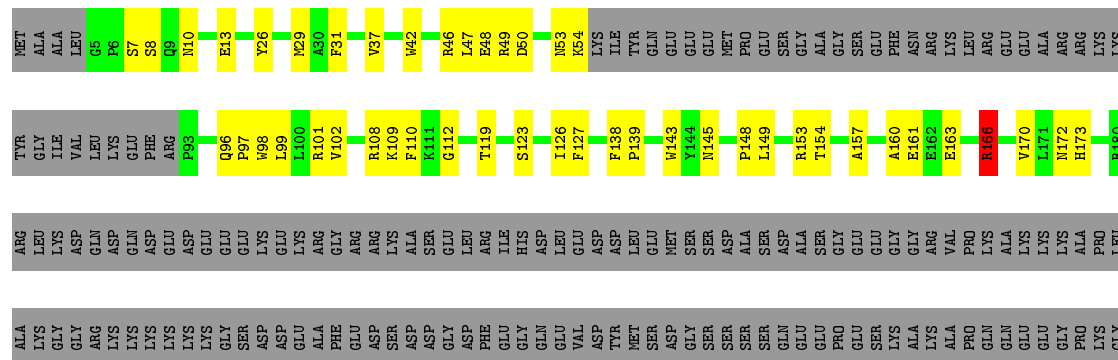




- Molecule 18: Transcription initiation factor IIE subunit beta



- Molecule 19: General transcription factor IIF subunit 1







G35	G49	A50	G53	A54	G55	G56	A57	G58	G59	A60	A61	G62	G63	G64	G65	G66	G67	G68	G69	G70	A71	G74	G75	T78	T79	T80	A81	A83	G84	G85	G86	G89	G90	T91	T92	G93
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	34728	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	Not provided	Depositor

## 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.27	0/11727	0.59	9/15833 (0.1%)
10	J	0.26	0/542	0.55	0/730
11	K	0.26	0/956	0.52	0/1294
12	L	0.26	0/394	0.61	0/524
13	M	0.26	0/2049	0.74	4/2769 (0.1%)
14	N	0.31	0/945	0.58	1/1274 (0.1%)
15	O	0.26	0/816	0.54	0/1105
16	P	0.31	0/1489	0.65	3/2005 (0.1%)
17	Q	0.29	0/1507	0.60	2/2023 (0.1%)
18	R	0.42	0/1380	0.91	2/1854 (0.1%)
19	S	0.29	0/1166	0.53	1/1575 (0.1%)
2	B	0.29	1/9503 (0.0%)	0.62	6/12831 (0.0%)
20	T	0.26	0/1817	0.58	1/2445 (0.0%)
21	U	0.33	0/1358	0.69	2/1820 (0.1%)
22	X	0.55	0/1369	0.90	0/2114
23	Y	0.55	0/1337	0.93	0/2059
3	C	0.27	0/2259	0.67	2/3073 (0.1%)
4	D	0.28	0/1077	0.51	0/1446
5	E	0.29	0/1753	0.63	2/2368 (0.1%)
6	F	0.25	0/700	0.51	0/946
7	G	0.27	0/1382	0.54	0/1874
8	H	0.27	0/1227	0.61	2/1654 (0.1%)
9	I	0.27	0/1038	0.90	2/1407 (0.1%)
All	All	0.31	1/47791 (0.0%)	0.65	39/65023 (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
1	A	0	2
17	Q	0	1
18	R	0	1
21	U	0	1
3	C	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1090	GLU	CD-OE1	7.40	1.33	1.25

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	84	HIS	C-N-CD	-24.01	67.78	120.60
18	R	194	ARG	C-N-CD	-22.48	71.14	120.60
13	M	10	LEU	C-N-CD	-20.59	75.30	120.60
3	C	6	GLN	C-N-CD	-20.16	76.26	120.60
2	B	497	LYS	C-N-CD	-20.03	76.53	120.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	PRO	Mainchain
1	A	85	PHE	Peptide
3	C	210	GLU	Mainchain
17	Q	100	VAL	Mainchain
18	R	230	GLU	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	11515	0	11607	677	0
2	B	9317	0	9307	574	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2213	0	2153	138	0
4	D	1062	0	1042	24	0
5	E	1723	0	1745	82	0
6	F	689	0	715	45	0
7	G	1351	0	1358	53	0
8	H	1205	0	1167	108	0
9	I	1013	0	931	81	0
10	J	533	0	553	39	0
11	K	937	0	959	46	0
12	L	388	0	393	65	0
13	M	2018	0	2060	136	0
14	N	930	0	888	64	0
15	O	806	0	818	51	0
16	P	1462	0	1548	117	0
17	Q	1484	0	1496	250	0
18	R	1357	0	1375	294	0
19	S	1137	0	1101	38	0
20	T	1788	0	1819	143	0
21	U	1343	0	1338	92	0
22	X	1218	0	661	25	0
23	Y	1195	0	663	30	0
24	A	1	0	0	0	0
24	B	1	0	0	0	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	Q	1	0	0	0	0
25	U	1	0	0	0	0
All	All	46697	0	45697	2635	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 29.

The worst 5 of 2635 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)
17:Q:110:MET:HB2	18:R:218:LYS:CG	1.11	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:MET:SD	2:B:256:ILE:HG23	1.45	1.53
17:Q:187:ILE:CD1	18:R:211:SER:CB	1.86	1.51
8:H:65:TYR:CE1	8:H:79:ASP:OD2	1.65	1.50
17:Q:110:MET:CE	18:R:213:ASP:CB	1.89	1.50

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	A	1450/1970 (74%)	1297 (89%)	100 (7%)	53 (4%)	4	38
2	B	1163/1174 (99%)	1044 (90%)	82 (7%)	37 (3%)	5	41
3	C	273/275 (99%)	244 (89%)	17 (6%)	12 (4%)	3	33
4	D	127/142 (89%)	118 (93%)	8 (6%)	1 (1%)	24	69
5	E	208/210 (99%)	198 (95%)	7 (3%)	3 (1%)	14	58
6	F	84/127 (66%)	78 (93%)	4 (5%)	2 (2%)	7	47
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	30	74
8	H	148/150 (99%)	121 (82%)	15 (10%)	12 (8%)	1	18
9	I	123/125 (98%)	102 (83%)	12 (10%)	9 (7%)	1	21
10	J	65/67 (97%)	53 (82%)	8 (12%)	4 (6%)	2	25
11	K	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	36 (82%)	4 (9%)	4 (9%)	1	16
13	M	256/316 (81%)	235 (92%)	11 (4%)	10 (4%)	4	36
14	N	109/376 (29%)	99 (91%)	6 (6%)	4 (4%)	4	38
15	O	97/109 (89%)	90 (93%)	7 (7%)	0	100	100
16	P	183/339 (54%)	167 (91%)	12 (7%)	4 (2%)	8	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	176/439 (40%)	159 (90%)	11 (6%)	6 (3%)	5	40
18	R	163/291 (56%)	129 (79%)	20 (12%)	14 (9%)	1	17
19	S	134/517 (26%)	123 (92%)	7 (5%)	4 (3%)	5	42
20	T	218/249 (88%)	191 (88%)	17 (8%)	10 (5%)	3	32
21	U	168/301 (56%)	135 (80%)	20 (12%)	13 (8%)	1	20
All	All	5473/7524 (73%)	4889 (89%)	381 (7%)	203 (4%)	7	38

5 of 203 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	205	VAL
1	A	531	ASN
1	A	610	PRO
1	A	619	LYS

### 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	A	1279/1748 (73%)	1243 (97%)	36 (3%)	51	79
2	B	1020/1028 (99%)	994 (98%)	26 (2%)	55	81
3	C	252/252 (100%)	247 (98%)	5 (2%)	63	85
4	D	119/126 (94%)	118 (99%)	1 (1%)	86	94
5	E	192/192 (100%)	187 (97%)	5 (3%)	54	80
6	F	74/111 (67%)	74 (100%)	0	100	100
7	G	152/153 (99%)	149 (98%)	3 (2%)	63	85
8	H	131/131 (100%)	128 (98%)	3 (2%)	58	83
9	I	112/112 (100%)	109 (97%)	3 (3%)	52	79
10	J	56/56 (100%)	55 (98%)	1 (2%)	66	87
11	K	106/106 (100%)	105 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	222/268 (83%)	211 (95%)	11 (5%)	30	66
14	N	105/324 (32%)	104 (99%)	1 (1%)	82	92
15	O	90/98 (92%)	89 (99%)	1 (1%)	80	91
16	P	159/293 (54%)	154 (97%)	5 (3%)	47	77
17	Q	164/373 (44%)	157 (96%)	7 (4%)	35	70
18	R	150/261 (58%)	140 (93%)	10 (7%)	20	58
19	S	121/448 (27%)	118 (98%)	3 (2%)	55	81
20	T	196/218 (90%)	189 (96%)	7 (4%)	42	74
21	U	148/266 (56%)	141 (95%)	7 (5%)	32	68
All	All	4891/6619 (74%)	4755 (97%)	136 (3%)	55	79

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1080	ARG
8	H	55	LYS
20	T	154	LYS
3	C	61	ASP
5	E	50	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1040	GLN
3	C	5	ASN
16	P	229	GLN
2	B	1117	HIS
1	A	1332	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 13 ligands modelled in this entry, 13 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.