



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

Jul 24, 2017 – 08:42 AM EDT

PDB ID : 5FUR  
EMDB ID: : EMD-3305  
Title : Structure of human TFIID-IIA bound to core promoter DNA  
Authors : Louder, R.K.; He, Y.; Lopez-Blanco, J.R.; Fang, J.; Chacon, P.; Nogales, E.  
Deposited on : unknown  
Resolution : 8.50 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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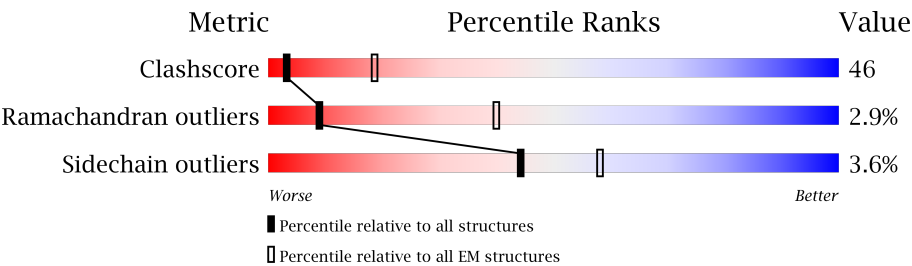
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.50 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	A	339	<div><div>44%</div><div>8%</div><div>.</div><div>47%</div></div>
2	B	43	<div><div>77%</div><div>21%</div><div>.</div></div>
3	C	47	<div><div>53%</div><div>45%</div><div>.</div></div>
4	D	97	<div><div>57%</div><div>41%</div><div>.</div></div>
5	E	89	<div><div>.</div><div>69%</div><div>18%</div><div>.</div><div>10%</div></div>
6	F	93	<div><div>.</div><div>68%</div><div>16%</div><div>14%</div></div>
7	G	1893	<div><div>19%</div><div>.</div><div>79%</div></div>
8	H	349	<div><div>31%</div><div>.</div><div>65%</div></div>
9	I	1199	<div><div>33%</div><div>31%</div><div>12%</div><div>.</div><div>24%</div></div>

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Mol	Chain	Length	Quality of chain
10	J	677	<div><div></div><div>22%8%..68%</div></div>
10	K	677	<div><div></div><div>18%8%..71%</div></div>
11	L	310	<div><div></div><div>.5%91%</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21485 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 TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	180	Total	C	N	O	S	0	0
			1429	927	252	243	7		

- Molecule 2 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	43	Total	C	N	O	S	0	0
			356	228	56	70	2		

- Molecule 3 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	47	Total	C	N	O	S	0	0
			393	250	70	71	2		

- Molecule 4 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	97	Total	C	N	O	S	0	0
			793	502	140	149	2		

- Molecule 5 is a DNA chain called SUPER CORE PROMOTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	80	Total	C	N	O	P	0	0
			1654	778	320	476	80		

- Molecule 6 is a DNA chain called SUPER CORE PROMOTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	P	0	0
			1626	770	292	484	80		

- Molecule 7 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	406	Total	C	N	O	P	S	0	0
			3290	2090	580	596	2	22		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	178	VAL	-	insertion	UNP P21675
G	179	SER	-	insertion	UNP P21675
G	180	GLU	-	insertion	UNP P21675
G	181	ASN	-	insertion	UNP P21675
G	182	GLY	-	insertion	UNP P21675
G	183	GLU	-	insertion	UNP P21675
G	184	GLY	-	insertion	UNP P21675
G	185	ILE	-	insertion	UNP P21675
G	186	ILE	-	insertion	UNP P21675
G	187	LEU	-	insertion	UNP P21675
G	188	PRO	-	insertion	UNP P21675
G	189	SER	-	insertion	UNP P21675
G	190	ILE	-	insertion	UNP P21675
G	191	ILE	-	insertion	UNP P21675
G	192	ALA	-	insertion	UNP P21675
G	193	PRO	-	insertion	UNP P21675
G	194	SER	-	insertion	UNP P21675
G	195	SER	-	insertion	UNP P21675
G	196	LEU	-	insertion	UNP P21675
G	197	ALA	-	insertion	UNP P21675
G	198	SER	-	insertion	UNP P21675

- Molecule 8 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			998	638	184	172	4		

- Molecule 9 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	914	Total	C	N	O	S	0	2
			7404	4761	1251	1336	56		

- Molecule 10 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	220	Total	C	N	O	S	0	0
			1741	1106	306	318	11		
10	K	198	Total	C	N	O	S	0	0
			1582	1006	276	290	10		

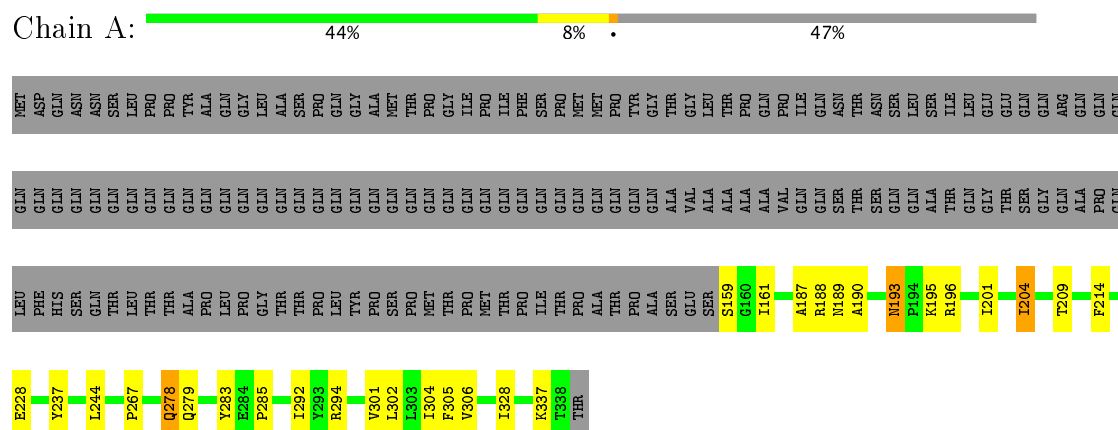
- Molecule 11 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	27	Total	C	N	O	S	0	1
			219	134	46	38	1		

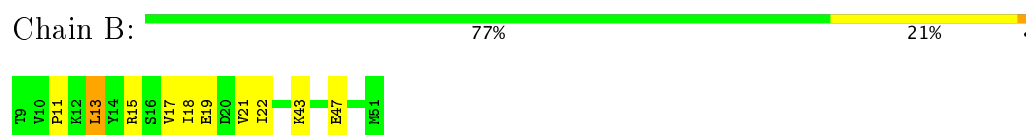
### 3 Residue-property plots [i](#)

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.

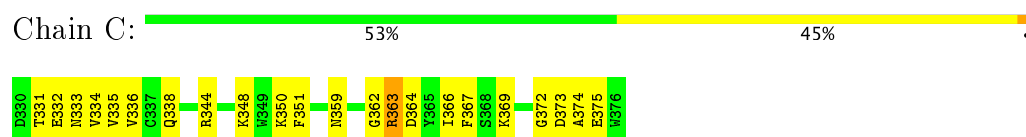
#### • Molecule 1: TATA-BOX-BINDING PROTEIN



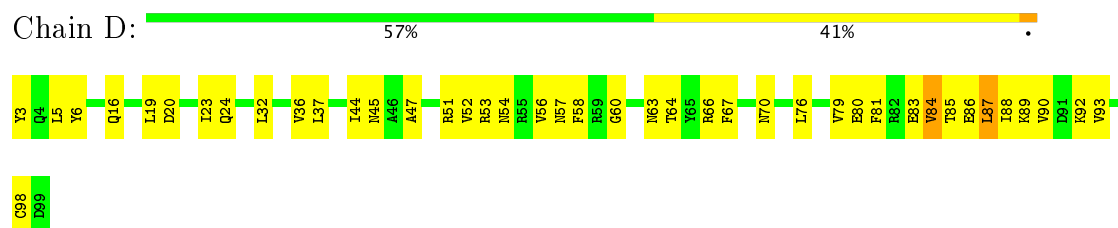
#### • Molecule 2: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1



#### • Molecule 3: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1

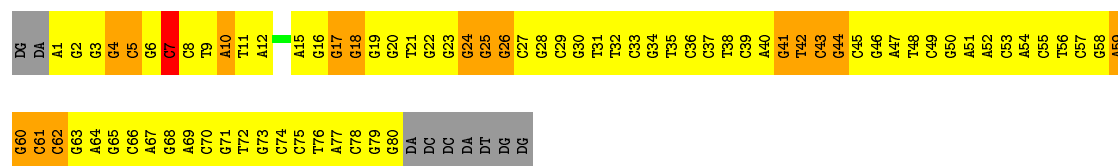


#### • Molecule 4: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2

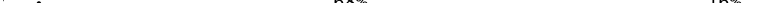


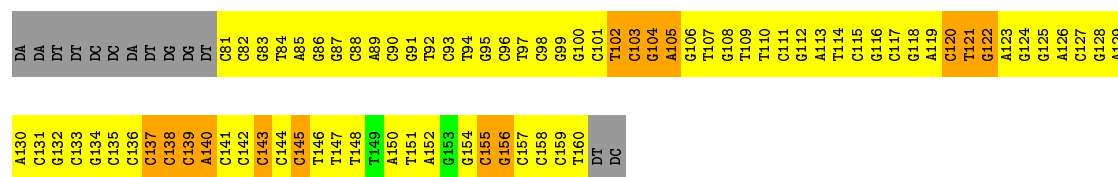
#### • Molecule 5: SUPER CORE PROMOTER

Chain E:  69% 18% 10%



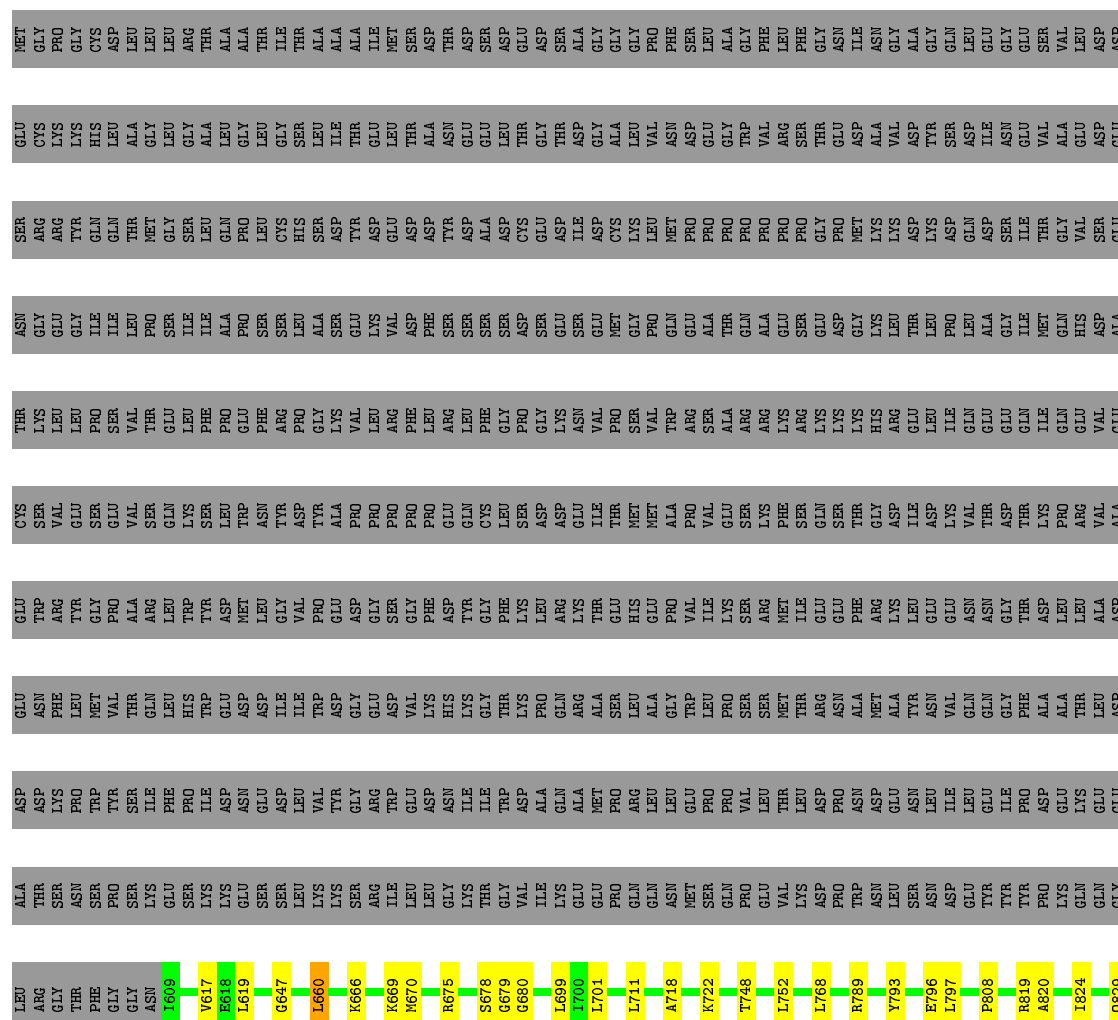
- Molecule 6: SUPER CORE PROMOTER

Chain F:  68% 16% 14%



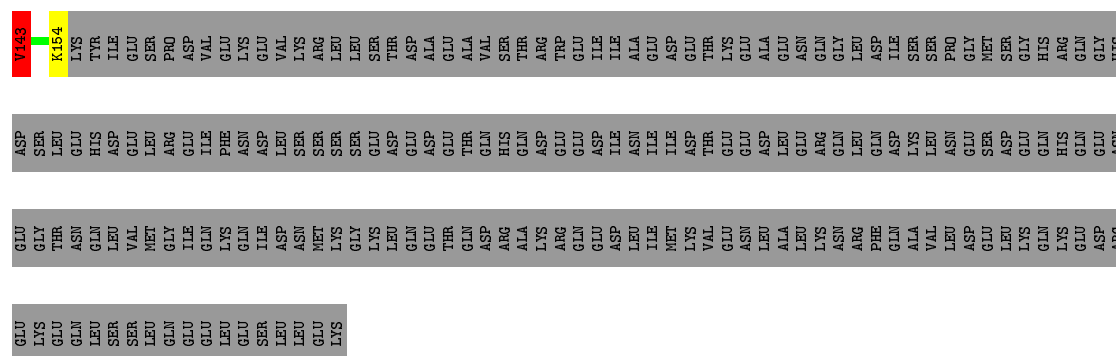
• Molecule 7: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 1

Chain G:  19% . 79%



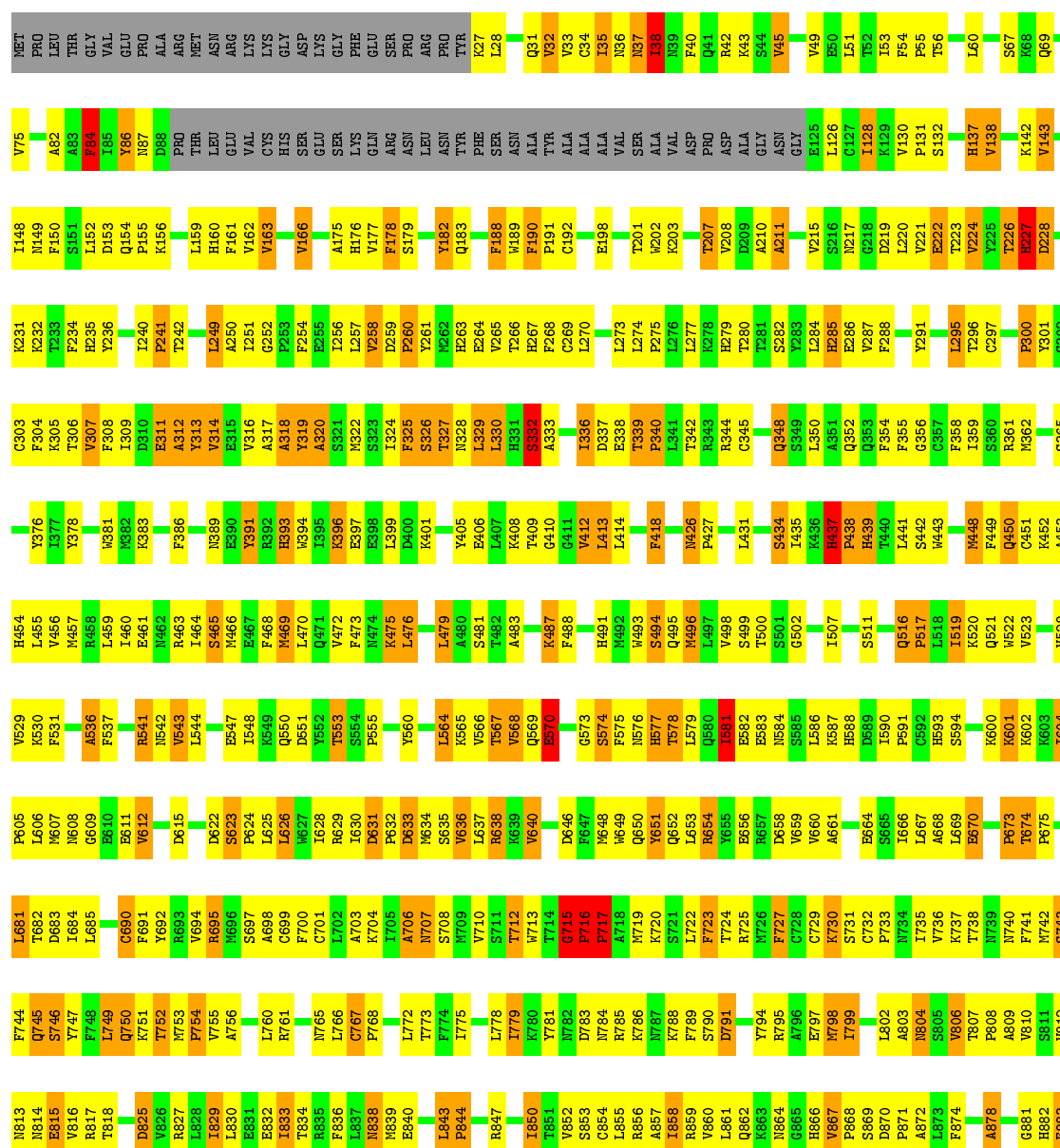


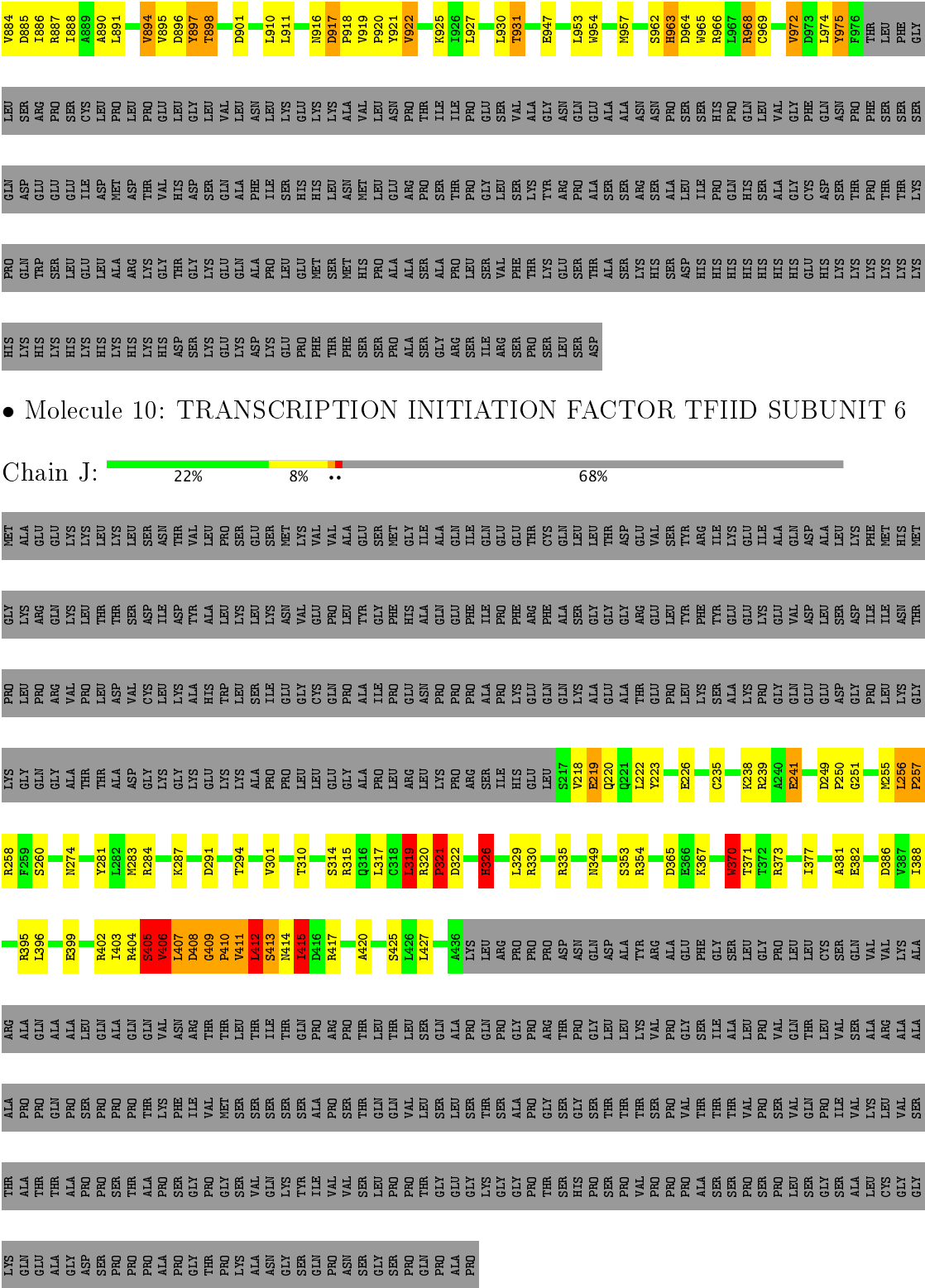




• Molecule 9: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 2

Chain I:  33% 31% 12% 1% 24%





• Molecule 10: TRANSCRIPTION INITIATION FACTOR TFIIID SUBUNIT 6

Chain K: 18% 8% .. 71%

[illegible]

- Molecule 11: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 8

Chain L:  5% 91%

LYS	ASP	R184	ALA	LEU	MET
LYS	GLN	D185	PRO	THR	ALA
SER	GLU	V186	PRO	GLU	ASP
LEU	THR	E187	VAL	MET	ALA
SER	ASP	R188	THR	LEU	ALA
	THR		ASN	GLN	ALA
	GLU	R192	GLN	SER	THR
	ASN	F193	PRO	TYR	ALA
	LEU	M194	VAL	ILE	GLY
	ALA	A195	THR	SER	ALA
	LEU	K196	PRO	GLU	GLY
	HIS	T197	LYS	ILE	GLY
	ILE	G198	ALA	GLY	SER
	SER	GLU	LEU	ARG	GLY
	MET	THR	THR	SER	THR
	GLU	GLN	ALA	ALA	ARG
	ASP	SER	GLY	LYS	SER
	SER	LEU	GLN	SER	GLY
	GLY	PHE	ASN	TYR	SER
	ALA	LYS	ARG	CYS	LYS
	GLU	ASP	PRO	GLU	GLN
	LYS	ASP	HIS	HIS	SER
	GLU	VAL	PRO	THR	THR
	ASN	SER	PRO	ALA	ASN
	THR	THR	HIS	PRO	PRO
	SER	PHE	ILE	THR	ALA
	LEU	LEU	PRO	GLN	ASP
	GLN	ILE	HIS	PRO	ASN
	GLN	ALA	PHE	THR	TYR
	ASN	ALA	PRO	LEU	HIS
	PRO	ARG	GLU	SER	LEU
	SER	PRO	PHE	ILE	ALA
	LEU	PHE	PRO	VAL	ARG
	SER	THR	ASP	VAL	ARG
	GLY	ILE	PRO	THR	ARG
	SER	PRO	HIS	THR	THR
	ARG	TYR	THR	VAL	LEU
	ASN	GLY	TYR	GLU	VAL
	GLY	THR	ILE	MET	VAL
	GLU	ALA	LYS	GLY	VAL
	GLU	LEU	THR	PHE	SER
	ASN	LEU	PRO	ASN	SER
	ILE	PRO	THR	VAL	SER
	ILE	SER	TYR	ASP	LEU
	ASP	GLU	ARG	THR	THR
	ASN	LEU	GLU	LEU	GLU
	PRO	GLU	PRO	PRO	ALA
	TYR	MET	VAL	ALA	GLY
	LEU	GLN	SER	TYR	PHE
	ARG	GLN	ASP	ALA	GLU
	PRO	MET	ASP	LYS	SER
	VAL	GLU	Y172	ARG	ALA
	LYS	GLU	L175	SER	GLU
	LYS	THR	K178	GLN	LYS
	PRO	ASP	A179	ARG	ALA
	LYS	SER		MET	SER
	ILE	SER		VAL	VAL
	ARG	GLN	Q182	ILE	THR
	ARG	GLN	P182	THR	GLU

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22050	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37879	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP

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	0.52	0/1455	0.69	0/1958
10	J	0.74	0/1773	1.42	26/2408 (1.1%)
10	K	0.75	0/1612	1.38	21/2188 (1.0%)
11	L	0.61	1/220 (0.5%)	1.10	0/292
2	B	0.34	0/360	0.53	0/487
3	C	0.40	0/402	0.83	1/539 (0.2%)
4	D	0.35	0/803	0.73	2/1088 (0.2%)
5	E	3.85	16/1806 (0.9%)	1.89	49/2658 (1.8%)
6	F	3.55	15/1764 (0.9%)	2.11	46/2582 (1.8%)
7	G	0.41	0/3349	0.55	0/4506
8	H	0.42	0/1017	0.59	1/1370 (0.1%)
9	I	0.84	8/7587 (0.1%)	0.82	5/10278 (0.0%)
All	All	1.61	40/22148 (0.2%)	1.16	151/30354 (0.5%)

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
10	J	2	16
10	K	1	12
5	E	0	2
7	G	0	1
9	I	0	235
All	All	3	266

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	43	DC	O3'-P	49.26	2.20	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	44	DG	O3'-P	48.90	2.19	1.61
5	E	62	DC	O3'-P	48.41	2.19	1.61
5	E	59	DA	O3'-P	46.14	2.16	1.61
6	F	105	DA	O3'-P	46.09	2.16	1.61

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	145	DC	O5'-P-OP2	-41.73	60.62	110.70
9	I	437	HIS	C-N-CD	-27.62	59.83	120.60
5	E	17	DG	P-O3'-C3'	-27.17	87.10	119.70
6	F	145	DC	P-O5'-C5'	-24.28	82.05	120.90
6	F	156	DG	O5'-P-OP1	-23.00	83.11	110.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	J	326	HIS	CA
10	J	411	VAL	CA
10	K	326	HIS	CA

5 of 266 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	DA	Sidechain
5	E	7	DC	Sidechain
7	G	1104	LEU	Peptide
9	I	32	VAL	Mainchain
9	I	33	VAL	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	1429	0	1521	49	0
2	B	356	0	360	7	0
3	C	393	0	380	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	793	0	801	39	0
5	E	1654	0	958	423	0
6	F	1626	0	962	396	0
7	G	3290	0	3276	61	0
8	H	998	0	1055	6	0
9	I	7404	0	7381	897	0
10	J	1741	0	1782	103	0
10	K	1582	0	1612	40	0
11	L	219	0	222	130	0
All	All	21485	0	20310	1916	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 46.

The worst 5 of 1916 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)
9:I:84:PHE:HZ	9:I:126:LEU:CG	1.10	1.64
5:E:70:DC:C5'	7:G:875:ARG:NH1	1.68	1.53
9:I:566:VAL:HB	9:I:579:LEU:CD1	1.36	1.51
9:I:309:ILE:CG2	9:I:312:ALA:HB2	1.42	1.48
9:I:84:PHE:CZ	9:I:126:LEU:CG	1.96	1.47

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 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	178/339 (52%)	175 (98%)	3 (2%)	0	100	100
2	B	41/43 (95%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
4	D	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	17	60
7	G	398/1893 (21%)	391 (98%)	7 (2%)	0	100	100
8	H	119/349 (34%)	117 (98%)	2 (2%)	0	100	100
9	I	910/1199 (76%)	753 (83%)	122 (13%)	35 (4%)	4	32
10	J	218/677 (32%)	185 (85%)	17 (8%)	16 (7%)	1	19
10	K	196/677 (29%)	163 (83%)	20 (10%)	13 (7%)	1	21
11	L	25/310 (8%)	25 (100%)	0	0	100	100
All	All	2225/5631 (40%)	1979 (89%)	181 (8%)	65 (3%)	9	38

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	84	VAL
9	I	222	GLU
9	I	413	LEU
9	I	438	PRO
9	I	577	HIS

### 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	155/293 (53%)	152 (98%)	3 (2%)	62	82
2	B	42/42 (100%)	41 (98%)	1 (2%)	54	78
3	C	42/42 (100%)	41 (98%)	1 (2%)	54	78
4	D	89/89 (100%)	87 (98%)	2 (2%)	57	79
7	G	355/1680 (21%)	331 (93%)	24 (7%)	18	51
8	H	113/322 (35%)	104 (92%)	9 (8%)	14	45
9	I	832/1083 (77%)	830 (100%)	2 (0%)	94	97
10	J	194/574 (34%)	177 (91%)	17 (9%)	12	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	176/574 (31%)	162 (92%)	14 (8%)	14	45
11	L	22/270 (8%)	22 (100%)	0	100	100
All	All	2020/4969 (41%)	1947 (96%)	73 (4%)	44	68

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	99	VAL
9	I	84	PHE
10	K	326	HIS
8	H	141	LYS
10	J	219	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	542	ASN
9	I	838	ASN
10	K	220	GLN
4	D	13	ASN
10	K	254	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SEP	G	1105	7	9,9,10	1.61	2 (22%)	9,12,14	1.08	1 (11%)
7	TPO	G	1106	7	9,10,11	1.24	1 (11%)	10,14,16	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SEP	G	1105	7	-	0/5/8/10	0/0/0/0
7	TPO	G	1106	7	-	0/8/11/13	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1106	TPO	CA-C	2.02	1.52	1.50
7	G	1105	SEP	CA-C	2.20	1.53	1.50
7	G	1105	SEP	P-O1P	3.26	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1105	SEP	OG-P-O1P	2.17	112.57	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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
6	F	68
5	E	65
9	I	1

The worst 5 of 134 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	158:DC	O3'	159:DC	P	4.06
1	E	2:DG	O3'	3:DG	P	3.41
1	F	159:DC	O3'	160:DT	P	3.14
1	E	1:DA	O3'	2:DG	P	2.67
1	F	142:DC	O3'	143:DC	P	2.56