



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 22, 2017 – 01:26 AM EDT

PDB ID : 4V1O
EMDB ID: : EMD-2786
Title : Architecture of the RNA polymerase II-Mediator core transcription initiation complex
Authors : Plaschka, C.; Lariviere, L.; Wenzek, L.; Hemann, M.; Tegunov, D.; Petrotchenko, E.V.; Borchers, C.H.; Baumeister, W.; Herzog, F.; Villa, E.; Cramer, P.
Deposited on : unknown
Resolution : 9.70 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

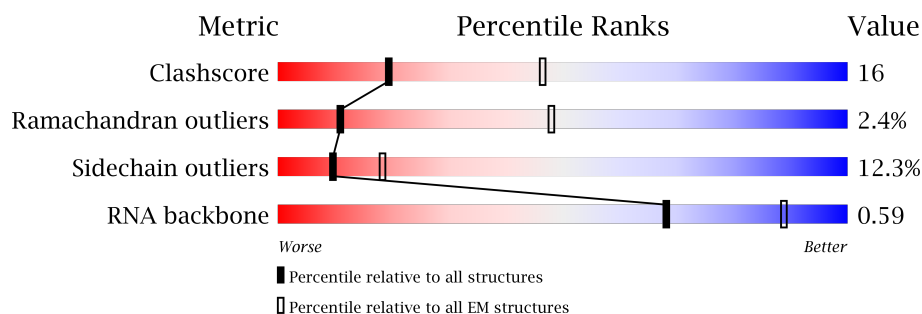
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.70 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.








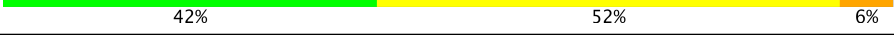



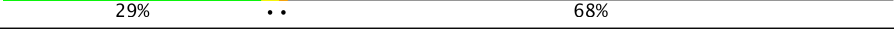
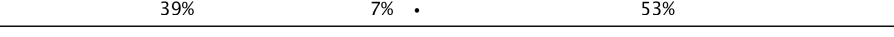


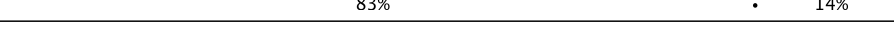




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 ≥ 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	1733	54% 23% . . 18%
2	B	1224	62% 29% . 6%
3	C	318	60% 20% . 16%
4	D	221	51% 24% 5% 19%
5	E	215	74% 23% .
6	F	155	33% 19% . 46%
7	G	171	69% 26% 5%
8	H	146	55% 30% 5% 9%

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Mol	Chain	Length	Quality of chain
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	50	
15	O	181	
16	P	6	
17	Q	734	
18	R	331	
19	S	295	
20	T	58	
21	U	222	
22	V	115	
23	W	687	
24	X	307	
25	Y	209	
26	Z	120	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 45091 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	1422	Total	C	N	O	S	0	0
			11174	7036	1954	2122	62		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1156	Total	C	N	O	S	0	0
			9140	5781	1606	1697	56		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	178	Total	C	N	O	S	0	0
			1434	887	257	288	2		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- 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
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	300	Total	C	N	O	S	0	1
			2202	1384	380	423	15		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	50	Total	C	N	O	P	0	0
			975	490	191	246	48		

- Molecule 15 is a protein called TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	60	MET	-	expression tag	UNP P13393

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	6	Total	C	N	O	P	0	0
			123	57	22	39	5		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	122	Total	C	N	O	0	0
			606	362	122	122		

- Molecule 18 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	105	Total	C	N	O	0	0
			521	311	105	105		

- Molecule 19 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	139	Total	C	N	O	0	0
			691	413	139	139		

- Molecule 20 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	58	Total	C	N	O	P	0	0
			1125	568	206	294	57		

- Molecule 21 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	158	Total	C	N	O	0	0
			787	471	158	158		

- Molecule 22 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	99	Total	C	N	O	0	0
			491	293	99	99		

- Molecule 23 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	419	Total	C	N	O	0	0
			2085	1247	419	419		

- Molecule 24 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	232	Total	C	N	O	0	0
			1146	682	232	232		

- Molecule 25 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	203	Total	C	N	O	0	0
			1003	597	203	203		

- Molecule 26 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	88	Total	C	N	O	1	0
			442	266	88	88		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	J	1	Total	Zn	0
			1	1	
27	B	1	Total	Zn	0
			1	1	
27	I	2	Total	Zn	0
			2	2	
27	C	1	Total	Zn	0
			1	1	
27	A	2	Total	Zn	0
			2	2	
27	L	1	Total	Zn	0
			1	1	
27	M	1	Total	Zn	0
			1	1	

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

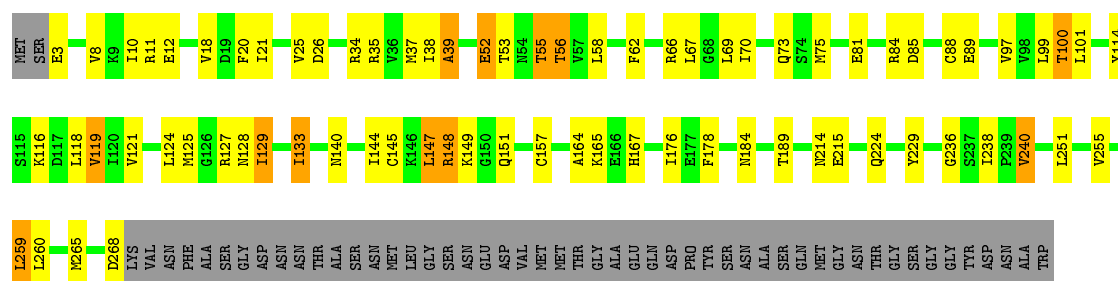
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Mg	0
			1	1	





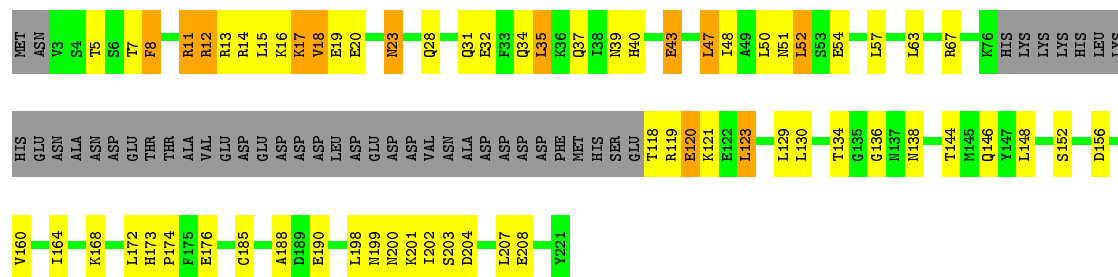
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 60% 20% 16%



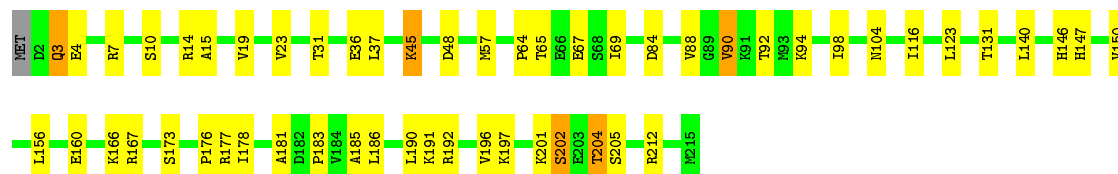
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D: 51% 24% 5% 19%



• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

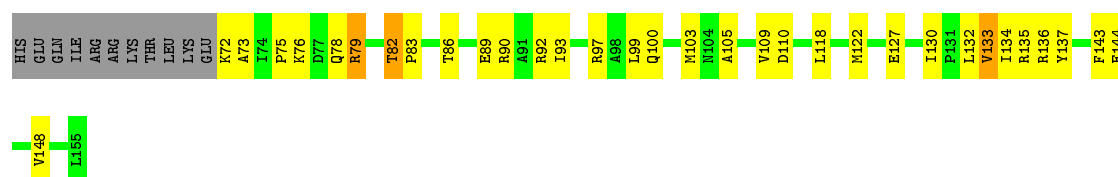
Chain E: 74% 23%



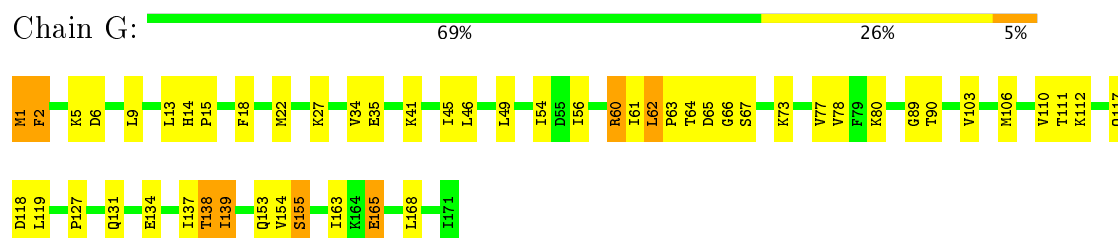
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 33% 19% 46%

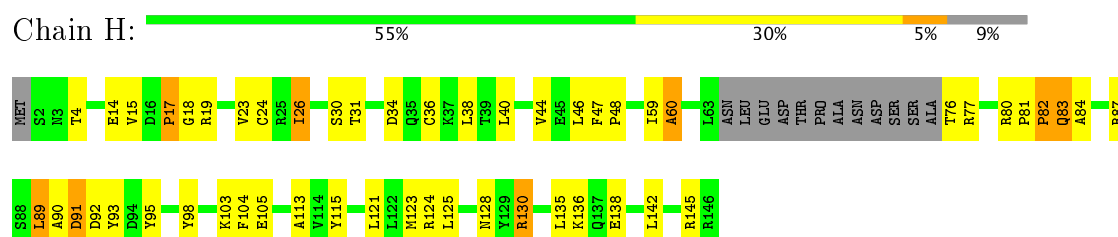




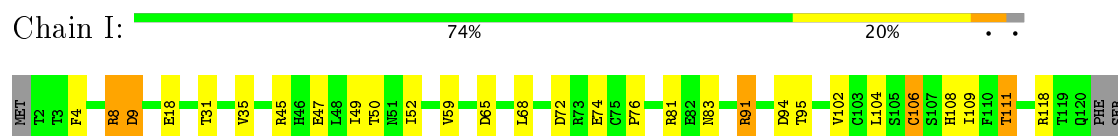
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



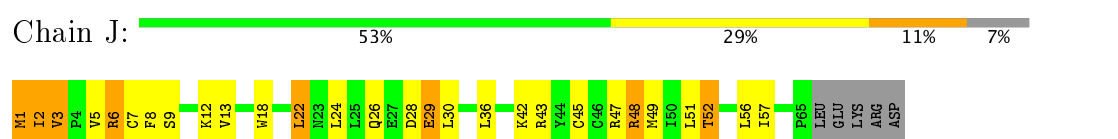
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



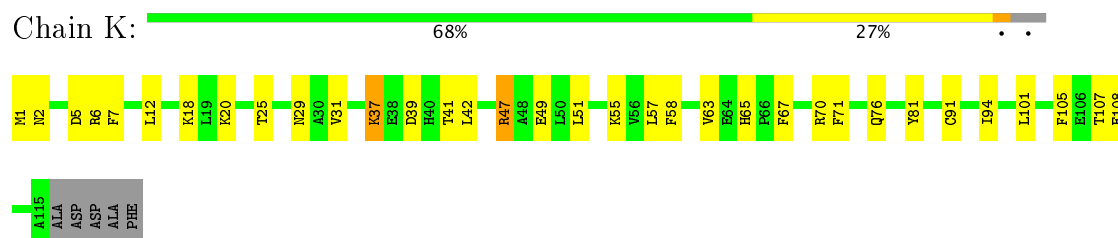
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

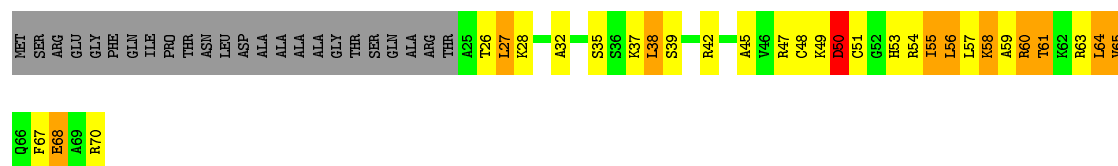


- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



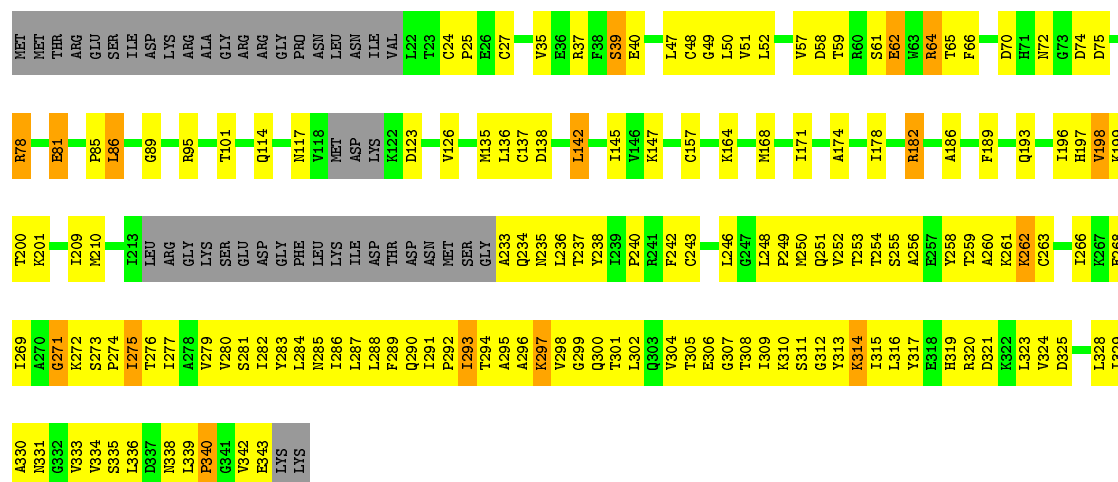
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 



• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

Chain M: 




• Molecule 14: NONTEMPLATE DNA

Chain N: 



• Molecule 15: TATA-BOX-BINDING PROTEIN

Chain O: 



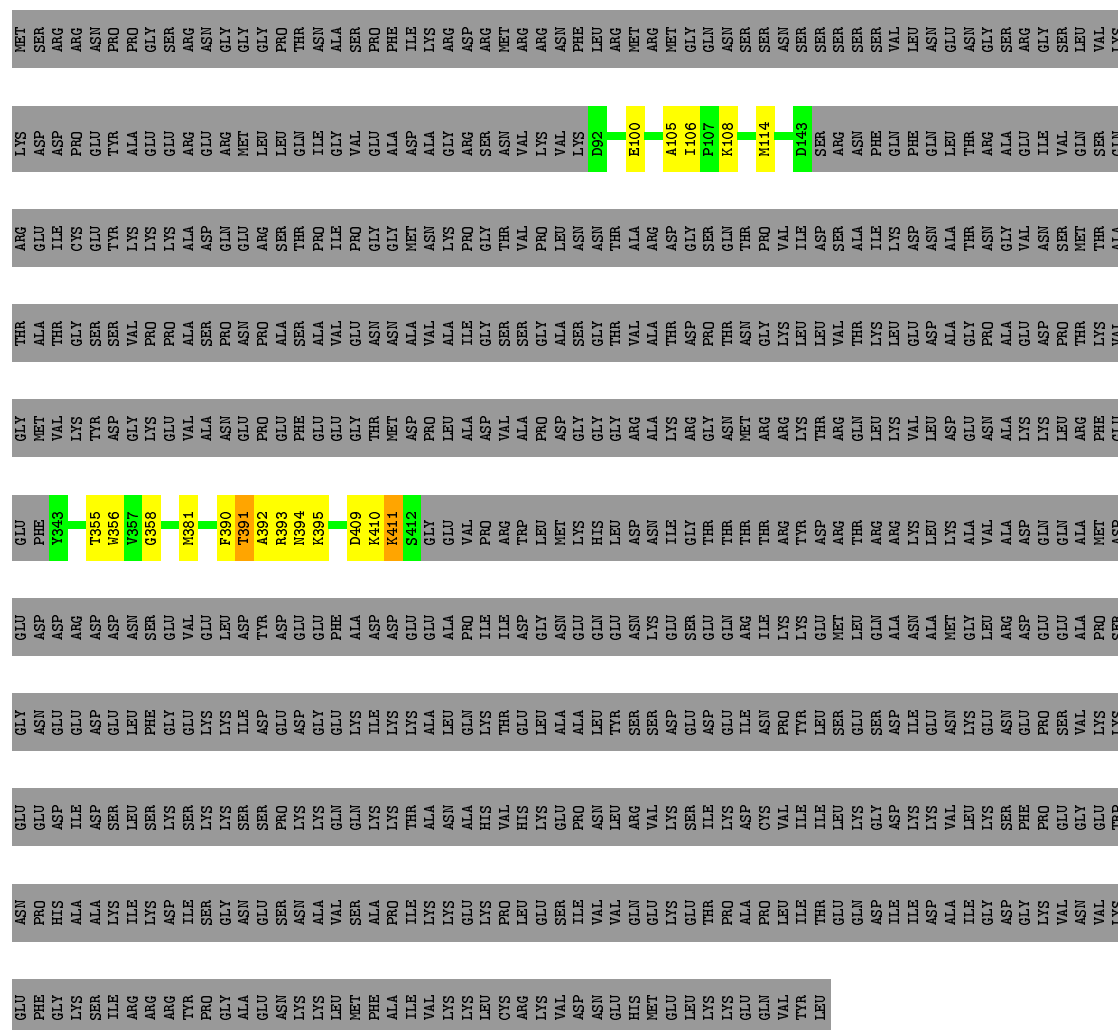
• Molecule 16: RNA

Chain P: 



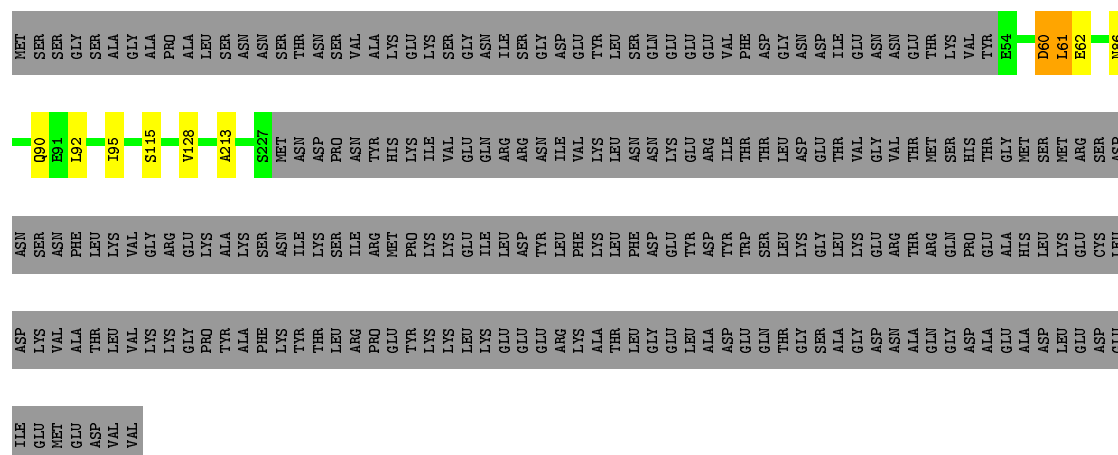
• Molecule 17: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA

Chain Q: 



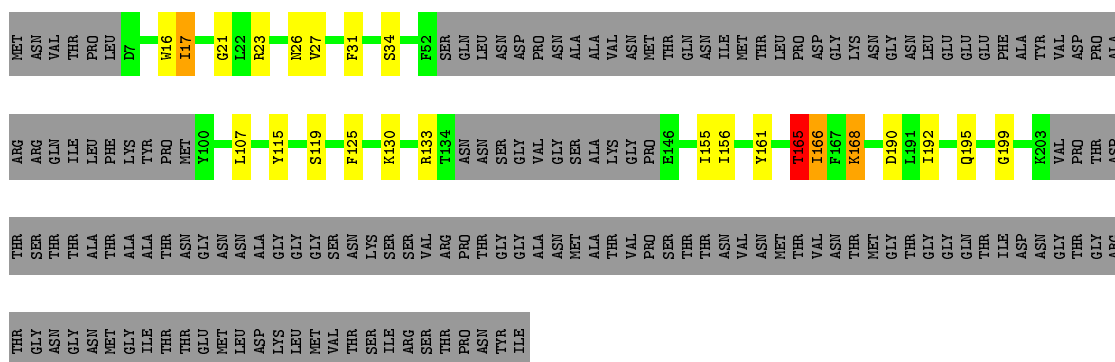
• Molecule 18: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA

Chain R: 29% .. 68%

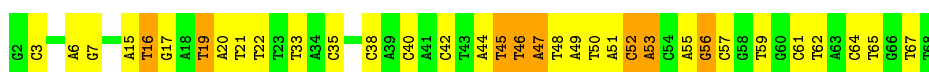


- Molecule 19: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 6

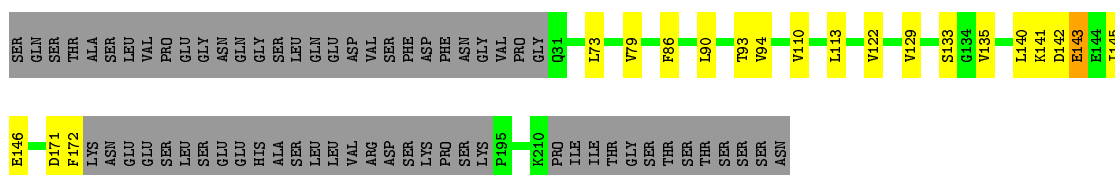
Chain S: 39% 7% 53%



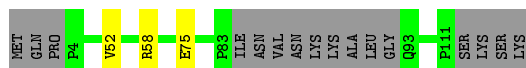
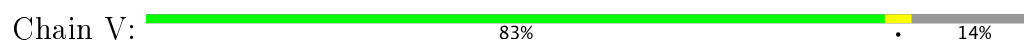
- Molecule 20: TEMPLATE DNA



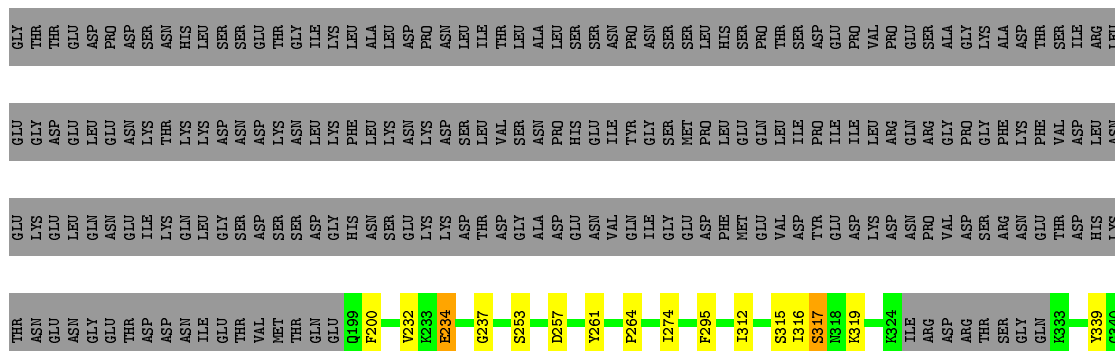
● Molecule 21: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 8

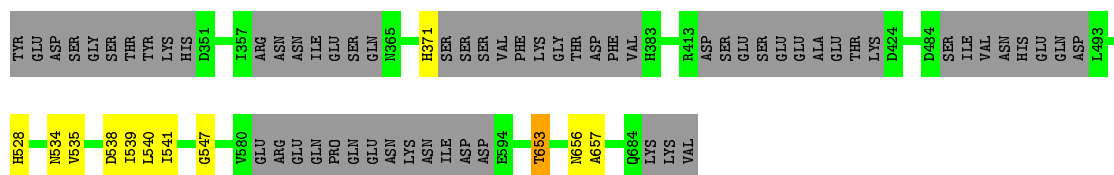


• Molecule 22: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20



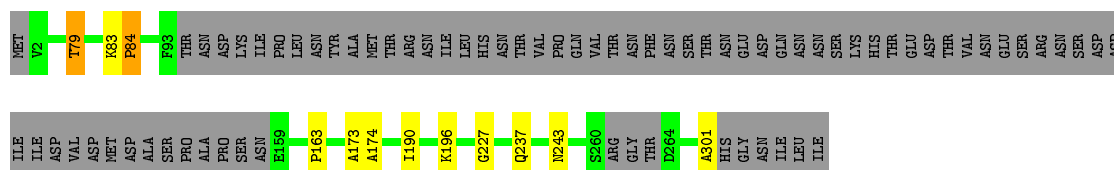
• Molecule 23: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 11





- Molecule 24: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 18

Chain X: 72% 24%



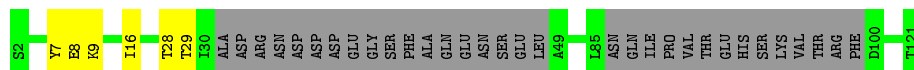
- Molecule 25: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20

Chain Y: 91% 6%



- Molecule 26: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 22

Chain Z: 68% 5% 27%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3267	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37169	Depositor
Image detector	GATAN K2 (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: 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	0.56	4/11374 (0.0%)	0.81	11/15384 (0.1%)
10	J	0.54	0/541	0.88	1/727 (0.1%)
11	K	0.47	0/938	0.71	0/1267
12	L	0.54	0/365	0.95	0/485
13	M	0.61	0/2232	0.77	1/3031 (0.0%)
14	N	1.13	15/1100 (1.4%)	1.32	5/1625 (0.3%)
15	O	0.58	0/1443	0.78	1/1942 (0.1%)
16	P	0.34	0/137	0.80	0/211
17	Q	0.95	0/604	1.19	3/840 (0.4%)
18	R	0.92	0/520	1.21	2/724 (0.3%)
19	S	0.53	0/688	1.40	15/956 (1.6%)
2	B	0.49	1/9316 (0.0%)	0.74	4/12564 (0.0%)
20	T	1.22	18/1265 (1.4%)	1.44	15/1866 (0.8%)
21	U	0.42	0/785	1.15	9/1094 (0.8%)
22	V	0.40	0/489	0.93	3/679 (0.4%)
23	W	0.40	0/2077	0.87	9/2889 (0.3%)
24	X	0.38	0/1143	0.76	2/1587 (0.1%)
25	Y	0.32	0/1001	0.69	2/1391 (0.1%)
26	Z	0.41	0/442	1.09	4/614 (0.7%)
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
4	D	0.38	0/1444	0.59	0/1935
5	E	0.48	0/1788	0.71	0/2406
6	F	0.62	0/691	0.81	0/933
7	G	0.43	0/1368	0.61	0/1844
8	H	0.50	0/1086	0.80	0/1470
9	I	0.47	0/989	0.78	0/1331
All	All	0.58	38/45959 (0.1%)	0.85	89/62686 (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
19	S	0	1
2	B	0	1
21	U	0	2
23	W	0	4
All	All	0	11

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1436	ILE	C-N	14.98	1.60	1.33
1	A	95	PHE	C-N	-14.46	1.00	1.34
20	T	53	DA	P-O5'	-11.80	1.48	1.59
1	A	234	MET	C-N	-11.60	1.07	1.34
20	T	47	DA	C1'-N9	-10.47	1.32	1.47

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	MET	O-C-N	-14.65	99.26	122.70
19	S	192	ILE	CB-CA-C	-12.19	87.22	111.60
20	T	46	DT	O4'-C4'-C3'	-11.78	98.93	106.00
22	V	52	VAL	CB-CA-C	-9.98	92.44	111.40
20	T	42	DC	O5'-P-OP1	-9.11	97.50	105.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	MET	Mainchain
1	A	95	PHE	Mainchain
2	B	43	LEU	Mainchain
17	Q	410	LYS	Peptide
19	S	165	THR	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	11174	0	11223	426	0
2	B	9140	0	9108	326	0
3	C	2095	0	2051	44	0
4	D	1434	0	1460	106	0
5	E	1752	0	1776	27	0
6	F	679	0	701	52	0
7	G	1340	0	1357	71	0
8	H	1068	0	1040	22	0
9	I	971	0	927	17	0
10	J	532	0	542	15	0
11	K	920	0	929	19	0
12	L	363	0	386	26	0
13	M	2202	0	2154	388	0
14	N	975	0	567	23	0
15	O	1416	0	1491	29	0
16	P	123	0	66	1	0
17	Q	606	0	256	30	0
18	R	521	0	216	5	0
19	S	691	0	279	6	0
20	T	1125	0	661	62	0
21	U	787	0	330	5	0
22	V	491	0	201	0	0
23	W	2085	0	871	13	0
24	X	1146	0	489	25	0
25	Y	1003	0	467	6	0
26	Z	442	0	190	1	0
27	A	2	0	0	0	0
27	B	1	0	0	0	0
27	C	1	0	0	0	0
27	I	2	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
27	M	1	0	0	0	0
28	A	1	0	0	0	0
All	All	45091	0	39738	1340	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 16.

The worst 5 of 1340 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)
2:B:868:MET:CE	13:M:182:ARG:HG2	1.34	1.57
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.83	1.52
17:Q:356:TRP:CA	17:Q:392:ALA:HA	1.06	1.51
17:Q:356:TRP:HA	17:Q:392:ALA:CA	0.93	1.39
2:B:1215:ARG:CD	4:D:15:LEU:HD13	1.19	1.39

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	1414/1733 (82%)	1248 (88%)	115 (8%)	51 (4%)	4	33
2	B	1140/1224 (93%)	1019 (89%)	85 (8%)	36 (3%)	5	36
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	22	67
4	D	174/221 (79%)	157 (90%)	12 (7%)	5 (3%)	5	38
5	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	9	47
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	152 (90%)	15 (9%)	2 (1%)	15	57
8	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1	19
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	6	40
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	2	28
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	3
13	M	294/345 (85%)	267 (91%)	24 (8%)	3 (1%)	18	61
15	O	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
17	Q	118/734 (16%)	106 (90%)	11 (9%)	1 (1%)	22	67
18	R	103/331 (31%)	96 (93%)	3 (3%)	4 (4%)	3	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	133/295 (45%)	122 (92%)	9 (7%)	2 (2%)	12	53
21	U	154/222 (69%)	148 (96%)	5 (3%)	1 (1%)	28	71
22	V	95/115 (83%)	94 (99%)	1 (1%)	0	100	100
23	W	403/687 (59%)	382 (95%)	18 (4%)	3 (1%)	25	68
24	X	226/307 (74%)	210 (93%)	13 (6%)	3 (1%)	14	56
25	Y	199/209 (95%)	180 (90%)	17 (8%)	2 (1%)	18	61
26	Z	83/120 (69%)	82 (99%)	1 (1%)	0	100	100
All	All	5907/8111 (73%)	5340 (90%)	425 (7%)	142 (2%)	11	42

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	96	ILE
1	A	189	ARG
1	A	195	ASP
1	A	286	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	1240/1520 (82%)	1066 (86%)	174 (14%)	4	23
2	B	985/1061 (93%)	868 (88%)	117 (12%)	6	27
3	C	234/274 (85%)	206 (88%)	28 (12%)	6	27
4	D	160/200 (80%)	140 (88%)	20 (12%)	5	26
5	E	196/197 (100%)	175 (89%)	21 (11%)	8	31
6	F	74/137 (54%)	67 (90%)	7 (10%)	10	36
7	G	152/152 (100%)	136 (90%)	16 (10%)	8	32
8	H	117/128 (91%)	103 (88%)	14 (12%)	6	27
9	I	113/116 (97%)	106 (94%)	7 (6%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	12
11	K	99/102 (97%)	87 (88%)	12 (12%)	6	27
12	L	40/57 (70%)	27 (68%)	13 (32%)	0	2
13	M	231/299 (77%)	208 (90%)	23 (10%)	9	33
15	O	152/153 (99%)	140 (92%)	12 (8%)	14	45
All	All	3853/4461 (86%)	3378 (88%)	475 (12%)	10	26

5 of 475 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	529	GLU
2	B	1045	SER
12	L	68	GLU
2	B	595	ARG
2	B	776	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	842	ASN
2	B	1193	GLN
13	M	300	GLN
2	B	1025	HIS
2	B	1195	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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
1	A	2
2	B	1
20	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	23:DT	O3'	33:DT	P	36.29
1	B	351:TYR	C	352:ALA	N	3.28
1	A	234:MET	C	235:ILE	N	1.07
1	A	95:PHE	C	96:ILE	N	1.00