wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:01 AM GMT

PDB ID	:	2JA7
Title	:	CPD lesion containing RNA Polymerase II elongation complex C
Authors	:	Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on	:	2006-11-23
Resolution	:	3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

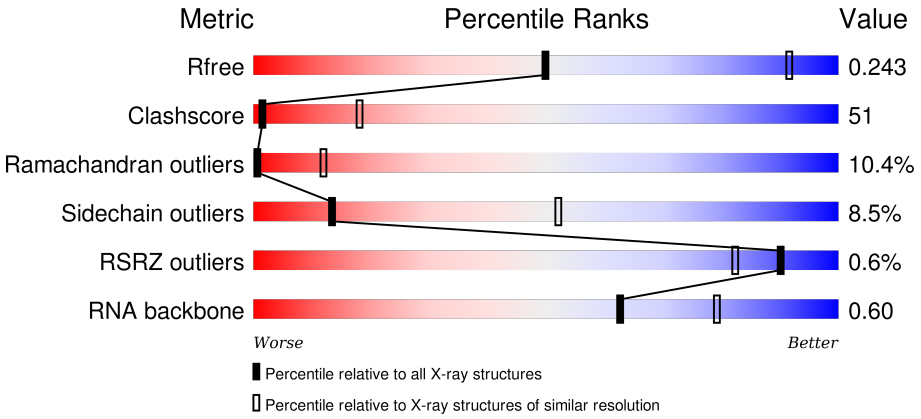
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	14	29% 21% 50%
1	4	14	29% 21% 50%
2	2	25	. 52% 16% 28%
2	5	25	8% 48% 16% 28%

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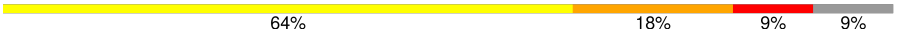
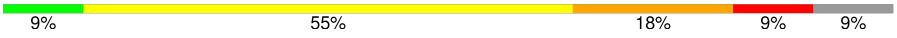
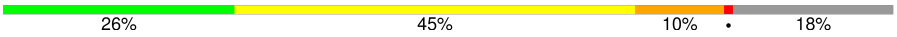
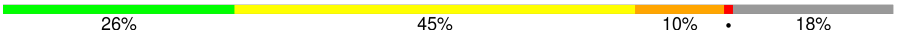
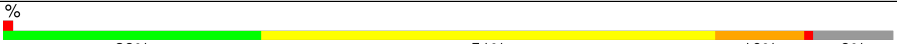
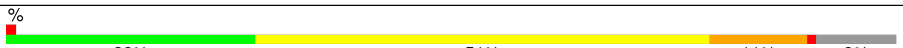
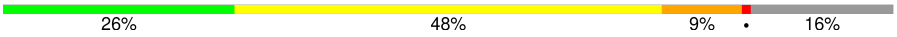
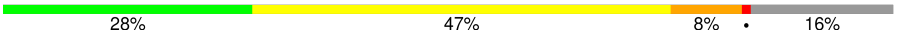
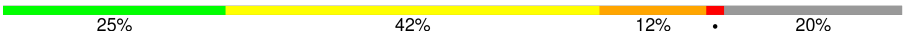
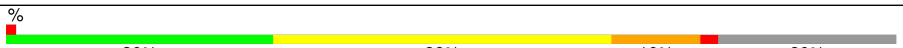
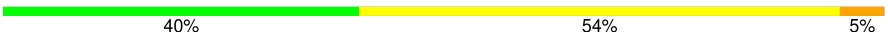
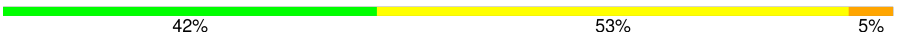
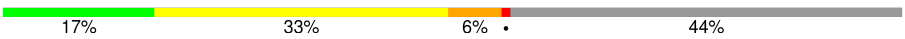
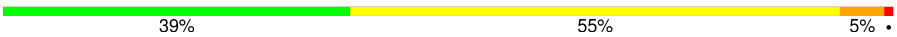
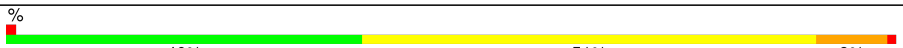
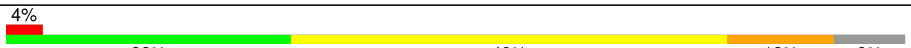
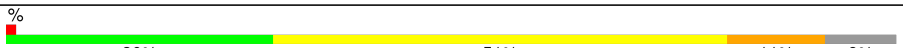
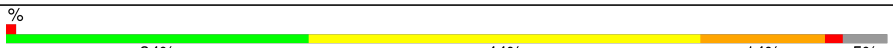
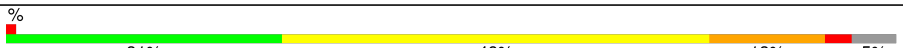
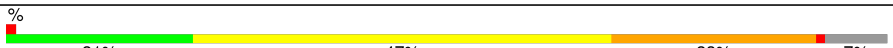
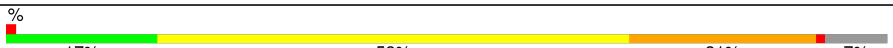
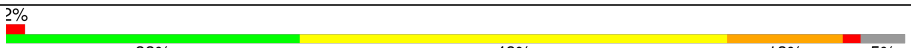
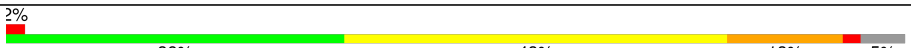
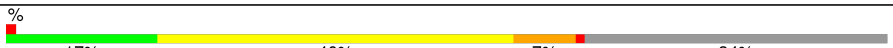
Mol	Chain	Length	Quality of chain
3	3	11	
3	6	11	
4	A	1733	
4	M	1733	
5	B	1224	
5	N	1224	
6	C	318	
6	O	318	
7	D	221	
7	P	221	
8	E	215	
8	Q	215	
9	F	155	
9	R	155	
10	G	171	
10	S	171	
11	H	146	
11	T	146	
12	I	122	
12	U	122	
13	J	70	
13	V	70	
14	K	120	
14	W	120	
15	L	70	

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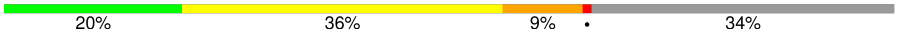
Mol	Chain	Length	Quality of chain
15	X	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	ZN	C	2457	-	-	-	X
17	ZN	I	2458	-	-	-	X
17	ZN	M	2457	-	-	-	X
17	ZN	O	2457	-	-	-	X
17	ZN	U	2457	-	-	-	X

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 63924 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	7	Total	C	N	O	P	0	0	0
			141	69	27	39	6			
1	4	7	Total	C	N	O	P	0	0	0
			141	69	27	39	6			

- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TP*TTP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	2	18	Total	Br	C	N	O	P	0	0	0
			380	1	186	60	116	17			
2	5	18	Total	Br	C	N	O	P	0	0	0
			380	1	186	60	116	17			

- Molecule 3 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	10	Total	C	N	O	P	0	0	0
			212	96	41	66	9			
3	6	10	Total	C	N	O	P	0	0	0
			212	96	41	66	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			
4	M	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1115	Total	C	N	O	S	0	0	0
			8866	5614	1553	1644	55			
5	N	1115	Total	C	N	O	S	0	0	0
			8866	5614	1553	1644	55			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			
6	O	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			
7	P	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			
9	R	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			
10	S	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			
11	T	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			
12	U	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

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

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			
14	W	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7

KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			
15	X	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	M	1	Total	Mg	0	0
			1	1		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total	Zn	0	0
			1	1		
17	B	1	Total	Zn	0	0
			1	1		
17	I	2	Total	Zn	0	0
			2	2		
17	C	1	Total	Zn	0	0
			1	1		
17	V	1	Total	Zn	0	0
			1	1		
17	A	2	Total	Zn	0	0
			2	2		
17	N	1	Total	Zn	0	0
			1	1		
17	U	2	Total	Zn	0	0
			2	2		
17	X	1	Total	Zn	0	0
			1	1		
17	O	1	Total	Zn	0	0
			1	1		
17	L	1	Total	Zn	0	0
			1	1		
17	M	2	Total	Zn	0	0
			2	2		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

Chain 1:

• Molecule 1: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

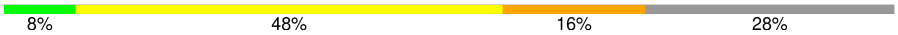
Chain 4:

• Molecule 2: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TP*TTP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain 2:

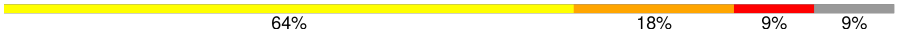
• Molecule 2: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TP*TTP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain 5:



• Molecule 3: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'

Chain 3:

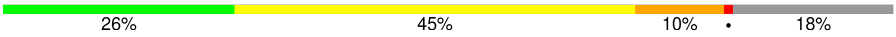


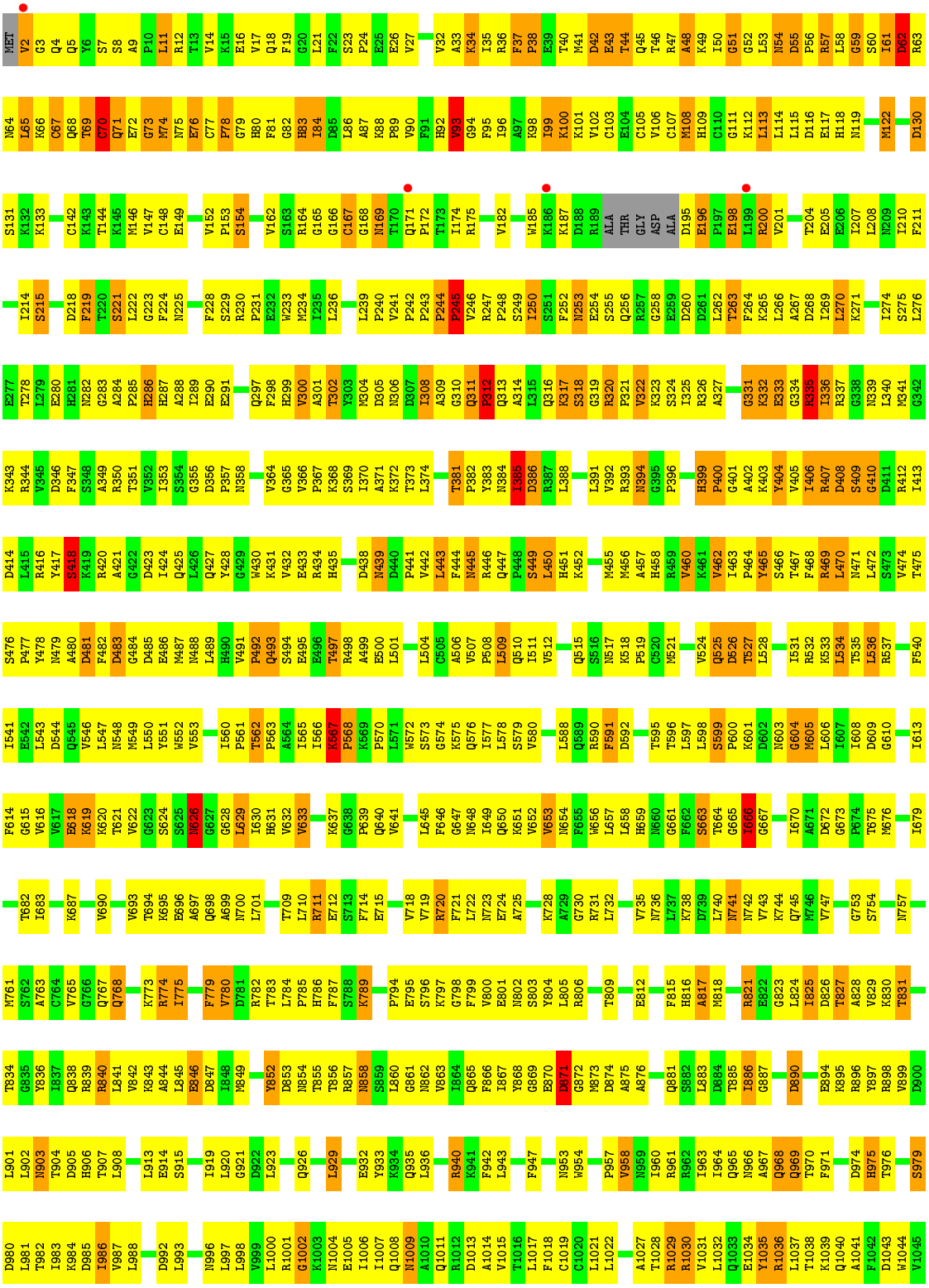
• Molecule 3: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'

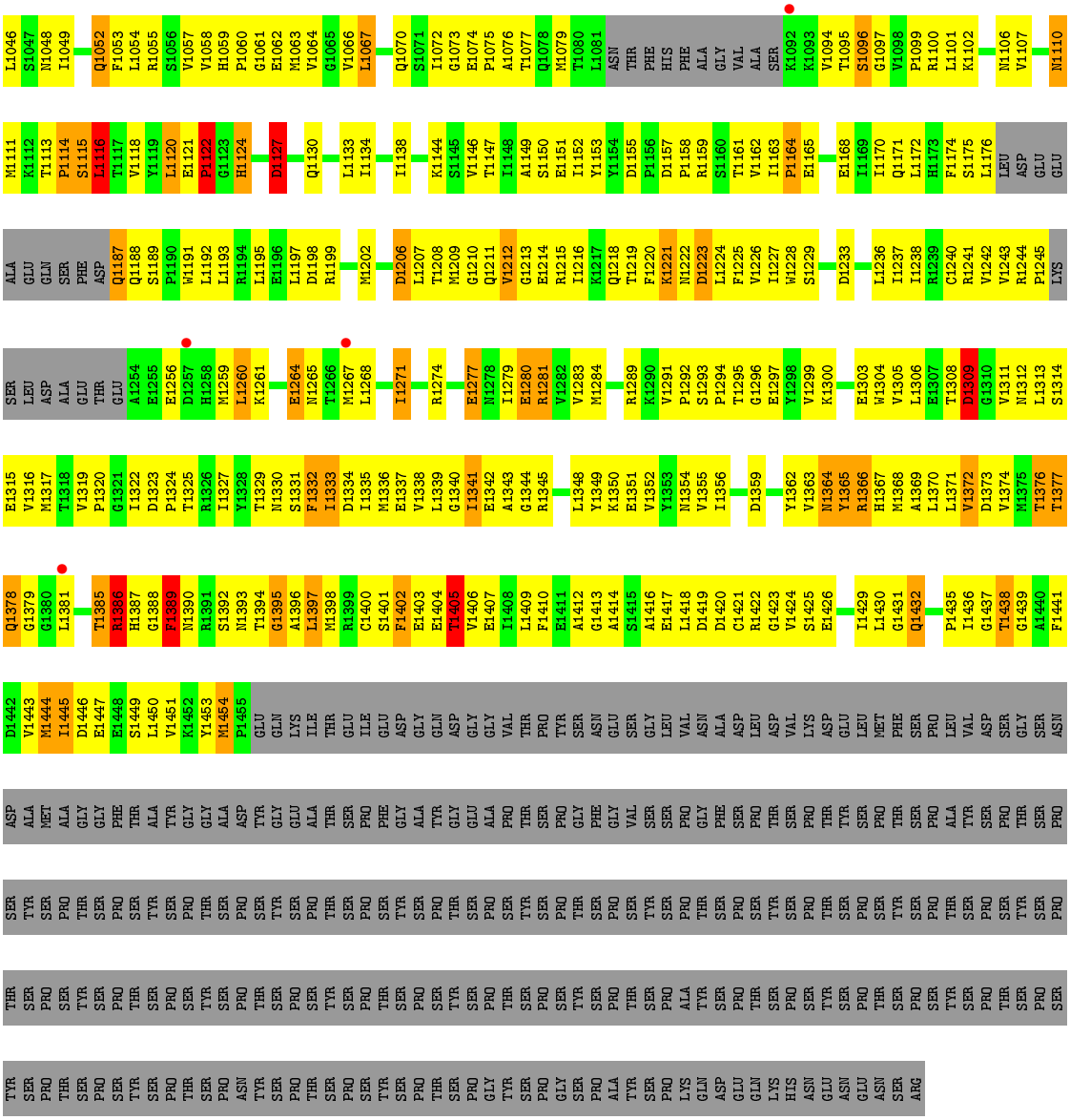
Chain 6:

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

Chain A:

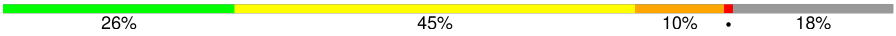


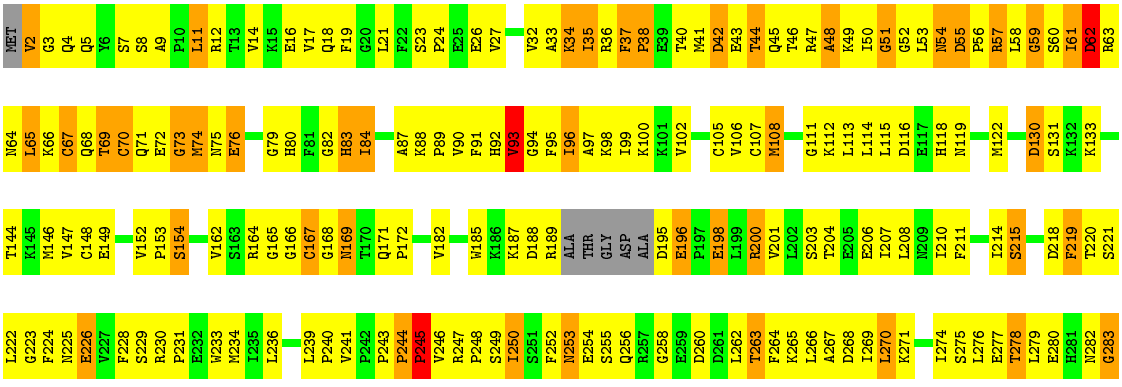


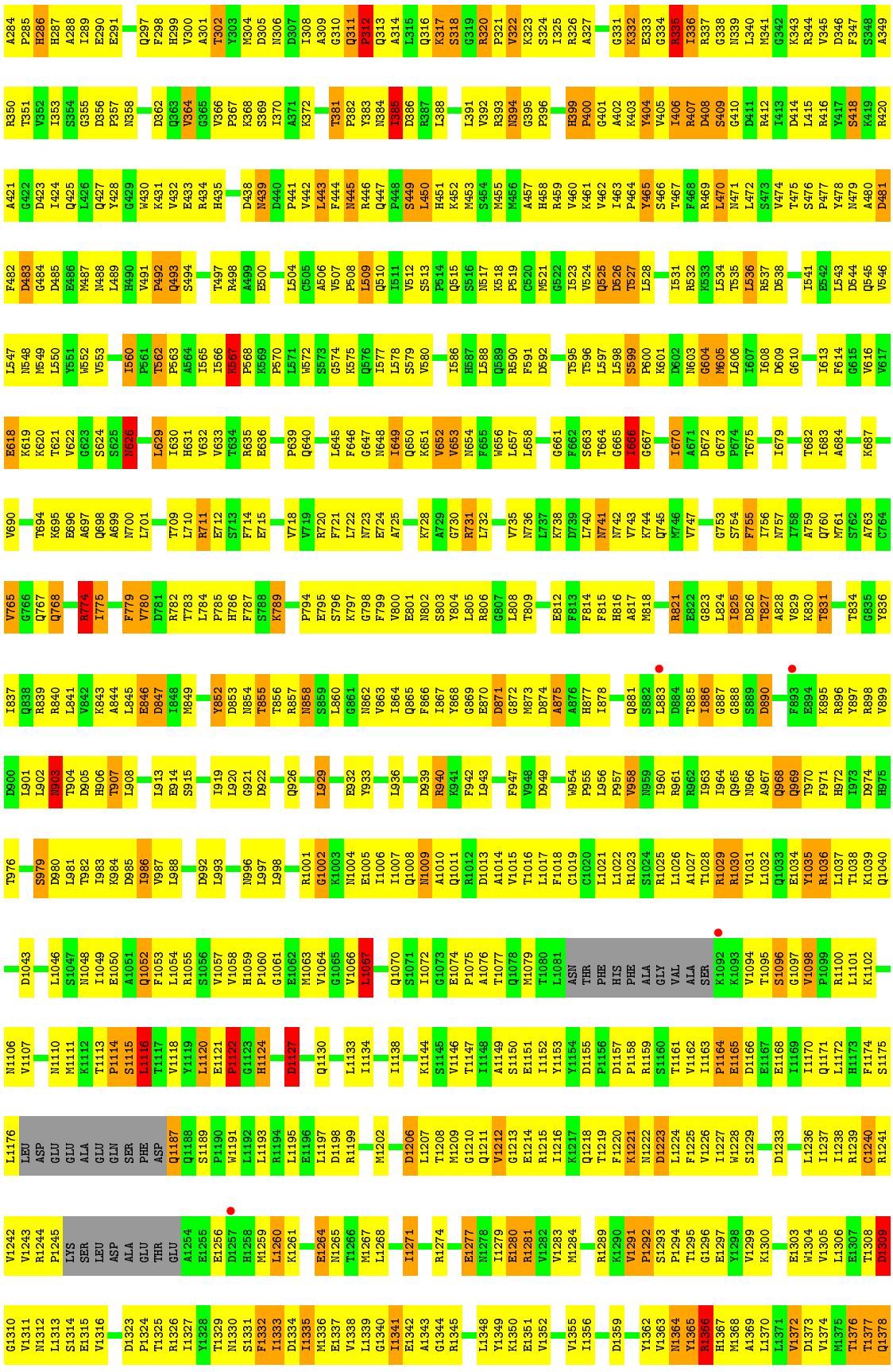


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

Chain M:



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V1242 V1243 R1244 P1245 LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 D1257 H1258 M1259 L1260 K1261 E1264 N1265 T1266 M1267 L1268 I1271 R1274 E1277 N1278 I1279 E1280 R1281 V1282 V1283 M1284 R1289 K1290 V1291 P1292 S1293 P1294 T1295 G1296 E1297 Y1298 V1299 K1300 E1303 W1304 V1305 L1306 E1307 T1308 D1309
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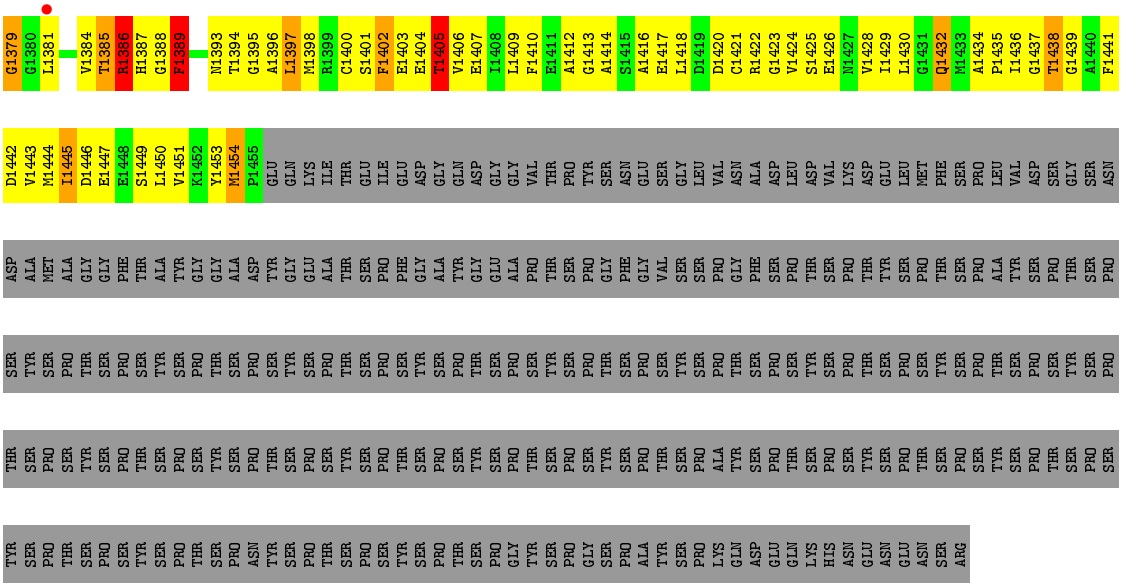
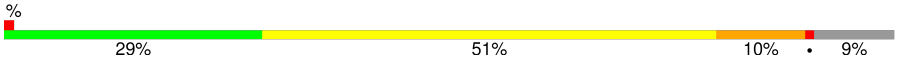
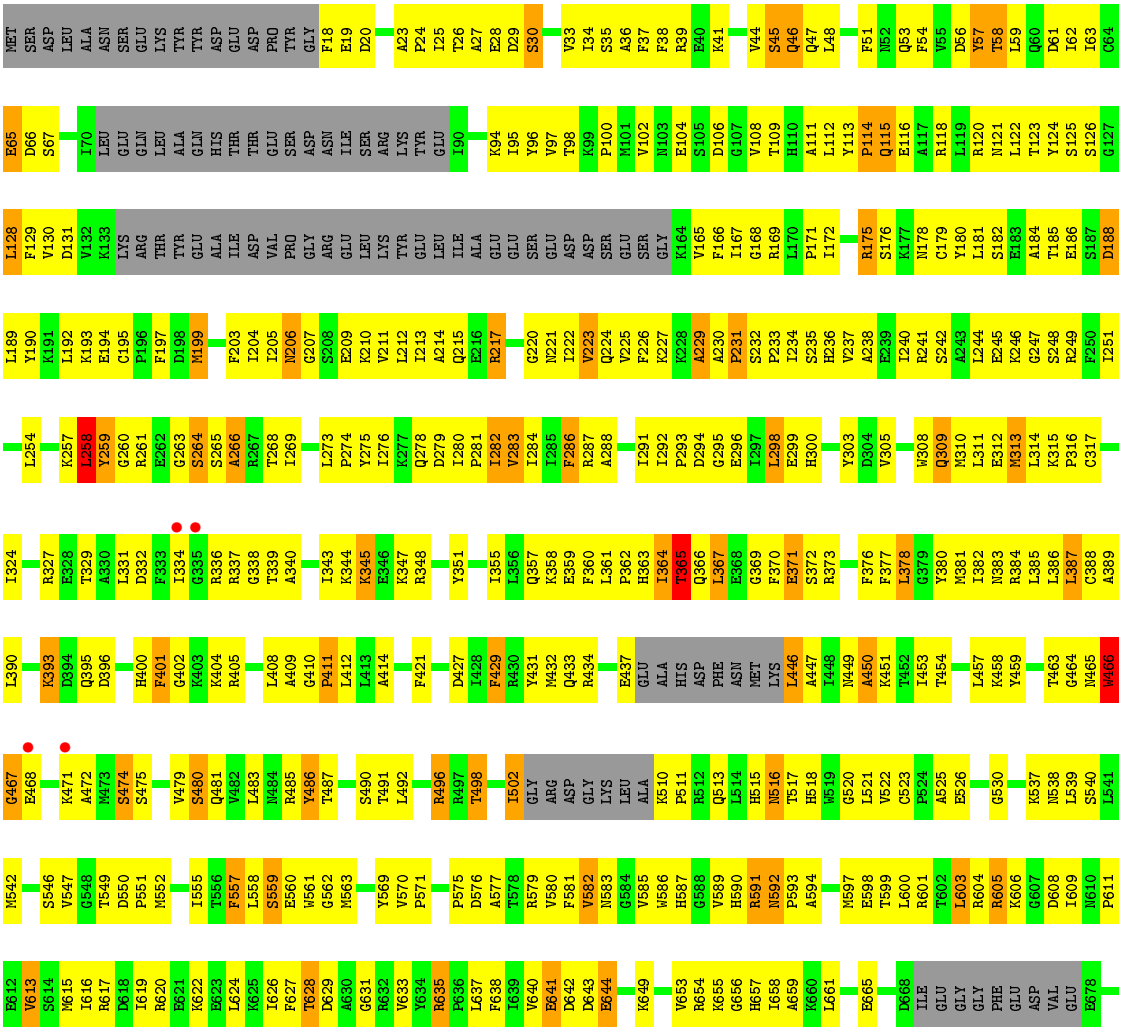
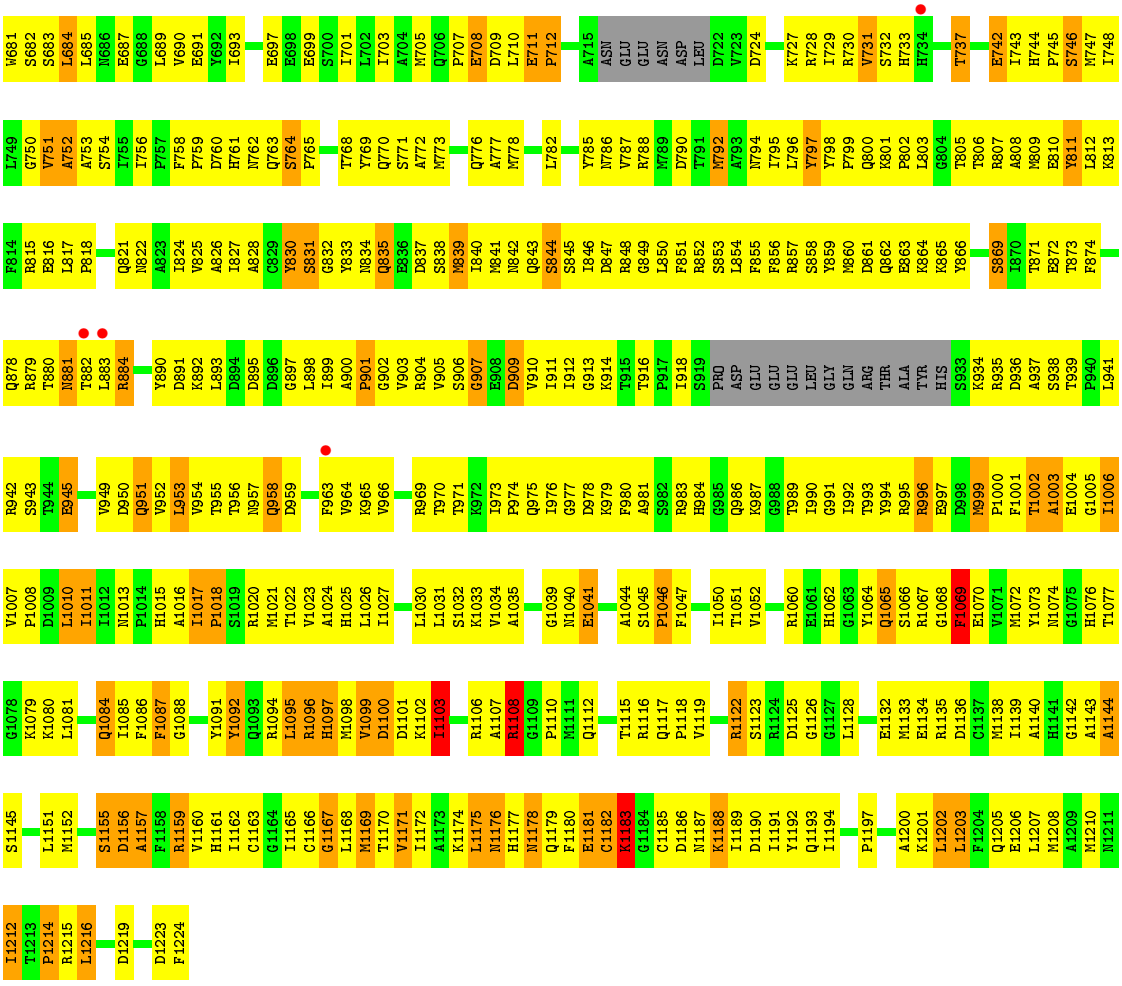


• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE

Chain B:

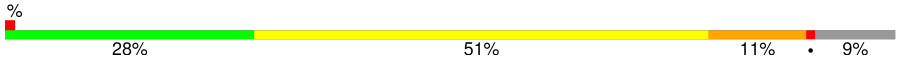


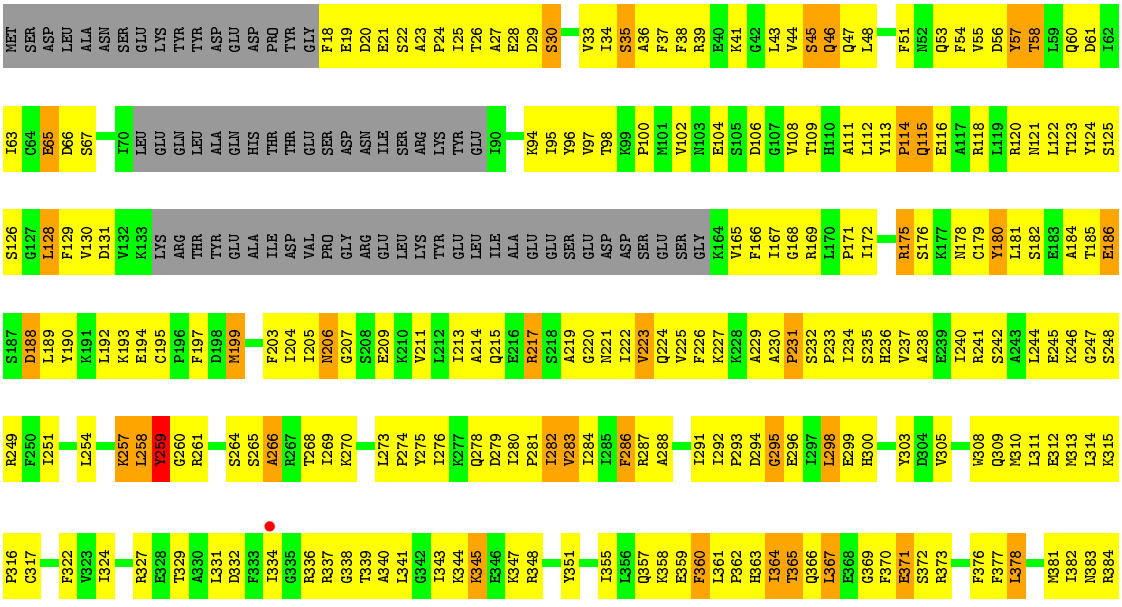


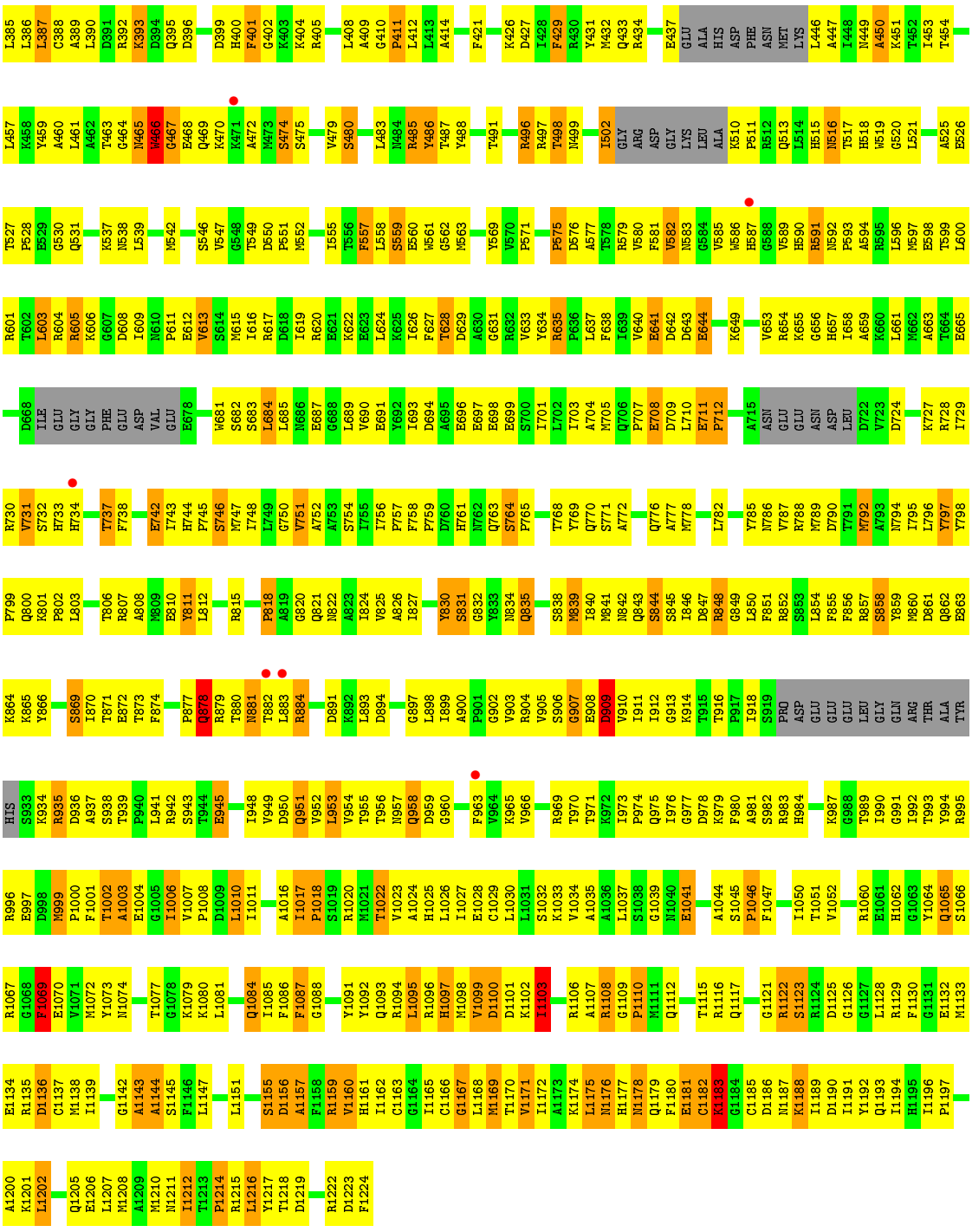


• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE

Chain N:

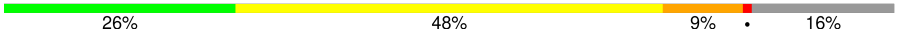


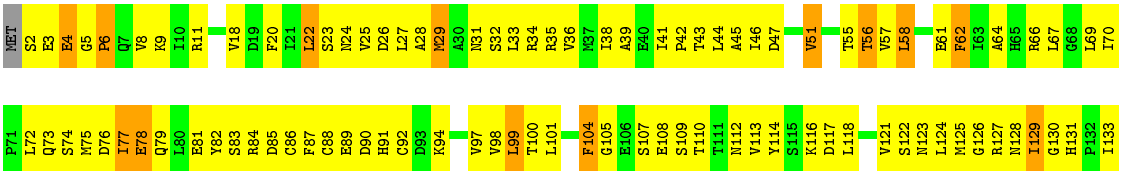


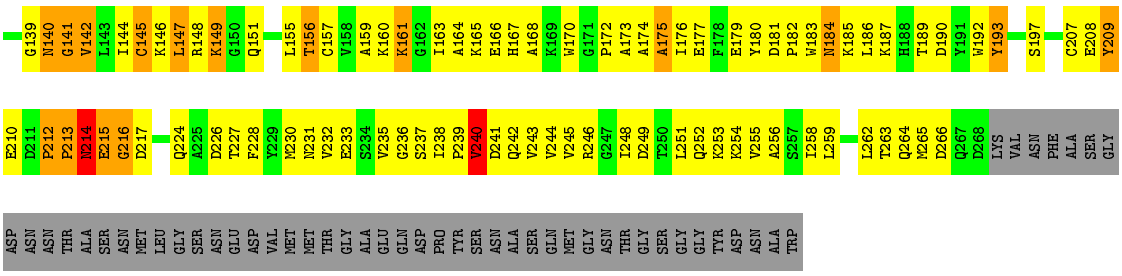


• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE

Chain C:

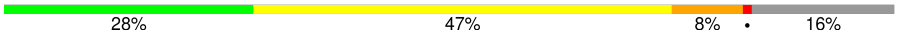


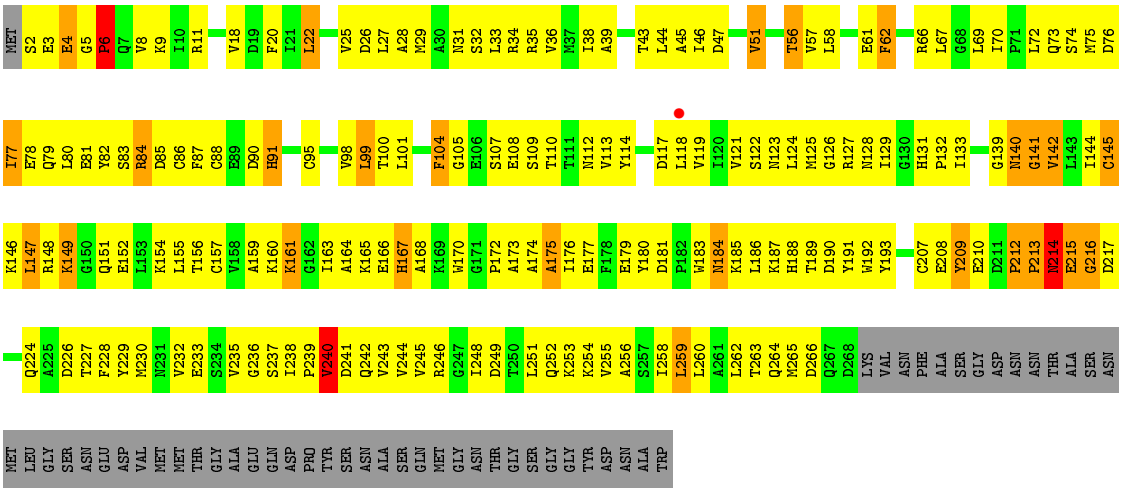




• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE

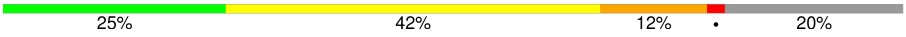
Chain O:

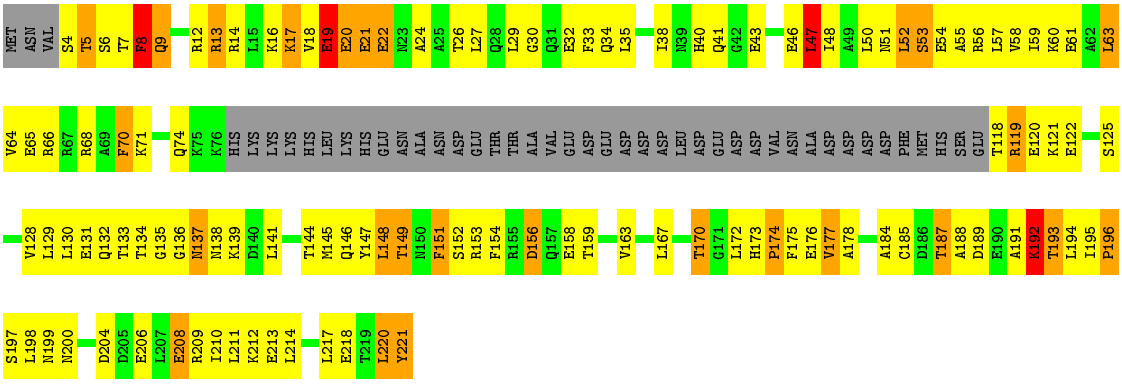




• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE

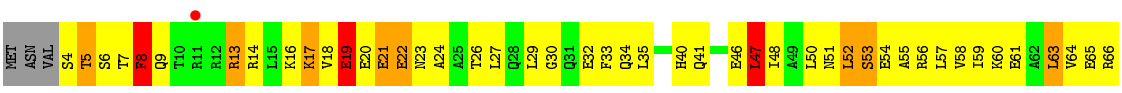
Chain D:

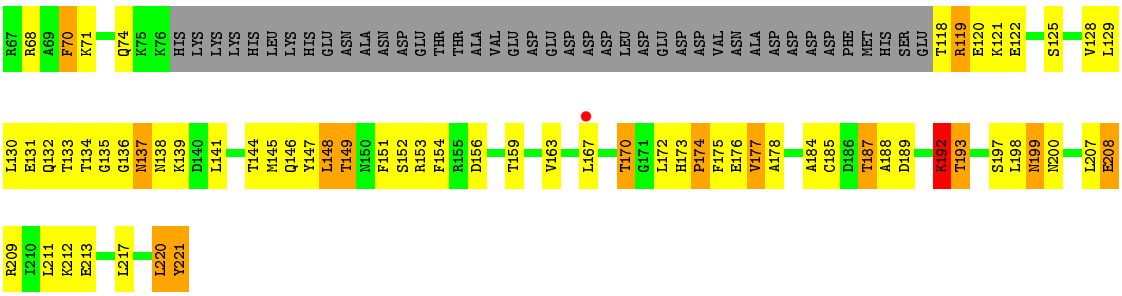




• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE

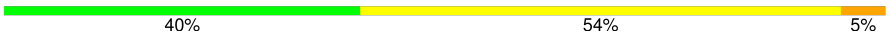
Chain P:

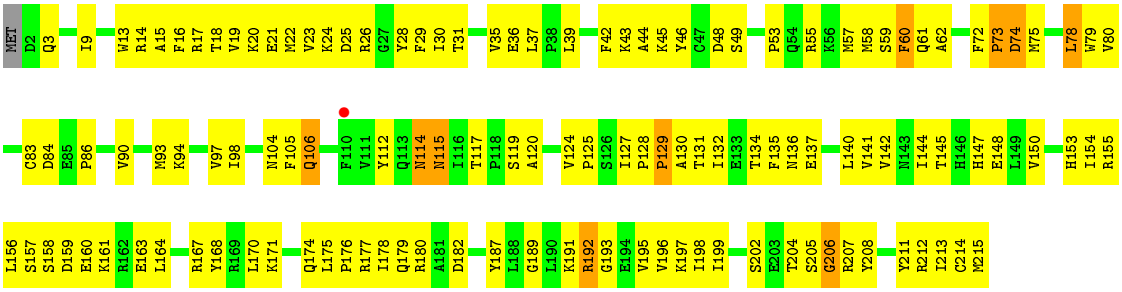




• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

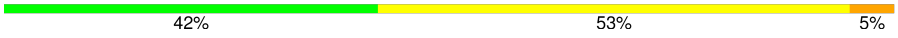
Chain E:

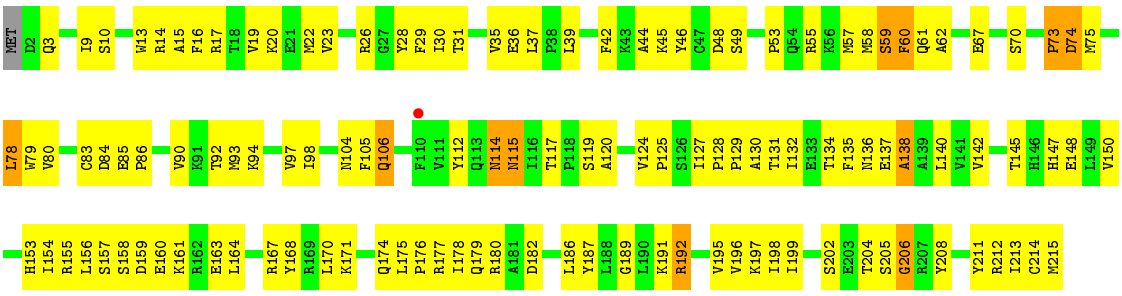




• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

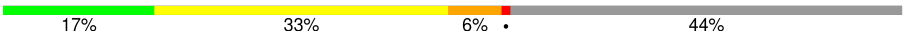
Chain Q:

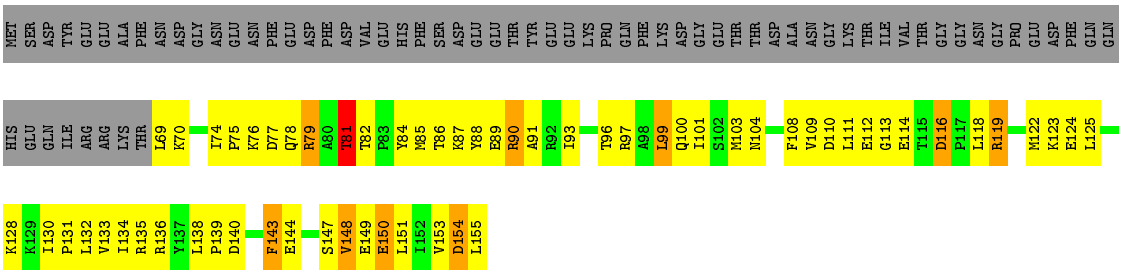




• Molecule 9: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

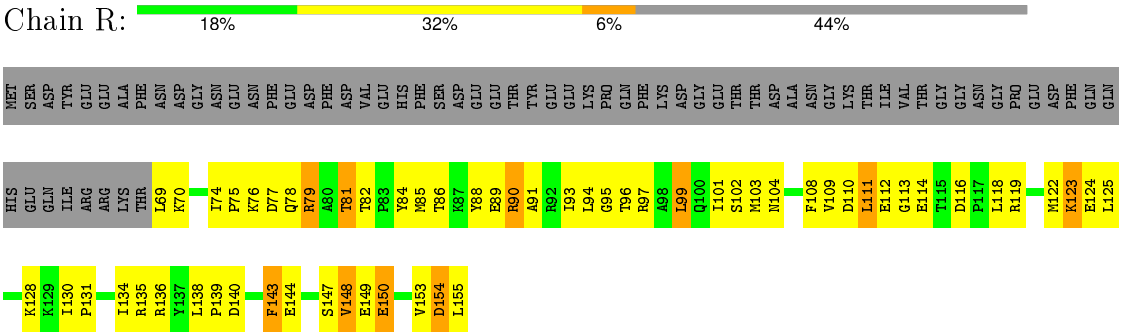
Chain F:





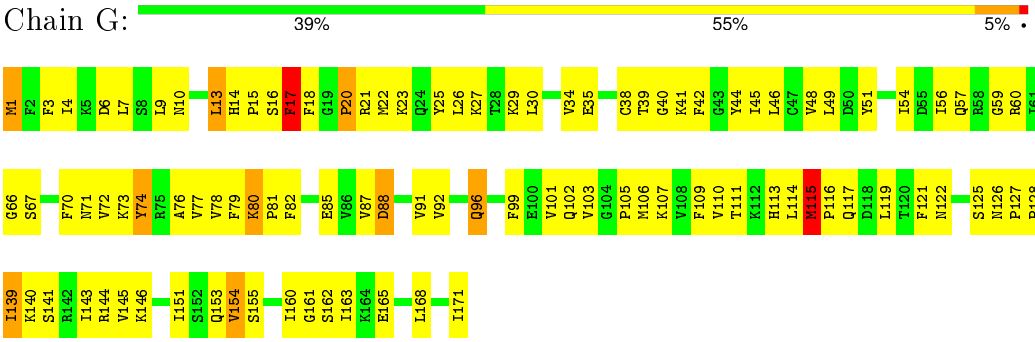
• Molecule 9: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

Chain R:



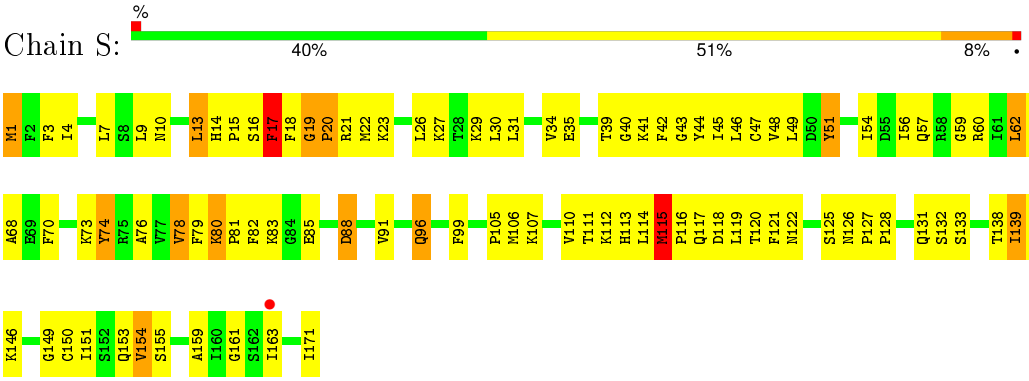
• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

Chain G:



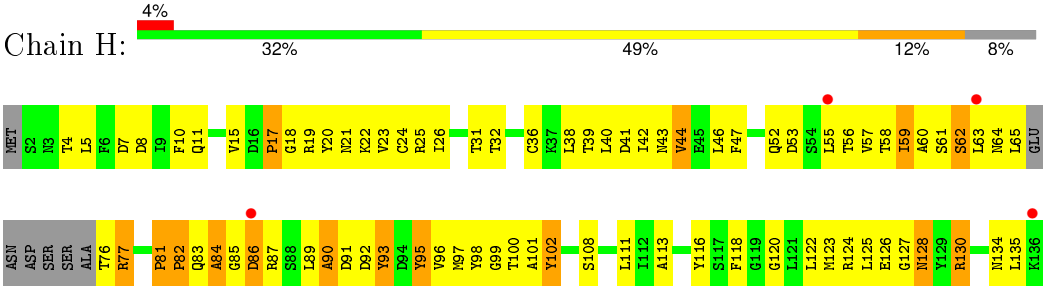
• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

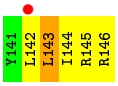
Chain S:



• Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

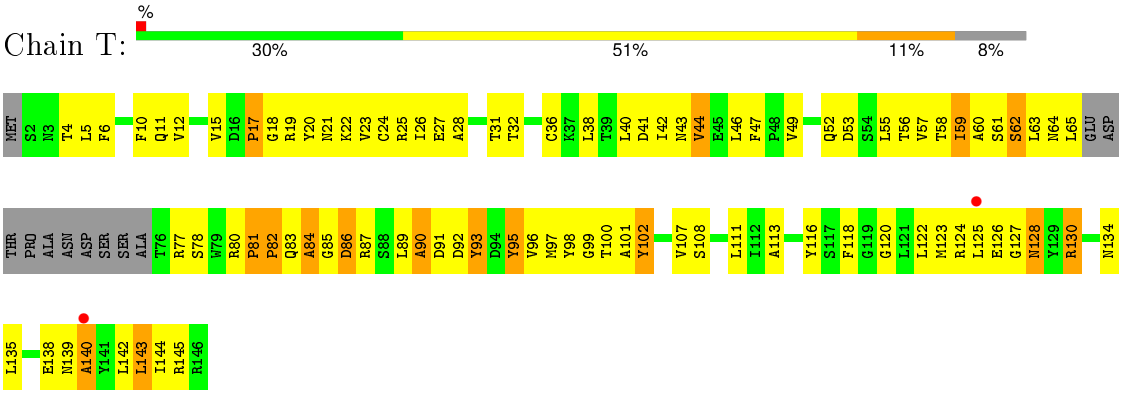
Chain H:





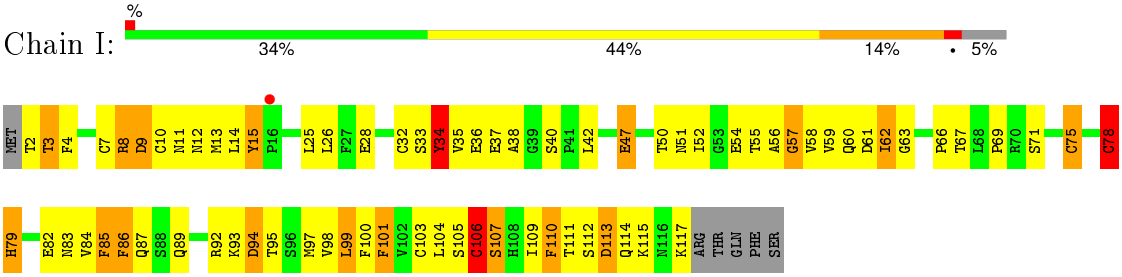
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

Chain T:



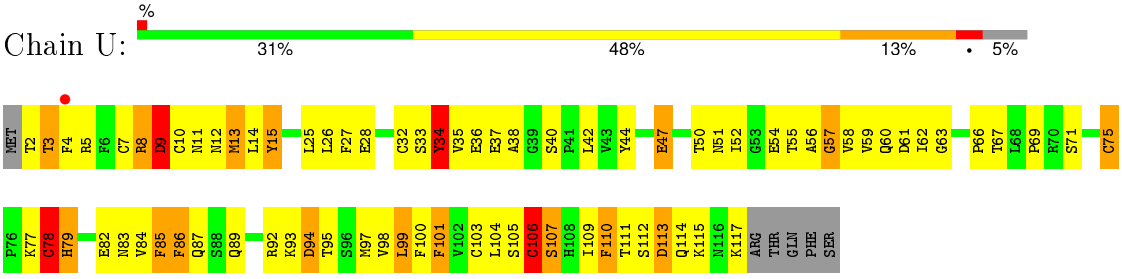
• Molecule 12: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

Chain I:



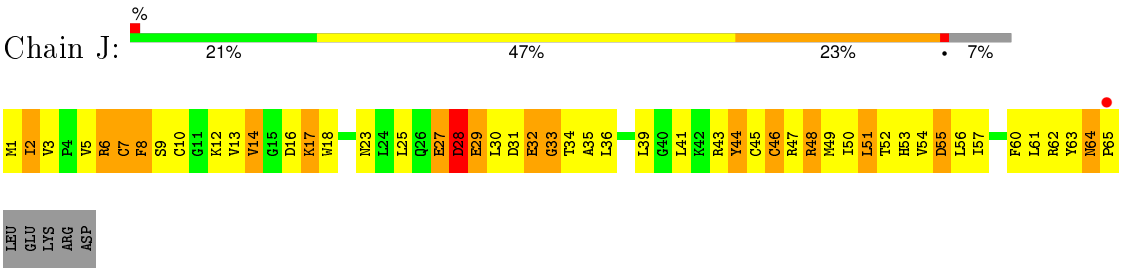
• Molecule 12: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

Chain U:



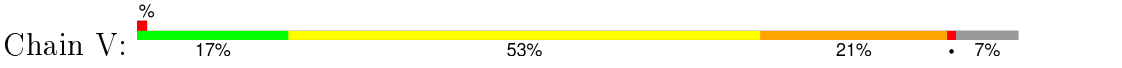
• Molecule 13: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

Chain J:



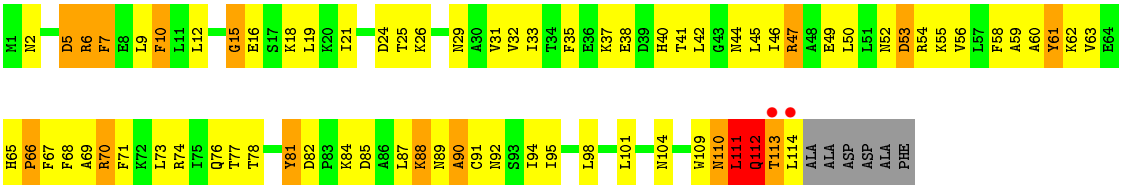
• Molecule 13: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

Chain V:



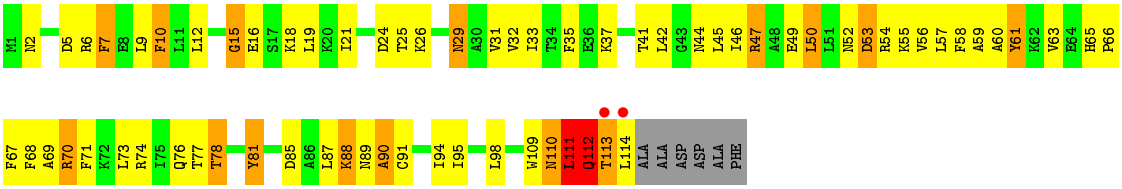
• Molecule 14: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K:



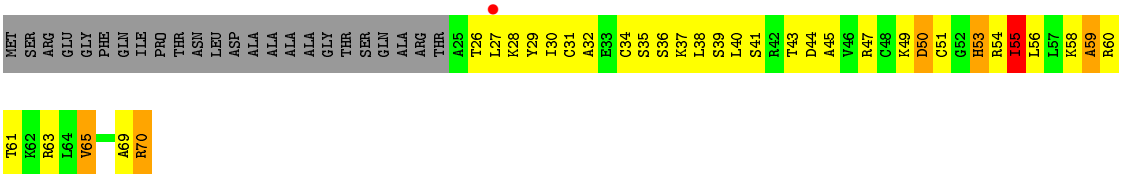
• Molecule 14: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain W:



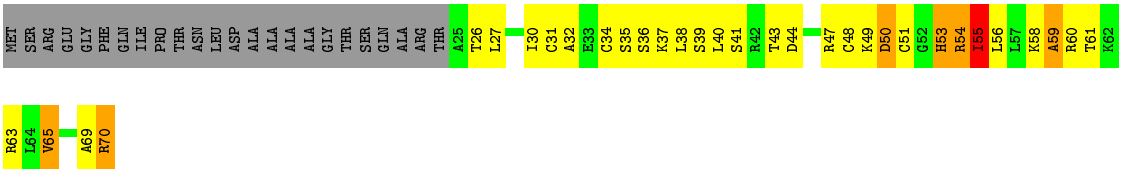
• Molecule 15: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain L:



• Molecule 15: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	394.36Å 221.86Å 283.11Å 90.00° 90.56° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 48.96 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-3.80) 96.7 (48.96-3.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.275 0.231 , 0.243	Depositor DCC
R_{free} test set	4608 reflections (1.97%)	DCC
Wilson B-factor (Å^2)	116.2	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.3	EDS
Estimated twinning fraction	0.024 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.024 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.024 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.020 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.308 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 463473 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	63924	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, BRU, TT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	1.37	0/158	1.57	3/242 (1.2%)
1	4	1.35	0/158	1.58	3/242 (1.2%)
2	2	1.47	1/357 (0.3%)	1.42	3/544 (0.6%)
2	5	1.46	1/357 (0.3%)	1.40	4/544 (0.7%)
3	3	1.55	4/237 (1.7%)	2.20	8/368 (2.2%)
3	6	1.59	4/237 (1.7%)	2.10	8/368 (2.2%)
4	A	0.48	0/11385	0.73	2/15393 (0.0%)
4	M	0.48	0/11385	0.73	2/15393 (0.0%)
5	B	0.47	0/9037	0.70	3/12181 (0.0%)
5	N	0.46	0/9037	0.70	2/12181 (0.0%)
6	C	0.48	0/2138	0.71	0/2896
6	O	0.50	0/2138	0.71	0/2896
7	D	0.44	0/1437	0.67	0/1925
7	P	0.46	0/1437	0.68	0/1925
8	E	0.43	0/1788	0.63	0/2406
8	Q	0.43	0/1788	0.63	0/2406
9	F	0.55	0/716	0.77	0/964
9	R	0.55	0/716	0.75	0/964
10	G	0.52	0/1368	0.74	0/1844
10	S	0.52	0/1368	0.74	0/1844
11	H	0.40	0/1102	0.65	0/1492
11	T	0.40	0/1102	0.65	0/1492
12	I	0.39	0/962	0.69	0/1295
12	U	0.41	0/962	0.69	0/1295
13	J	0.49	0/541	0.77	0/727
13	V	0.52	0/541	0.79	1/727 (0.1%)
14	K	0.92	6/937 (0.6%)	1.00	11/1265 (0.9%)
14	W	0.93	6/937 (0.6%)	0.99	11/1265 (0.9%)
15	L	0.43	0/366	0.71	0/485
15	X	0.45	0/366	0.72	0/485
All	All	0.53	22/65058 (0.0%)	0.76	61/88054 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	2
2	5	0	1
5	B	0	1
5	N	0	1
All	All	0	5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	W	112	GLN	CA-C	10.22	1.79	1.52
14	K	112	GLN	CA-C	10.06	1.79	1.52
14	W	113	THR	N-CA	9.11	1.64	1.46
14	K	113	THR	N-CA	9.06	1.64	1.46
14	W	112	GLN	N-CA	8.71	1.63	1.46

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	2	C	OP1-P-O3'	-22.50	55.69	105.20
3	3	3	G	O5'-P-OP1	22.31	137.47	110.70
3	6	3	G	O5'-P-OP1	21.67	136.70	110.70
3	6	2	C	OP1-P-O3'	-20.00	61.20	105.20
14	W	113	THR	N-CA-C	9.88	137.68	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	20	DC	Sidechain
2	2	26	DC	Sidechain
2	5	20	DC	Sidechain
5	B	486	TYR	Sidechain
5	N	486	TYR	Sidechain

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	1	141	0	81	11	0
1	4	141	0	81	12	0
2	2	380	0	218	36	0
2	5	380	0	218	33	0
3	3	212	0	110	14	0
3	6	212	0	110	10	0
4	A	11186	0	11266	1277	0
4	M	11186	0	11266	1263	0
5	B	8866	0	8898	968	0
5	N	8866	0	8898	1006	0
6	C	2101	0	2055	256	0
6	O	2101	0	2055	237	0
7	D	1427	0	1451	142	0
7	P	1427	0	1451	144	0
8	E	1752	0	1776	131	0
8	Q	1752	0	1776	124	0
9	F	705	0	730	82	0
9	R	705	0	730	80	0
10	G	1340	0	1357	154	0
10	S	1340	0	1357	164	0
11	H	1084	0	1057	122	0
11	T	1084	0	1057	122	0
12	I	944	0	899	112	0
12	U	944	0	899	113	0
13	J	532	0	542	98	0
13	V	532	0	542	110	0
14	K	919	0	929	113	0
14	W	919	0	929	99	0
15	L	364	0	386	41	0
15	X	364	0	386	41	0
16	A	1	0	0	0	0
16	M	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1	0	0	0	0
17	M	2	0	0	0	0
17	N	1	0	0	0	0
17	O	1	0	0	0	0
17	U	2	0	0	0	0
17	V	1	0	0	0	0
17	X	1	0	0	0	0
All	All	63924	0	63510	6519	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 51.

The worst 5 of 6519 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)
14:W:112:GLN:CB	14:W:112:GLN:CG	1.76	1.59
14:K:112:GLN:CB	14:K:112:GLN:CG	1.75	1.56
14:K:112:GLN:CA	14:K:112:GLN:C	1.79	1.49
14:W:112:GLN:C	14:W:112:GLN:CA	1.79	1.47
4:A:855:THR:HG21	4:A:857:ARG:HE	1.09	1.18

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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	1410/1733 (81%)	968 (69%)	288 (20%)	154 (11%)	0 11
4	M	1410/1733 (81%)	964 (68%)	291 (21%)	155 (11%)	0 10
5	B	1096/1224 (90%)	762 (70%)	222 (20%)	112 (10%)	1 13
5	N	1096/1224 (90%)	765 (70%)	217 (20%)	114 (10%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	C	264/318 (83%)	172 (65%)	64 (24%)	28 (11%)	0 11
6	O	264/318 (83%)	171 (65%)	63 (24%)	30 (11%)	0 9
7	D	173/221 (78%)	125 (72%)	27 (16%)	21 (12%)	0 8
7	P	173/221 (78%)	124 (72%)	32 (18%)	17 (10%)	1 14
8	E	212/215 (99%)	155 (73%)	42 (20%)	15 (7%)	1 23
8	Q	212/215 (99%)	156 (74%)	42 (20%)	14 (7%)	1 25
9	F	84/155 (54%)	67 (80%)	11 (13%)	6 (7%)	1 23
9	R	84/155 (54%)	67 (80%)	12 (14%)	5 (6%)	2 27
10	G	169/171 (99%)	125 (74%)	37 (22%)	7 (4%)	3 37
10	S	169/171 (99%)	132 (78%)	28 (17%)	9 (5%)	2 30
11	H	131/146 (90%)	87 (66%)	27 (21%)	17 (13%)	0 7
11	T	131/146 (90%)	83 (63%)	30 (23%)	18 (14%)	0 6
12	I	114/122 (93%)	83 (73%)	19 (17%)	12 (10%)	1 11
12	U	114/122 (93%)	81 (71%)	22 (19%)	11 (10%)	1 14
13	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0 1
13	V	63/70 (90%)	36 (57%)	15 (24%)	12 (19%)	0 3
14	K	112/120 (93%)	86 (77%)	14 (12%)	12 (11%)	0 11
14	W	112/120 (93%)	86 (77%)	17 (15%)	9 (8%)	1 19
15	L	44/70 (63%)	16 (36%)	21 (48%)	7 (16%)	0 5
15	X	44/70 (63%)	17 (39%)	19 (43%)	8 (18%)	0 3
All	All	7744/9130 (85%)	5363 (69%)	1574 (20%)	807 (10%)	1 12

5 of 807 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	44	THR
4	A	48	ALA
4	A	57	ARG
4	A	62	ASP
4	A	65	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	1244/1520 (82%)	1138 (92%)	106 (8%)	13 52
4	M	1244/1520 (82%)	1142 (92%)	102 (8%)	14 53
5	B	967/1061 (91%)	888 (92%)	79 (8%)	14 53
5	N	967/1061 (91%)	886 (92%)	81 (8%)	14 52
6	C	235/274 (86%)	216 (92%)	19 (8%)	15 54
6	O	235/274 (86%)	215 (92%)	20 (8%)	13 52
7	D	159/200 (80%)	136 (86%)	23 (14%)	4 27
7	P	159/200 (80%)	138 (87%)	21 (13%)	5 31
8	E	196/197 (100%)	191 (97%)	5 (3%)	54 82
8	Q	196/197 (100%)	191 (97%)	5 (3%)	54 82
9	F	77/137 (56%)	68 (88%)	9 (12%)	7 36
9	R	77/137 (56%)	69 (90%)	8 (10%)	9 42
10	G	152/152 (100%)	141 (93%)	11 (7%)	18 58
10	S	152/152 (100%)	140 (92%)	12 (8%)	15 55
11	H	119/128 (93%)	112 (94%)	7 (6%)	24 66
11	T	119/128 (93%)	112 (94%)	7 (6%)	24 66
12	I	110/116 (95%)	96 (87%)	14 (13%)	5 32
12	U	110/116 (95%)	95 (86%)	15 (14%)	5 30
13	J	60/65 (92%)	53 (88%)	7 (12%)	7 36
13	V	60/65 (92%)	54 (90%)	6 (10%)	9 43
14	K	99/102 (97%)	89 (90%)	10 (10%)	9 43
14	W	99/102 (97%)	88 (89%)	11 (11%)	8 39
15	L	40/57 (70%)	36 (90%)	4 (10%)	9 43
15	X	40/57 (70%)	36 (90%)	4 (10%)	9 43
All	All	6916/8018 (86%)	6330 (92%)	586 (8%)	13 52

5 of 586 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	I	78	CYS
4	M	470	LEU

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Mol	Chain	Res	Type
10	S	126	ASN
12	I	110	PHE
4	M	37	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
12	I	60	GLN
4	M	631	HIS
8	Q	147	HIS
13	J	64	ASN
4	M	68	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	3	9/11 (81%)	1 (11%)	0
3	6	9/11 (81%)	1 (11%)	0
All	All	18/22 (81%)	2 (11%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	3	3	G
3	6	3	G

There are no RNA pucker outliers to report.

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

4 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	$\#\|Z\|>2$
2	TT	2	18	2	38,43,44	4.61	7 (18%)	54,69,72	2.15	13 (24%)
2	BRU	2	22	3,2	13,21,22	1.81	3 (23%)	16,30,33	4.27	4 (25%)
2	TT	5	18	2	38,43,44	4.59	6 (15%)	54,69,72	2.15	12 (22%)
2	BRU	5	22	3,2	13,21,22	1.98	3 (23%)	16,30,33	4.33	5 (31%)

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
2	TT	2	18	2	-	0/18/105/106	0/3/6/6
2	BRU	2	22	3,2	-	0/3/21/22	0/2/2/2
2	TT	5	18	2	-	0/18/105/106	0/3/6/6
2	BRU	5	22	3,2	-	0/3/21/22	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	18	TT	C5-C6	-20.23	1.31	1.55
2	2	18	TT	C5-C6	-20.09	1.31	1.55
2	2	18	TT	C5T-C6T	-18.68	1.33	1.55
2	5	18	TT	C5T-C6T	-18.36	1.33	1.55
2	2	18	TT	C6-N1	-3.90	1.39	1.46

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	22	BRU	C5-C4-N3	-8.42	115.01	124.00
2	2	22	BRU	C5-C4-N3	-8.33	115.11	124.00
2	5	18	TT	C5-C6-C6T	-5.94	79.23	89.27
2	2	18	TT	C5-C6-C6T	-5.76	79.54	89.27
2	5	18	TT	C5-C5T-C6T	-5.27	81.69	88.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	18	TT	4	0
2	2	22	BRU	4	0
2	5	18	TT	4	0
2	5	22	BRU	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 18 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	7/14 (50%)	-0.72	0 100 100	123, 130, 149, 149	0
1	4	7/14 (50%)	-0.66	0 100 100	120, 128, 147, 148	0
2	2	16/25 (64%)	-0.66	0 100 100	84, 130, 151, 155	0
2	5	16/25 (64%)	-0.55	0 100 100	87, 132, 150, 153	0
3	3	10/11 (90%)	-0.42	0 100 100	95, 100, 152, 155	0
3	6	10/11 (90%)	-0.38	0 100 100	95, 102, 153, 156	0
4	A	1421/1733 (81%)	-0.06	8 (0%) 90 82	22, 88, 163, 200	0
4	M	1421/1733 (81%)	-0.04	5 (0%) 93 87	20, 88, 163, 200	0
5	B	1115/1224 (91%)	-0.01	8 (0%) 89 80	24, 101, 175, 200	0
5	N	1115/1224 (91%)	-0.01	7 (0%) 90 82	23, 101, 174, 200	0
6	C	267/318 (83%)	-0.11	0 100 100	49, 88, 147, 173	0
6	O	267/318 (83%)	-0.04	1 (0%) 93 87	52, 87, 148, 170	0
7	D	177/221 (80%)	-0.03	0 100 100	72, 121, 166, 183	0
7	P	177/221 (80%)	-0.04	2 (1%) 82 69	71, 124, 166, 182	0
8	E	214/215 (99%)	-0.12	1 (0%) 91 85	60, 145, 193, 197	0
8	Q	214/215 (99%)	-0.11	1 (0%) 91 85	58, 145, 194, 197	0
9	F	87/155 (56%)	-0.05	0 100 100	31, 62, 108, 140	0
9	R	87/155 (56%)	-0.02	0 100 100	31, 63, 109, 138	0
10	G	171/171 (100%)	-0.07	0 100 100	64, 91, 136, 146	0
10	S	171/171 (100%)	-0.05	1 (0%) 90 82	65, 93, 136, 143	0
11	H	135/146 (92%)	-0.01	6 (4%) 38 25	101, 145, 182, 192	0
11	T	135/146 (92%)	0.03	2 (1%) 76 62	99, 146, 181, 191	0
12	I	116/122 (95%)	-0.08	1 (0%) 85 74	82, 139, 170, 195	0
12	U	116/122 (95%)	-0.11	1 (0%) 85 74	81, 138, 170, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	J	65/70 (92%)	-0.11	1 (1%)	76	62	52, 83, 128, 133	0
13	V	65/70 (92%)	-0.07	1 (1%)	76	62	46, 81, 130, 136	0
14	K	114/120 (95%)	0.02	2 (1%)	71	56	48, 92, 120, 170	0
14	W	114/120 (95%)	-0.02	2 (1%)	71	56	47, 92, 118, 167	0
15	L	46/70 (65%)	0.09	1 (2%)	65	50	86, 155, 179, 186	0
15	X	46/70 (65%)	0.08	0	100	100	84, 156, 179, 185	0
All	All	7922/9230 (85%)	-0.05	51 (0%)	90	82	20, 99, 173, 200	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	K	114	LEU	8.5
14	K	113	THR	8.0
14	W	114	LEU	6.6
14	W	113	THR	6.2
4	M	1092	LYS	5.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BRU	5	22	20/21	0.92	0.14	-	77,84,87,89	0
2	BRU	2	22	20/21	0.90	0.17	-	69,76,80,84	0
2	TT	2	18	38/39	0.94	0.21	-	93,106,123,125	0
2	TT	5	18	38/39	0.94	0.16	-	95,108,126,127	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
17	ZN	I	2458	1/1	0.99	0.29	5.83	94,94,94,94	0
17	ZN	U	2457	1/1	0.99	0.30	5.66	91,91,91,91	0
17	ZN	O	2457	1/1	0.99	0.30	3.58	39,39,39,39	0
17	ZN	M	2457	1/1	0.98	0.27	2.67	87,87,87,87	0
17	ZN	C	2457	1/1	0.99	0.30	2.54	48,48,48,48	0
17	ZN	N	2457	1/1	1.00	0.28	1.03	54,54,54,54	0
17	ZN	X	2457	1/1	0.98	0.25	0.98	120,120,120,120	0
17	ZN	B	2457	1/1	0.97	0.28	0.96	53,53,53,53	0
17	ZN	L	2457	1/1	0.98	0.24	0.92	116,116,116,116	0
17	ZN	I	2457	1/1	0.97	0.24	0.77	199,199,199,199	0
17	ZN	A	2471	1/1	0.99	0.24	0.67	90,90,90,90	0
17	ZN	J	2457	1/1	0.99	0.25	0.40	70,70,70,70	0
17	ZN	V	2457	1/1	0.99	0.24	0.33	67,67,67,67	0
17	ZN	U	2458	1/1	0.98	0.19	0.12	178,178,178,178	0
17	ZN	M	2458	1/1	0.99	0.24	-0.23	51,51,51,51	0
17	ZN	A	2472	1/1	1.00	0.22	-0.50	52,52,52,52	0
16	MG	A	2457	1/1	0.99	0.19	-	50,50,50,50	0
16	MG	M	2459	1/1	0.99	0.24	-	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.