wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 06:21 PM EDT

PDB ID	:	2O5I
Title	:	Crystal structure of the T. thermophilus RNA polymerase elongation complex
Authors	:	Vassylyev, D.G.; Tahirov, T.H.; Vassylyeva, M.N.
Deposited on	:	2006-12-06
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

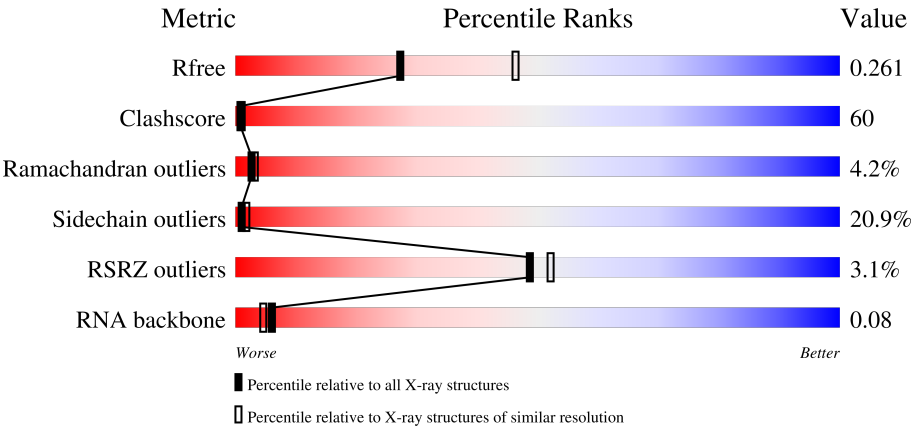
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	G	23	13% 61% 17% 9%
1	X	23	13% 70% 13% .
2	H	16	19% 81%
2	Y	16	31% 69%

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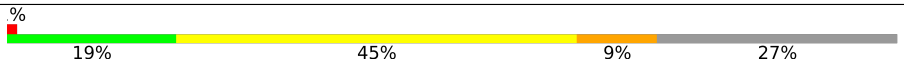
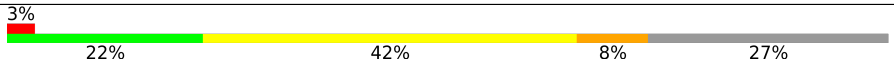
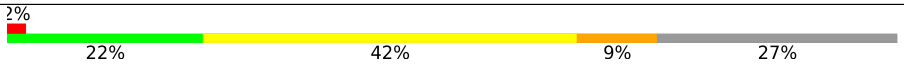
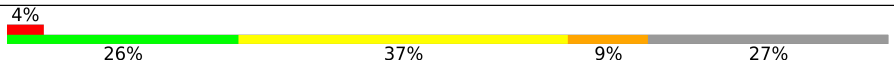
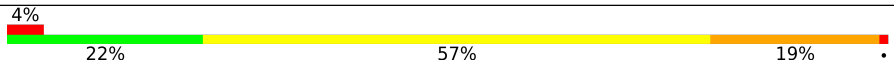
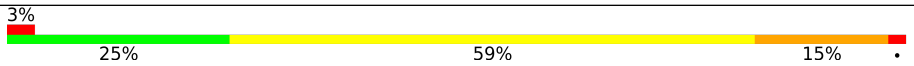
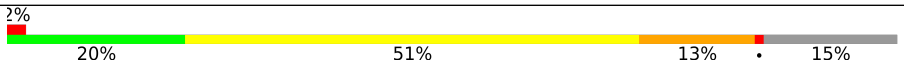
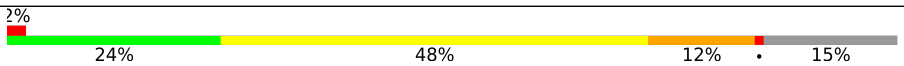
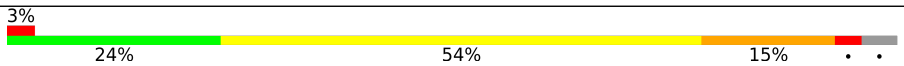
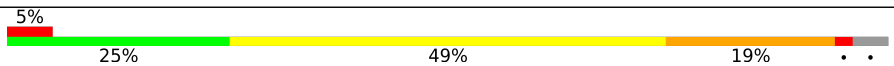
Mol	Chain	Length	Quality of chain
3	I	14	
3	Z	14	
4	A	315	
4	B	315	
4	K	315	
4	L	315	
5	C	1119	
5	M	1119	
6	D	1524	
6	N	1524	
7	E	99	
7	O	99	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 52719 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(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			
1	X	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			

- Molecule 2 is a RNA chain called 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			
2	Y	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			

- Molecule 3 is a DNA chain called 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			
3	Z	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 5 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
5	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 6 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	1303	Total	C	N	O	S	0	0	0
			10280	6508	1821	1919	32			
6	N	1303	Total	C	N	O	S	0	0	0
			10280	6508	1821	1919	32			

- Molecule 7 is a protein called DNA-directed RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
7	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	N	1	Total Mg 1 1	0	0

- Molecule 10 is water.

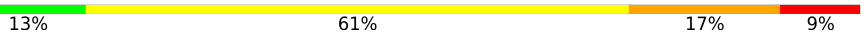
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	G	22	Total O 22 22	0	0
10	H	18	Total O 18 18	0	0
10	I	36	Total O 36 36	0	0
10	X	25	Total O 25 25	0	0
10	Y	16	Total O 16 16	0	0
10	Z	16	Total O 16 16	0	0
10	A	144	Total O 144 144	0	0
10	B	159	Total O 159 159	0	0
10	C	658	Total O 658 658	0	0
10	D	760	Total O 760 760	0	0
10	E	70	Total O 70 70	0	0
10	K	132	Total O 132 132	0	0
10	L	121	Total O 121 121	0	0
10	M	575	Total O 575 575	0	0
10	N	750	Total O 750 750	0	0
10	O	61	Total O 61 61	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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.

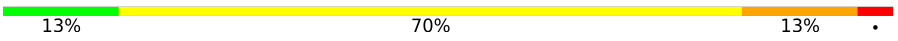
• Molecule 1: 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'

Chain G:



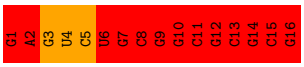
• Molecule 1: 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'

Chain X:



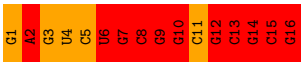
• Molecule 2: 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3'

Chain H:



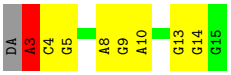
• Molecule 2: 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3'

Chain Y:



• Molecule 3: 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'

Chain I:

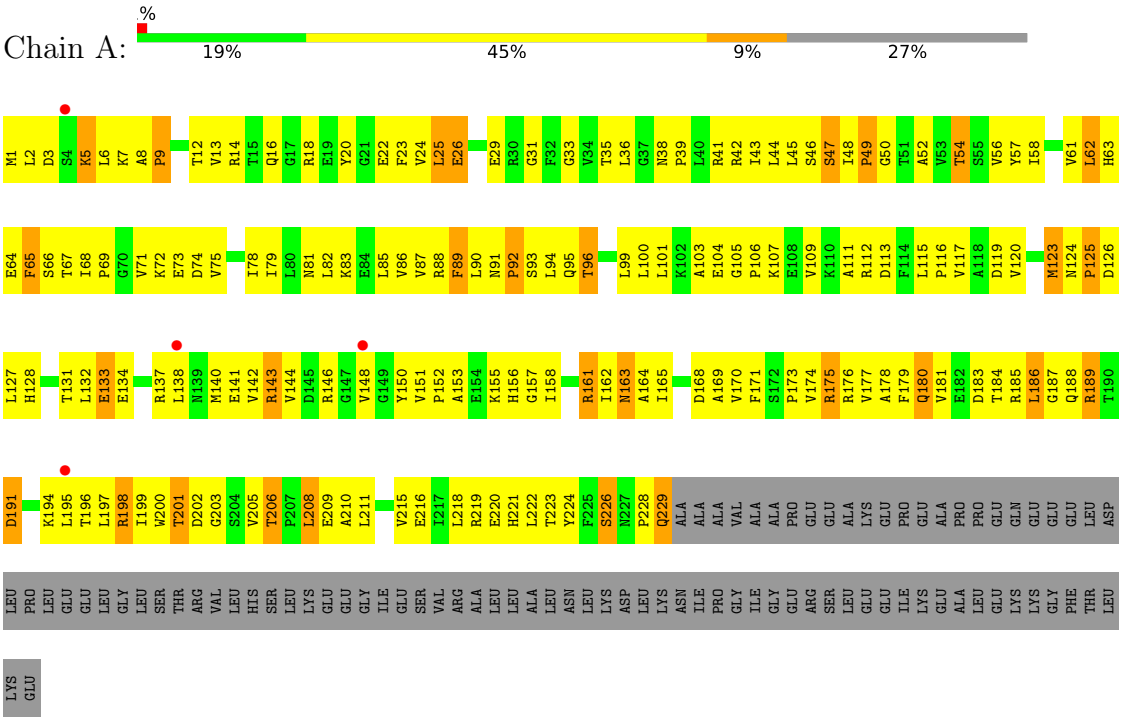


• Molecule 3: 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'

Chain Z:

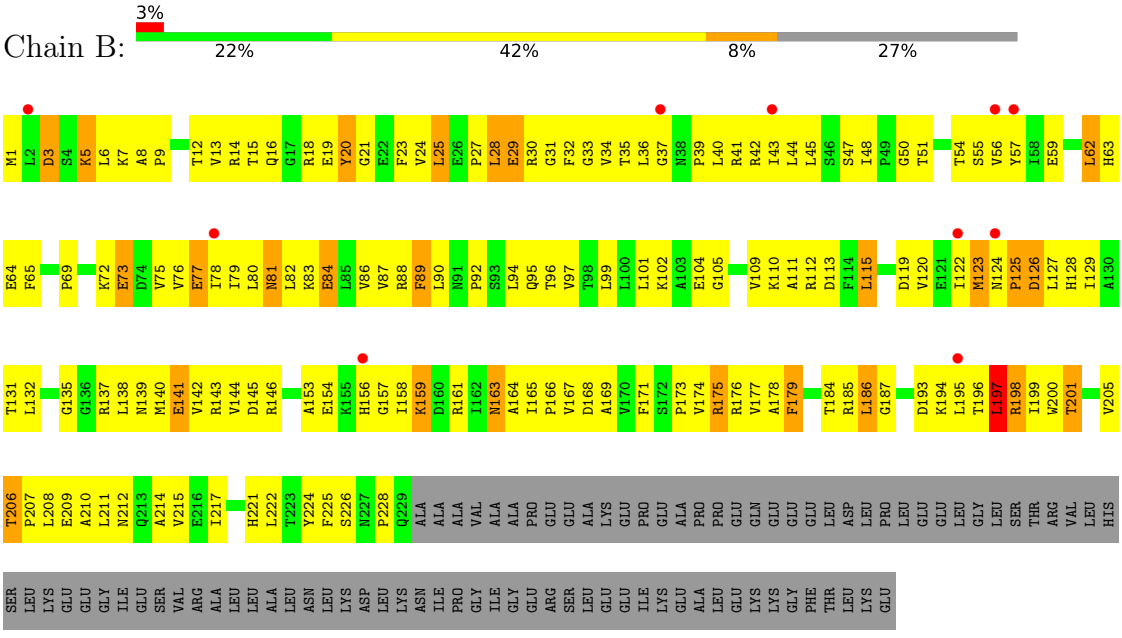
• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain A:



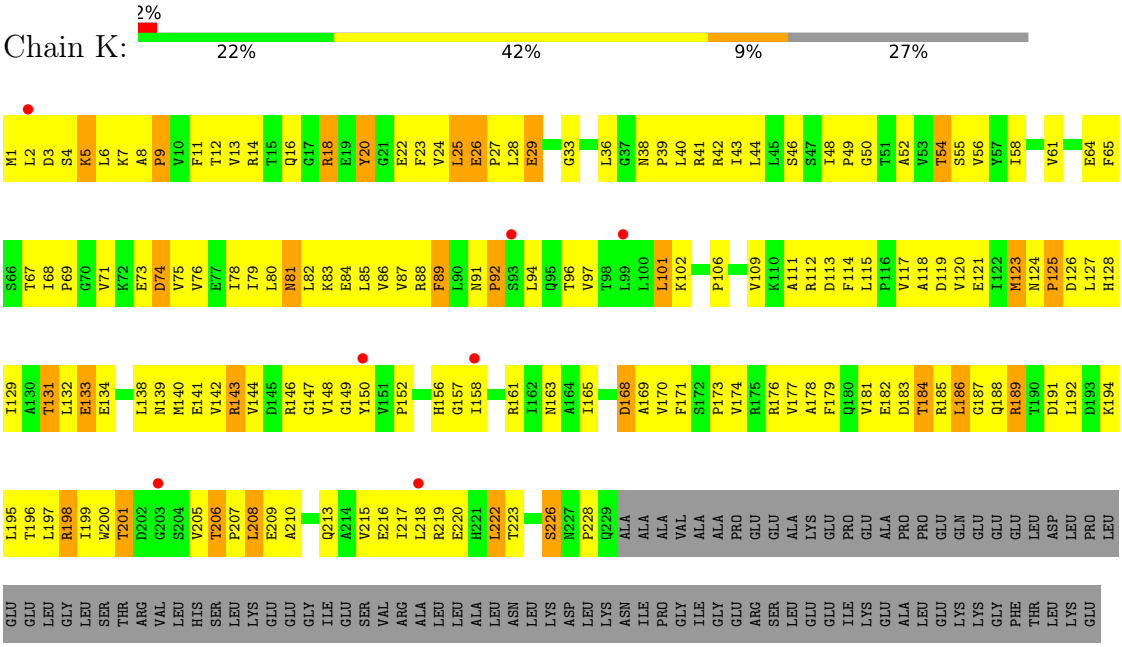
• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain B:



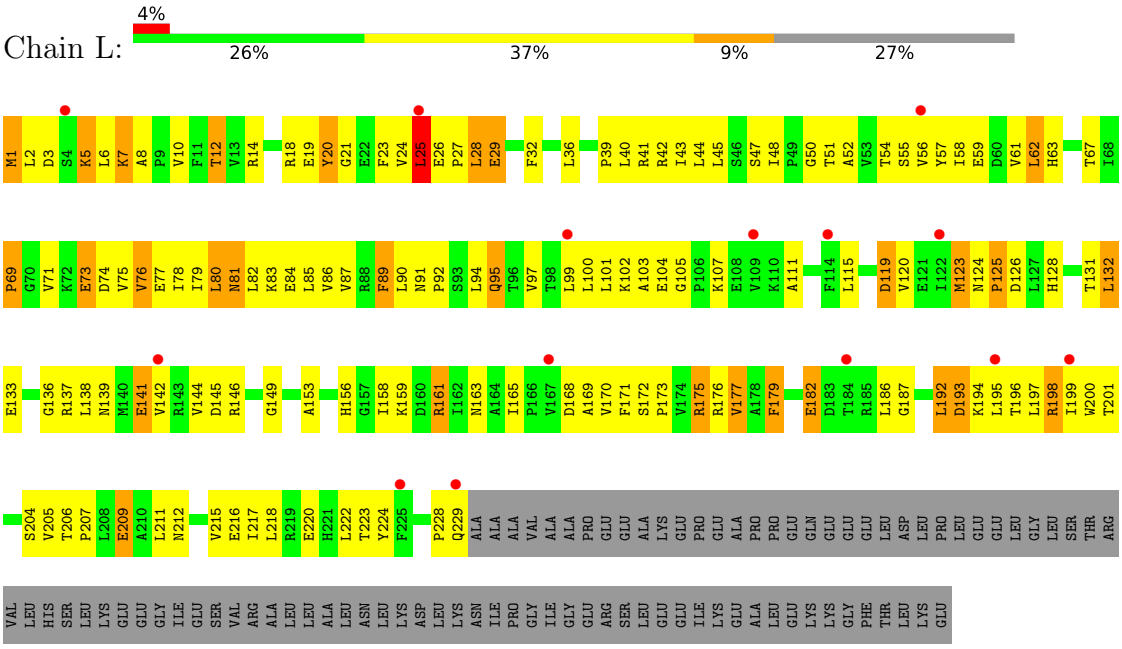
• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain K:



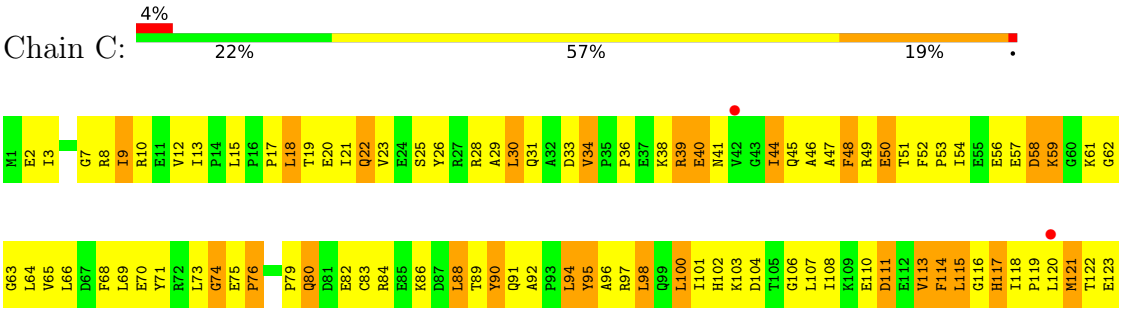
• Molecule 4: DNA-directed RNA polymerase alpha chain

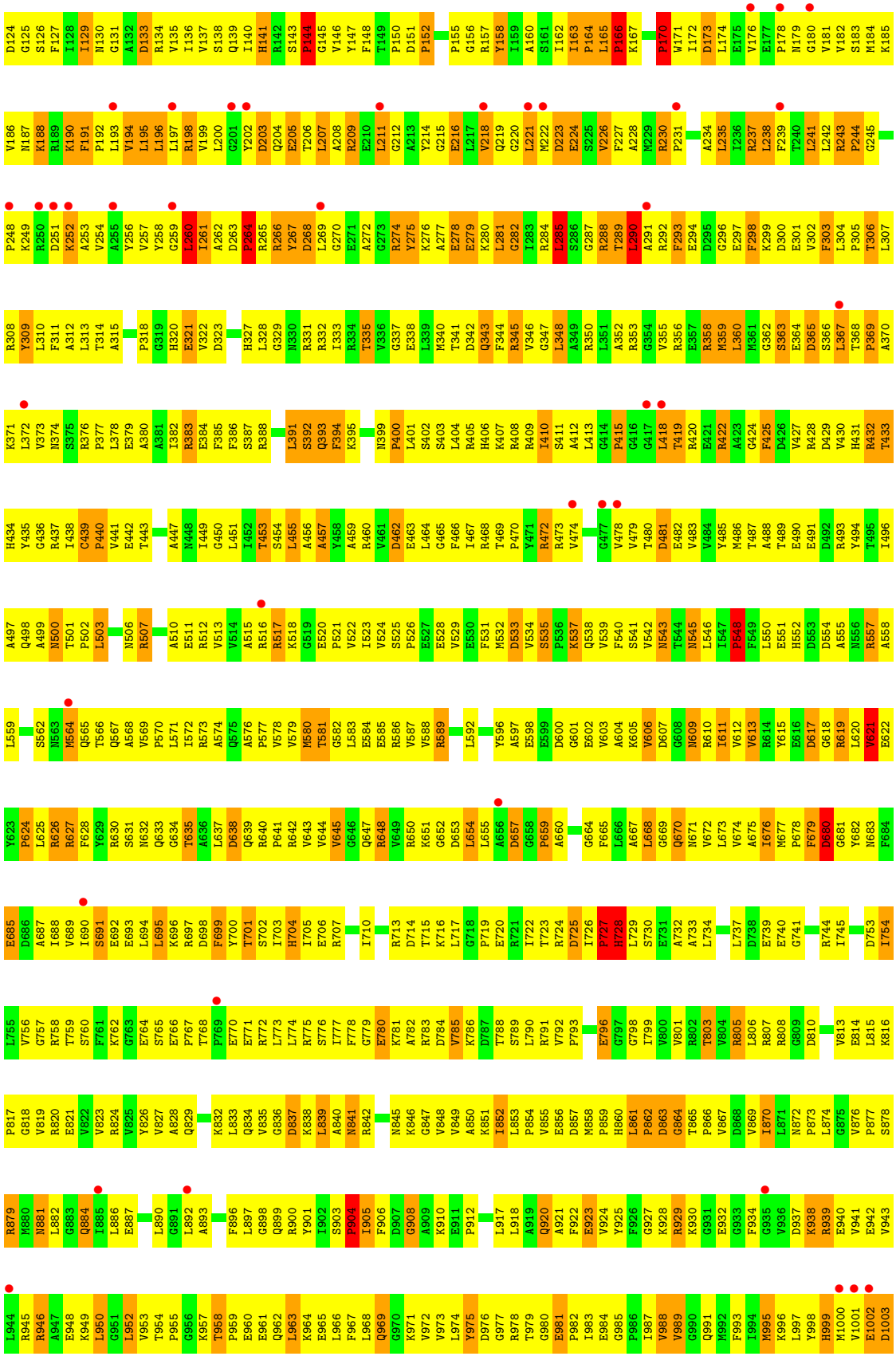
Chain L:

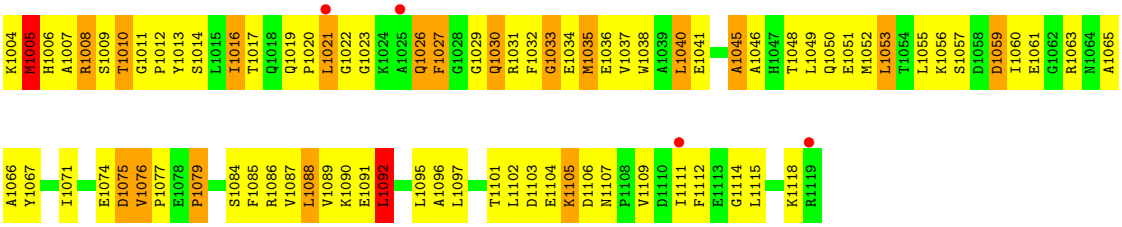


• Molecule 5: DNA-directed RNA polymerase beta chain

Chain C:

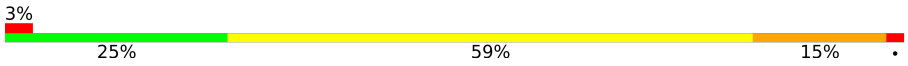


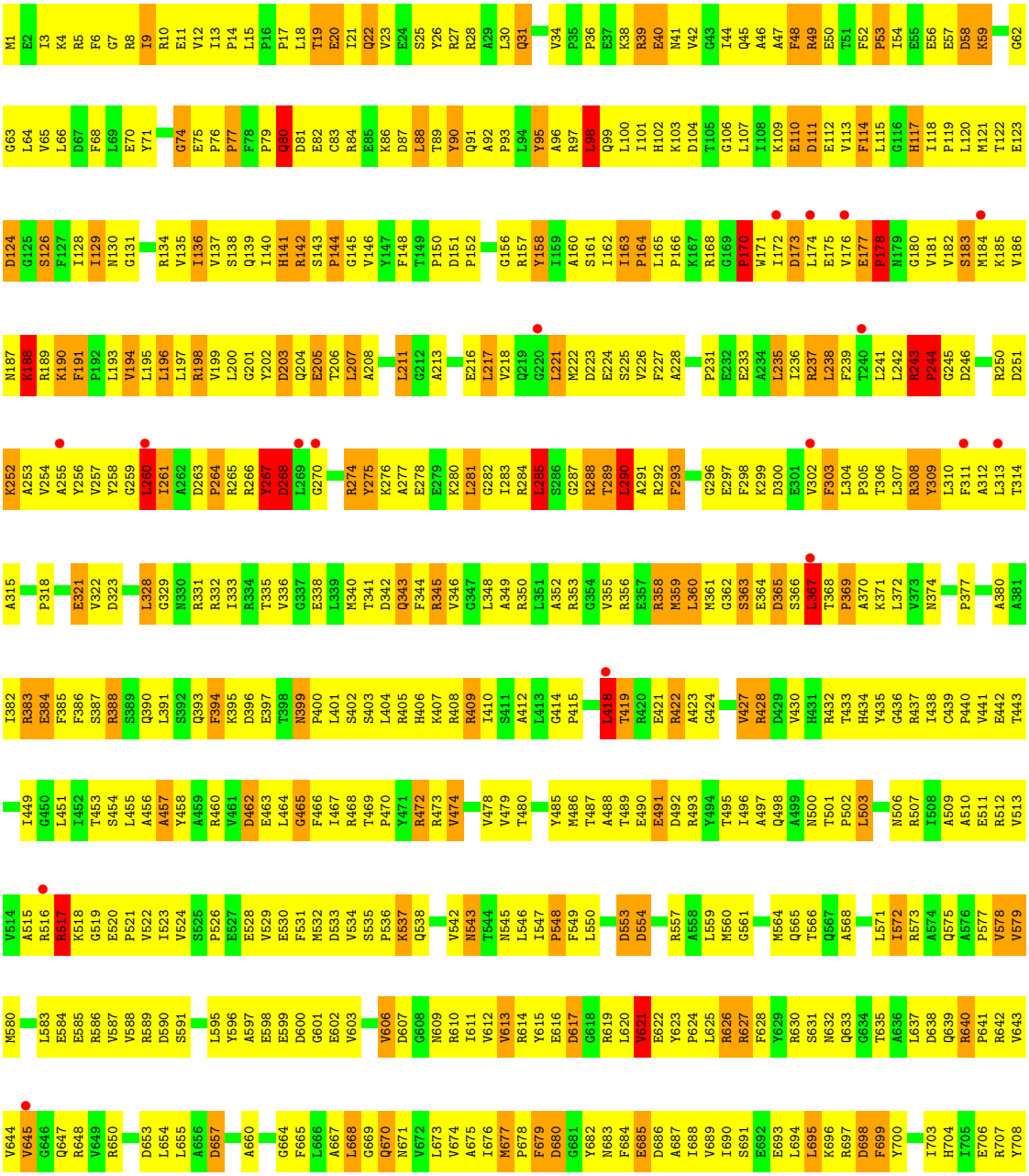


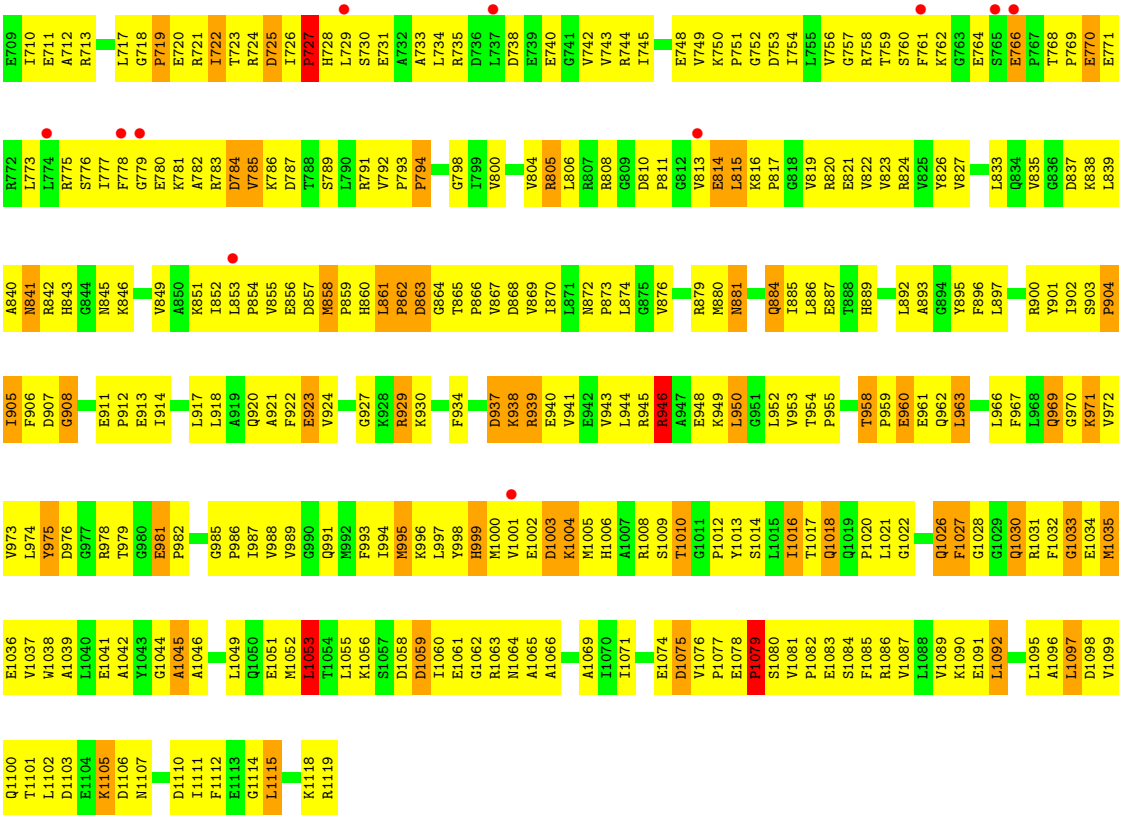


• Molecule 5: DNA-directed RNA polymerase beta chain

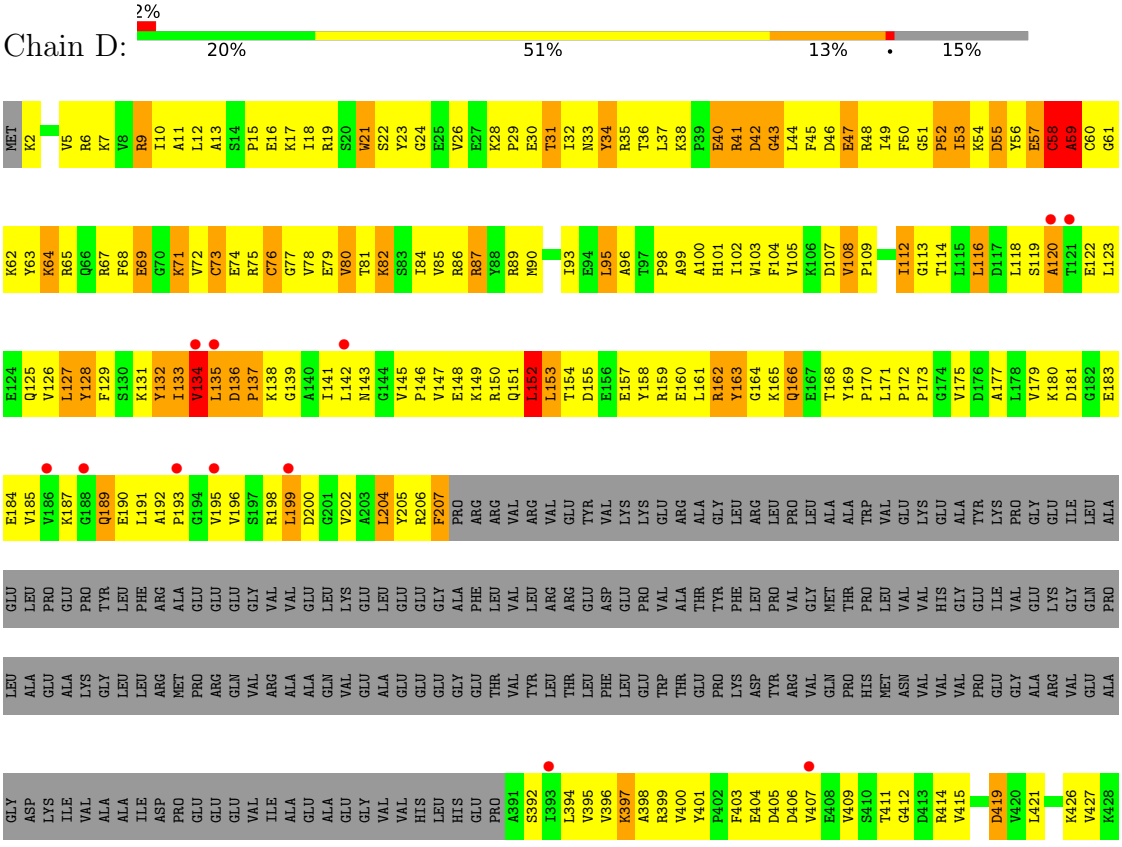
Chain M:

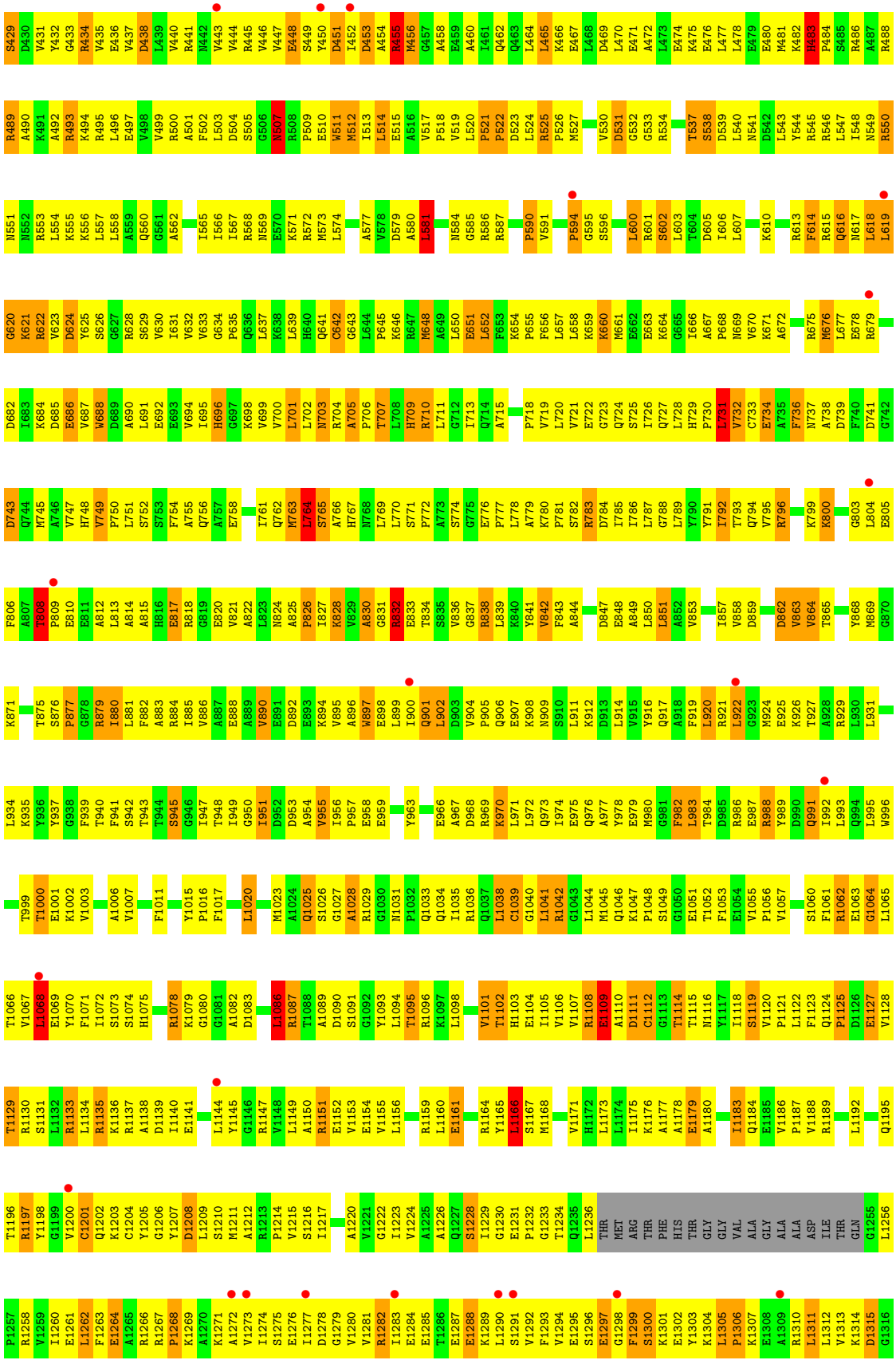


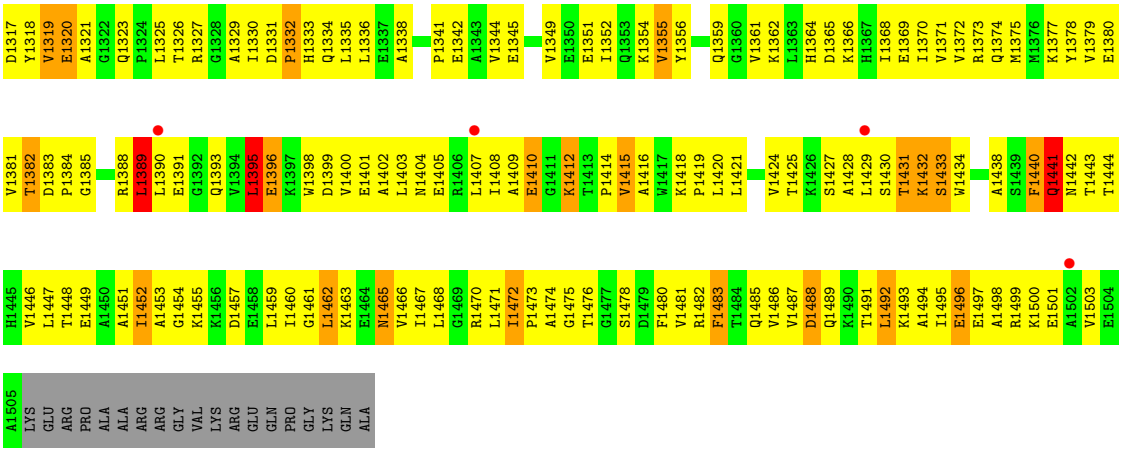




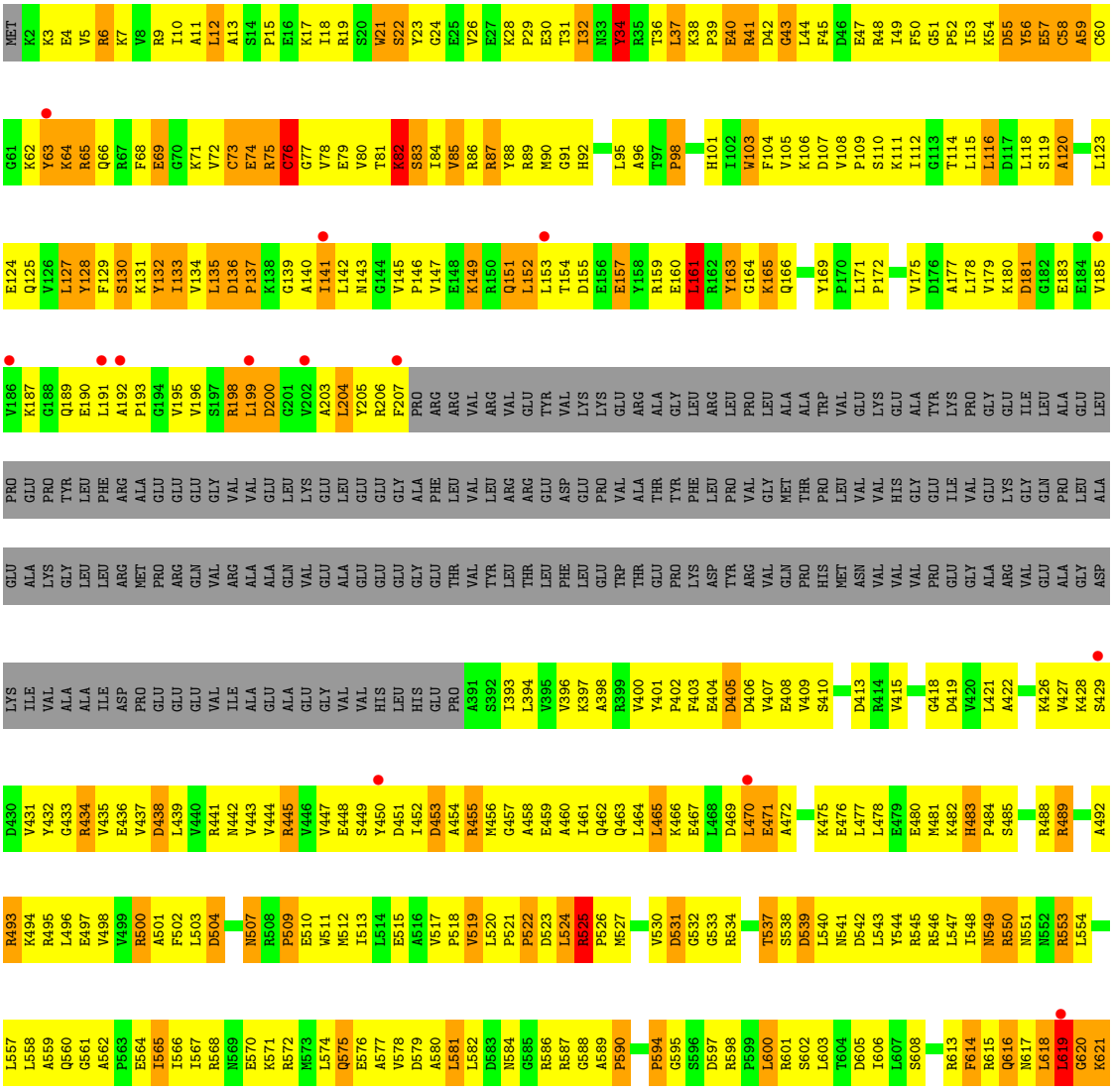
• Molecule 6: DNA-directed RNA polymerase beta' chain

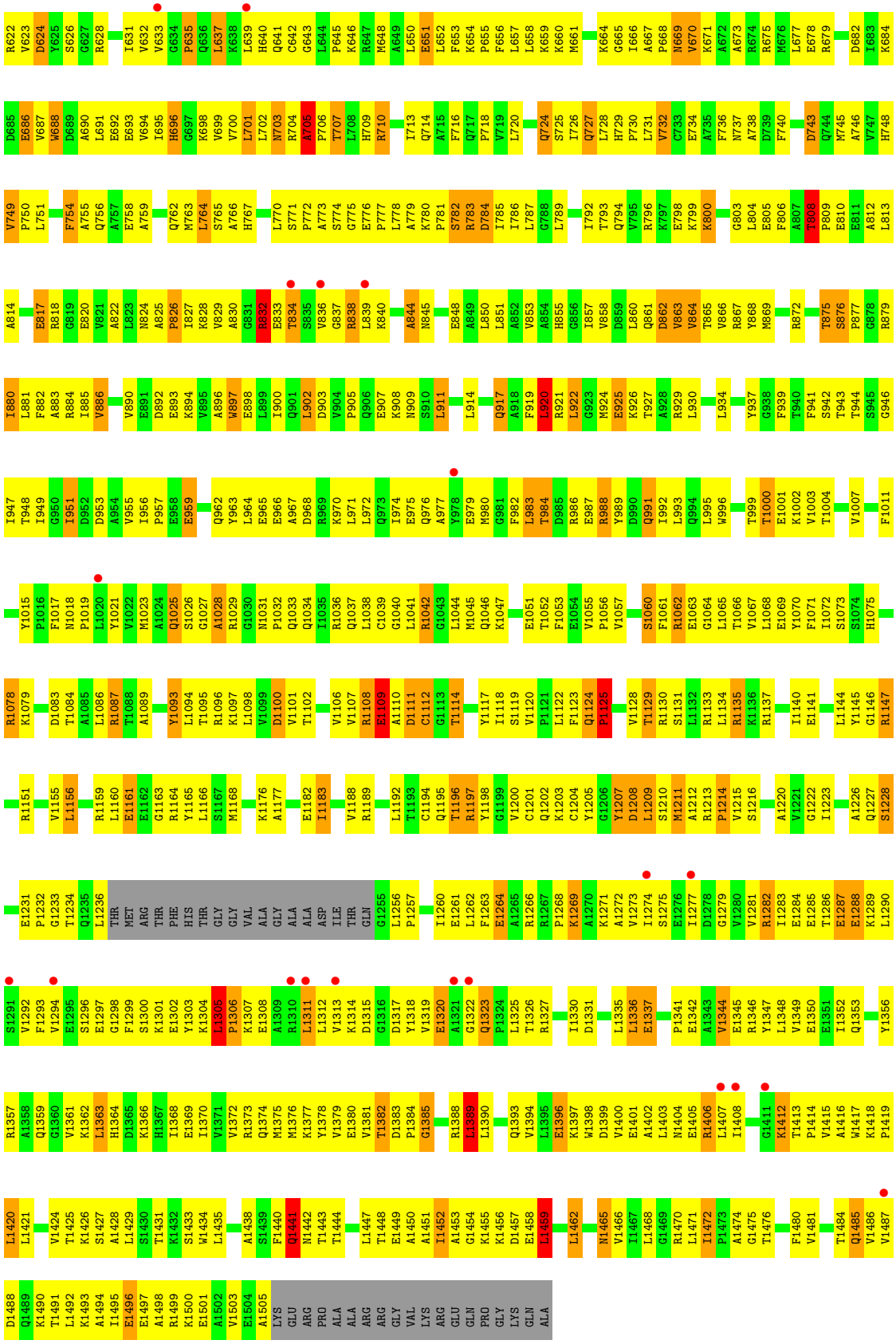






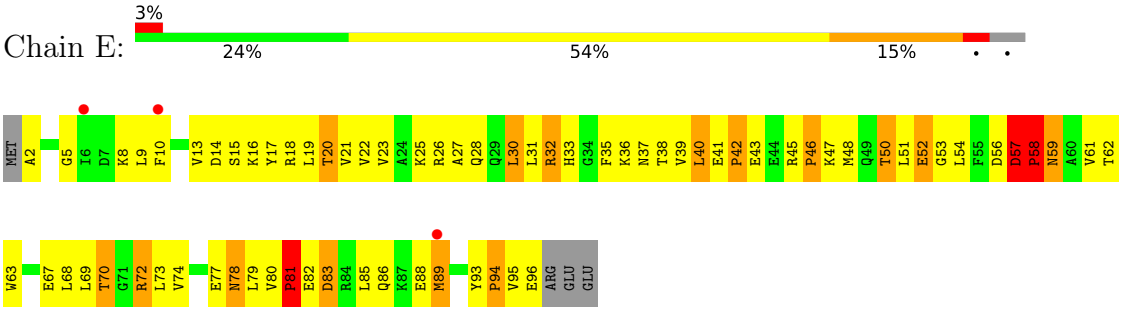
• Molecule 6: DNA-directed RNA polymerase beta' chain





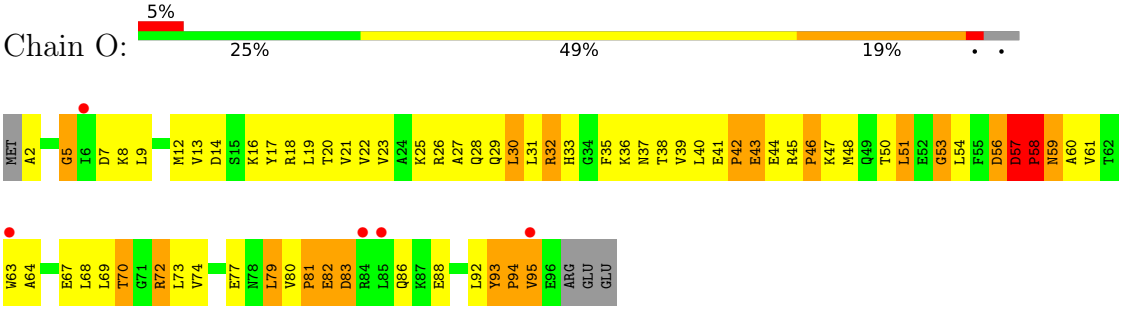
• Molecule 7: DNA-directed RNA polymerase omega chain

Chain E:



• Molecule 7: DNA-directed RNA polymerase omega chain

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	156.21Å 156.21Å 499.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.2 (20.00-2.50) 83.7 (19.99-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.267 0.238 , 0.261	Depositor DCC
R_{free} test set	19570 reflections (5.74%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 124.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	52719	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	G	1.12	2/520 (0.4%)	1.17	5/798 (0.6%)
1	X	1.05	1/520 (0.2%)	1.13	2/798 (0.3%)
2	H	1.84	1/387 (0.3%)	2.39	37/601 (6.2%)
2	Y	1.31	1/387 (0.3%)	2.56	40/601 (6.7%)
3	I	0.94	1/304 (0.3%)	0.89	0/467
3	Z	0.84	1/304 (0.3%)	0.90	0/467
4	A	0.74	0/1838	0.82	1/2498 (0.0%)
4	B	0.76	0/1838	0.79	3/2498 (0.1%)
4	K	0.72	0/1838	0.82	1/2498 (0.0%)
4	L	0.72	0/1838	0.80	4/2498 (0.2%)
5	C	0.78	0/8997	0.93	17/12164 (0.1%)
5	M	0.79	1/8997 (0.0%)	0.93	20/12164 (0.2%)
6	D	0.83	9/10452 (0.1%)	0.92	21/14116 (0.1%)
6	N	0.80	2/10452 (0.0%)	0.91	15/14116 (0.1%)
7	E	0.85	1/784 (0.1%)	1.18	6/1057 (0.6%)
7	O	0.82	1/784 (0.1%)	1.08	5/1057 (0.5%)
All	All	0.82	21/50240 (0.0%)	0.97	177/68398 (0.3%)

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	G	0	5
1	X	0	3
2	H	0	2
2	Y	0	3
3	I	0	1
3	Z	0	1
All	All	0	15

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	G	OP3-P	25.71	1.92	1.61
6	D	133	ILE	N-CA	9.15	1.64	1.46
6	D	132	TYR	CA-C	8.40	1.74	1.52
1	X	1	DC	OP3-P	-8.00	1.51	1.61
1	G	1	DC	OP3-P	-7.45	1.52	1.61

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	2	A	N9-C1'-C2'	-18.13	90.43	114.00
7	E	94	PRO	CA-N-CD	-16.74	88.07	111.50
2	Y	3	G	O4'-C1'-N9	-13.31	97.55	108.20
2	H	7	G	N9-C1'-C2'	-11.21	99.43	114.00
2	Y	7	G	N9-C1'-C2'	-11.05	99.63	114.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1	DC	Sidechain
1	G	13	DT	Sidechain
1	G	16	DG	Sidechain
1	G	17	DC	Sidechain
1	G	18	DG	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	G	467	0	259	45	0
1	X	467	0	259	34	0
2	H	347	0	174	68	0
2	Y	347	0	175	77	0
3	I	270	0	144	13	0
3	Z	270	0	144	15	0
4	A	1806	0	1861	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1806	0	1861	179	0
4	K	1806	0	1861	192	0
4	L	1806	0	1861	172	0
5	C	8829	0	8933	1212	0
5	M	8829	0	8933	1123	0
6	D	10280	0	10510	1429	0
6	N	10280	0	10510	1343	0
7	E	770	0	784	104	0
7	O	770	0	784	108	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	D	1	0	0	0	0
9	N	1	0	0	0	0
10	A	144	0	0	51	0
10	B	159	0	0	38	0
10	C	658	0	0	189	0
10	D	760	0	0	210	0
10	E	70	0	0	15	0
10	G	22	0	0	4	0
10	H	18	0	0	1	0
10	I	36	0	0	4	0
10	K	132	0	0	39	0
10	L	121	0	0	23	0
10	M	575	0	0	168	0
10	N	750	0	0	226	0
10	O	61	0	0	23	0
10	X	25	0	0	5	0
10	Y	16	0	0	2	0
10	Z	16	0	0	2	0
All	All	52719	0	49053	5880	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 60.

The worst 5 of 5880 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)
6:D:132:TYR:C	6:D:132:TYR:CA	1.74	1.56
7:O:95:VAL:CG1	10:O:2132:HOH:O	1.89	1.21
2:H:2:A:OP2	6:D:671:LYS:HD2	1.47	1.14
6:D:165:LYS:HB2	6:D:397:LYS:HB2	1.31	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:619:LEU:HD12	6:N:621:LYS:HZ3	1.08	1.12

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	227/315 (72%)	206 (91%)	16 (7%)	5 (2%)	6	10
4	B	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	8	14
4	K	227/315 (72%)	205 (90%)	17 (8%)	5 (2%)	6	10
4	L	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	8	14
5	C	1117/1119 (100%)	916 (82%)	142 (13%)	59 (5%)	2	2
5	M	1117/1119 (100%)	918 (82%)	145 (13%)	54 (5%)	2	2
6	D	1297/1524 (85%)	1081 (83%)	165 (13%)	51 (4%)	3	4
6	N	1297/1524 (85%)	1100 (85%)	147 (11%)	50 (4%)	3	4
7	E	93/99 (94%)	76 (82%)	8 (9%)	9 (10%)	0	0
7	O	93/99 (94%)	75 (81%)	9 (10%)	9 (10%)	0	0
All	All	5922/6744 (88%)	4987 (84%)	685 (12%)	250 (4%)	3	3

5 of 250 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	29	GLU
4	A	187	GLY
4	B	29	GLU
4	B	187	GLY
5	C	40	GLU

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	202/273 (74%)	164 (81%)	38 (19%)	1	2
4	B	202/273 (74%)	171 (85%)	31 (15%)	2	5
4	K	202/273 (74%)	170 (84%)	32 (16%)	2	4
4	L	202/273 (74%)	166 (82%)	36 (18%)	2	3
5	C	941/941 (100%)	710 (76%)	231 (24%)	0	1
5	M	941/941 (100%)	740 (79%)	201 (21%)	1	2
6	D	1100/1279 (86%)	874 (80%)	226 (20%)	1	2
6	N	1100/1279 (86%)	879 (80%)	221 (20%)	1	2
7	E	84/88 (96%)	62 (74%)	22 (26%)	0	0
7	O	84/88 (96%)	66 (79%)	18 (21%)	1	2
All	All	5058/5708 (89%)	4002 (79%)	1056 (21%)	1	2

5 of 1056 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	N	808	THR
6	N	944	THR
6	N	805	GLU
7	O	38	THR
6	D	651	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	1100	GLN
6	N	166	GLN
6	N	762	GLN
6	D	462	GLN
6	D	189	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	16/16 (100%)	12 (75%)	8 (50%)
2	Y	15/16 (93%)	11 (73%)	7 (46%)
All	All	31/32 (96%)	23 (74%)	15 (48%)

5 of 23 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	2	A
2	H	3	G
2	H	6	U
2	H	7	G
2	H	8	C

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	15	C
2	Y	13	C
2	Y	6	U
2	Y	15	C
2	Y	9	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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	G	23/23 (100%)	-0.38	0 100 100	16, 38, 58, 69	0
1	X	23/23 (100%)	-0.45	0 100 100	18, 41, 74, 89	0
2	H	16/16 (100%)	-0.74	0 100 100	35, 64, 80, 84	0
2	Y	16/16 (100%)	-0.84	0 100 100	31, 54, 90, 95	0
3	I	13/14 (92%)	-0.56	0 100 100	32, 42, 61, 78	0
3	Z	13/14 (92%)	-0.54	0 100 100	37, 49, 76, 84	0
4	A	229/315 (72%)	0.09	4 (1%) 70 72	45, 74, 94, 101	0
4	B	229/315 (72%)	0.08	10 (4%) 34 37	57, 79, 94, 104	0
4	K	229/315 (72%)	0.09	7 (3%) 49 52	56, 76, 91, 97	0
4	L	229/315 (72%)	0.21	14 (6%) 21 22	48, 82, 94, 101	0
5	C	1119/1119 (100%)	0.08	46 (4%) 37 40	19, 68, 98, 119	0
5	M	1119/1119 (100%)	0.06	28 (2%) 57 61	32, 68, 96, 108	0
6	D	1303/1524 (85%)	0.07	38 (2%) 51 55	34, 68, 94, 110	0
6	N	1303/1524 (85%)	0.06	34 (2%) 56 59	35, 69, 95, 108	0
7	E	95/99 (95%)	-0.00	3 (3%) 47 51	50, 70, 90, 96	0
7	O	95/99 (95%)	0.22	5 (5%) 26 28	41, 72, 98, 102	0
All	All	6054/6850 (88%)	0.07	189 (3%) 49 52	16, 70, 95, 119	0

The worst 5 of 189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	135	LEU	7.9
6	N	1408	ILE	7.5
5	M	779	GLY	7.3
5	C	221	LEU	6.9
6	D	452	ILE	6.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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. 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	B-factors(Å^2)	Q<0.9
8	ZN	D	4058	1/1	0.96	0.10	82,82,82,82	0
8	ZN	N	5058	1/1	0.96	0.17	71,71,71,71	0
9	MG	N	8002	1/1	0.98	0.08	25,25,25,25	0
8	ZN	N	7112	1/1	0.99	0.14	73,73,73,73	0
9	MG	D	8001	1/1	0.99	0.11	27,27,27,27	0
8	ZN	D	6112	1/1	0.99	0.14	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.