wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:30 AM GMT

PDB ID	:	3EQL
Title	:	Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic myxopyronin
Authors	:	Vassylyev, D.G.; Vassylyeva, M.N.; Artsimovitch, I.
Deposited on	:	2008-09-30
Resolution	:	2.70 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:

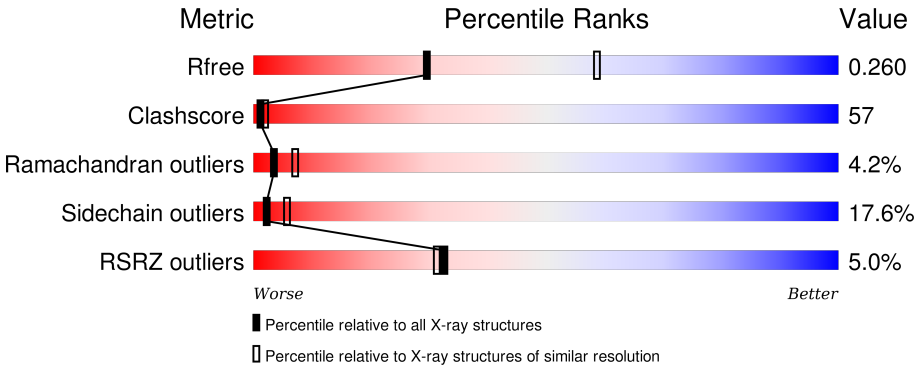
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	A	315	2% 18% 44% 10% 27%
1	B	315	6% 19% 44% 9% 27%
1	K	315	2% 20% 42% 10% 27%
1	L	315	5% 17% 46% 9% 27%
2	C	1119	5% 25% 58% 16%

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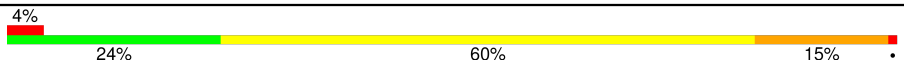
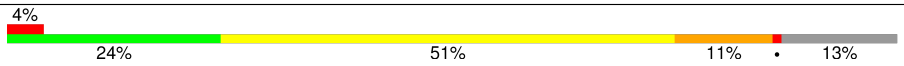
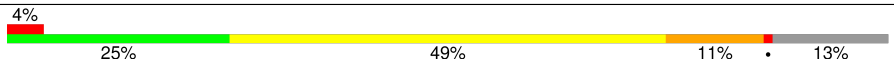
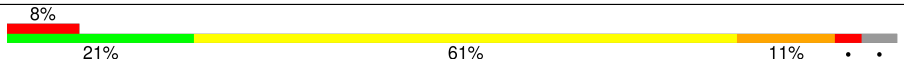
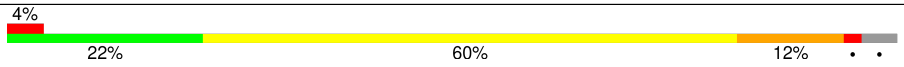
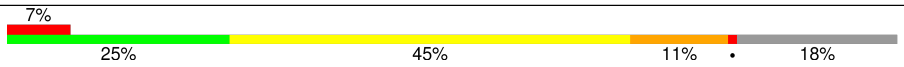
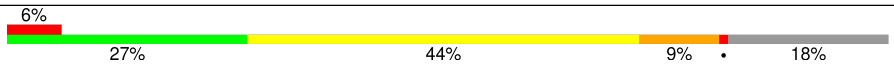
Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 57340 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 protein called DNA-directed RNA polymerase subunit alpha.

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

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

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

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			
3	N	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			

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

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

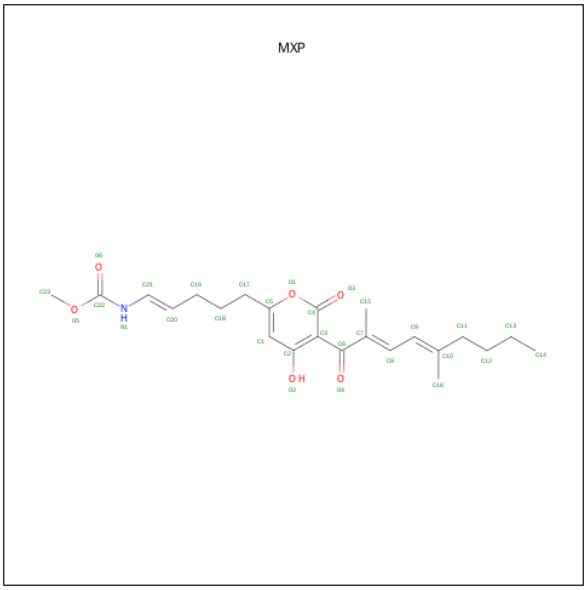
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is MYXOPYRONIN B (three-letter code: MXP) (formula: $C_{23}H_{31}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			30	23	1	6		
7	N	1	Total	C	N	O	0	0
			30	23	1	6		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0

- Molecule 9 is water.

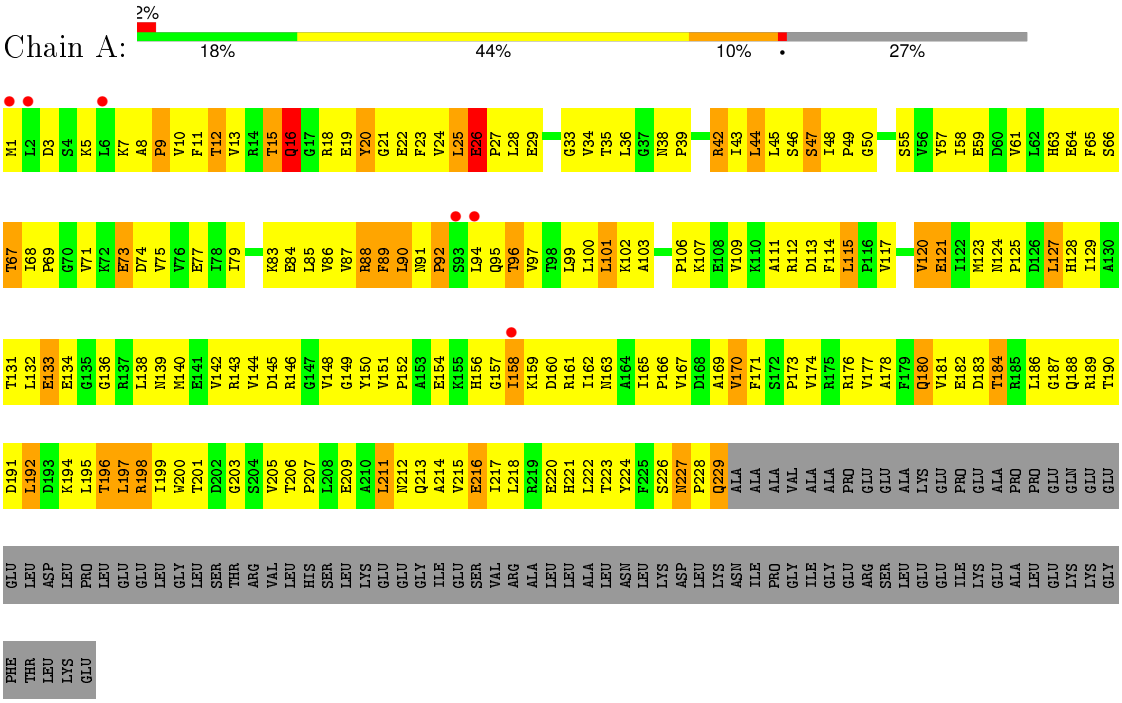
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	141	Total O 141 141	0	0
9	B	149	Total O 149 149	0	0
9	C	704	Total O 704 704	0	0
9	D	927	Total O 927 927	0	0
9	E	82	Total O 82 82	0	0
9	F	305	Total O 305 305	0	0
9	K	152	Total O 152 152	0	0
9	L	148	Total O 148 148	0	0
9	M	680	Total O 680 680	0	0
9	N	864	Total O 864 864	0	0
9	O	84	Total O 84 84	0	0
9	P	260	Total O 260 260	0	0

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.

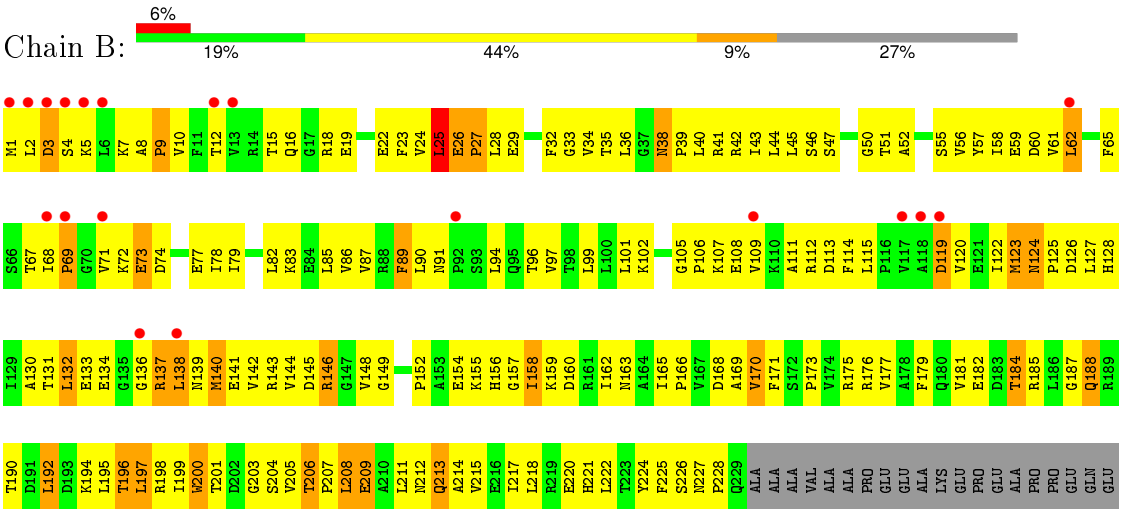
- Molecule 1: DNA-directed RNA polymerase subunit alpha

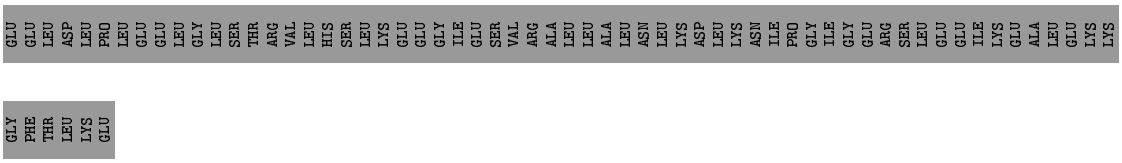
Chain A:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

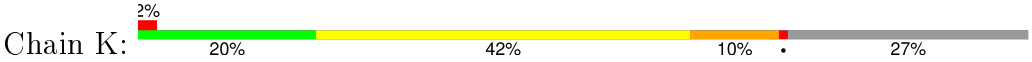
Chain B:

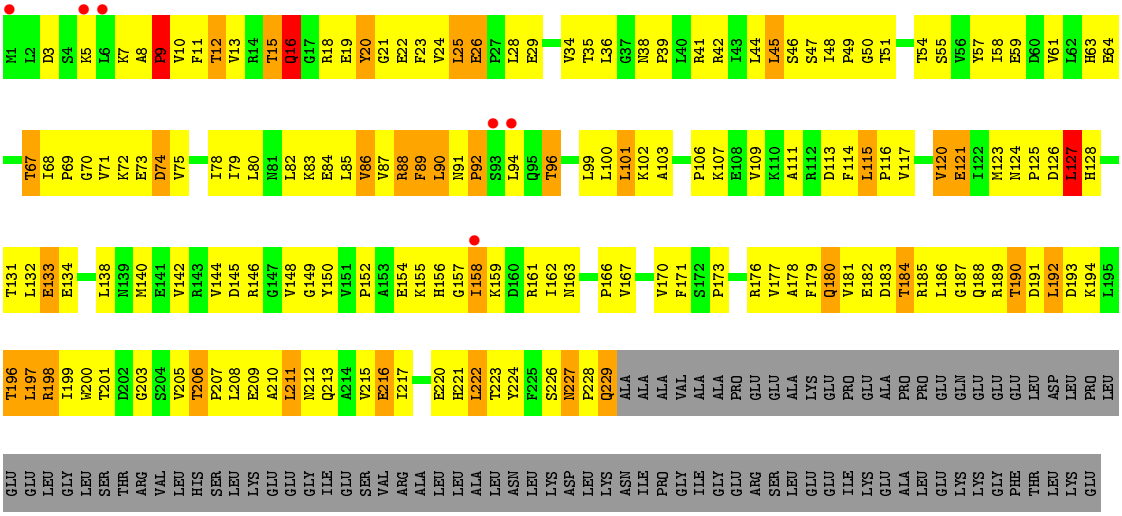




• Molecule 1: DNA-directed RNA polymerase subunit alpha

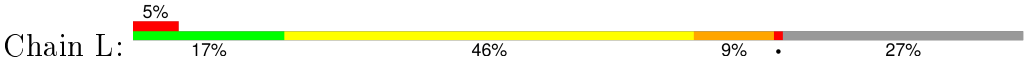
Chain K:

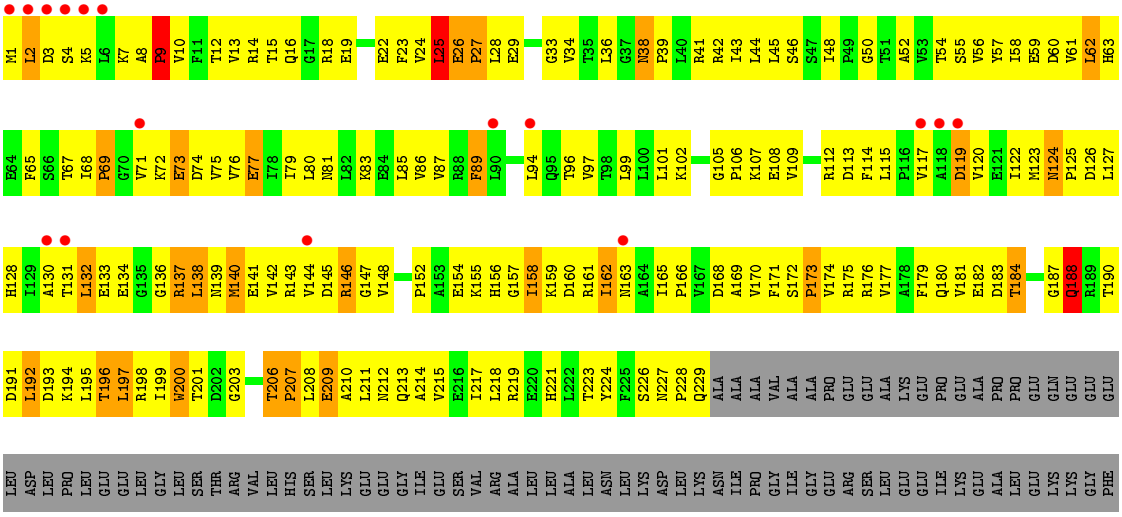




• Molecule 1: DNA-directed RNA polymerase subunit alpha

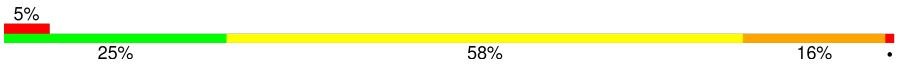
Chain L:

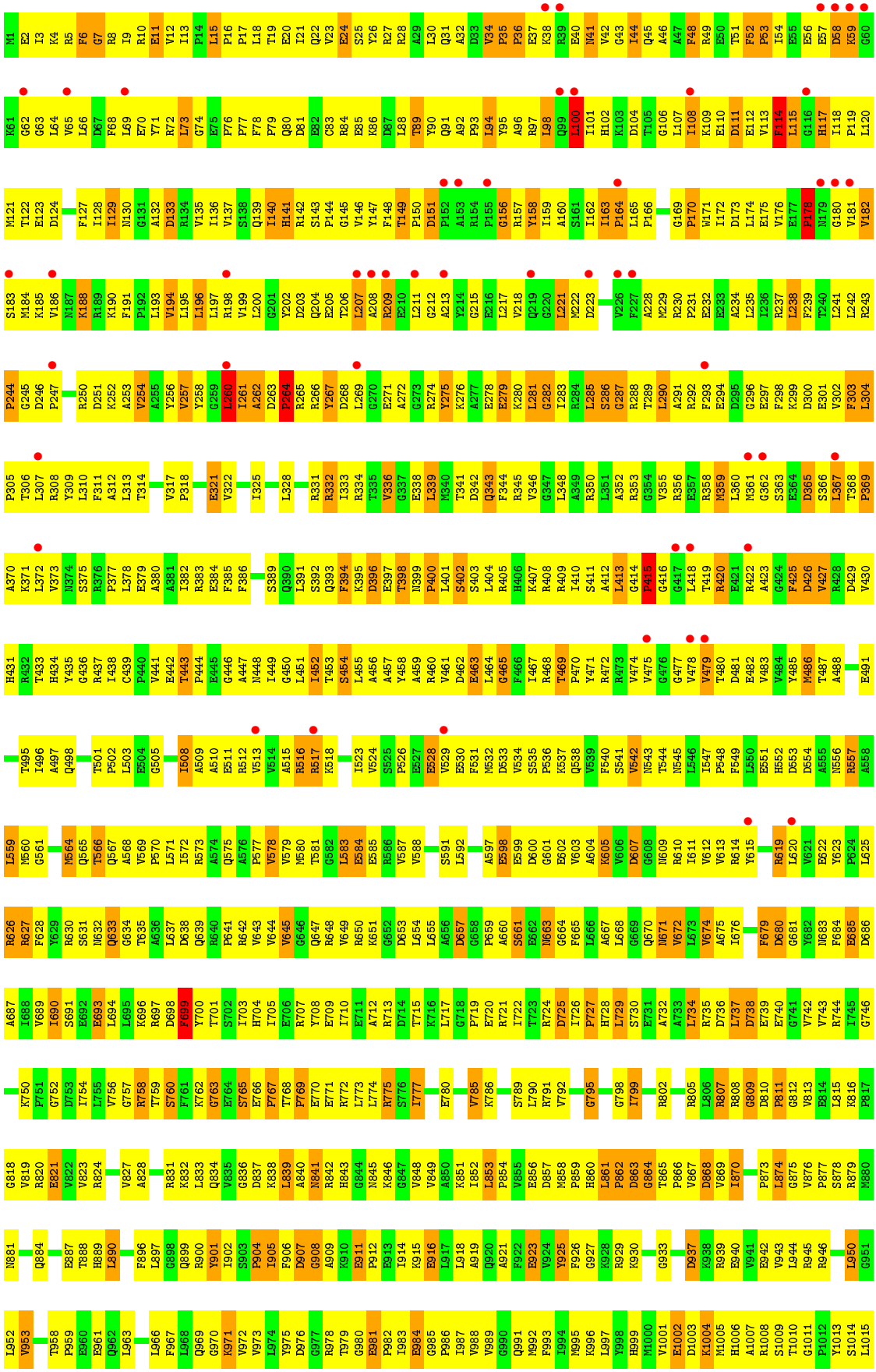


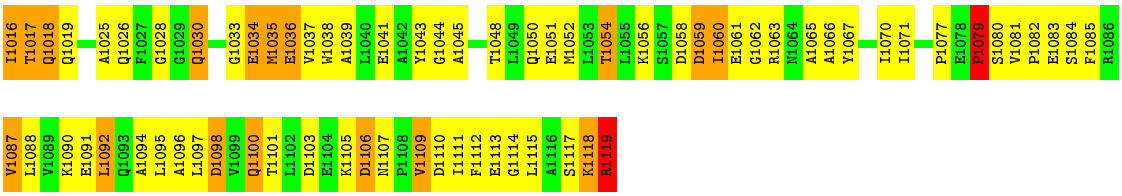


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

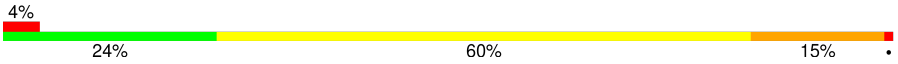


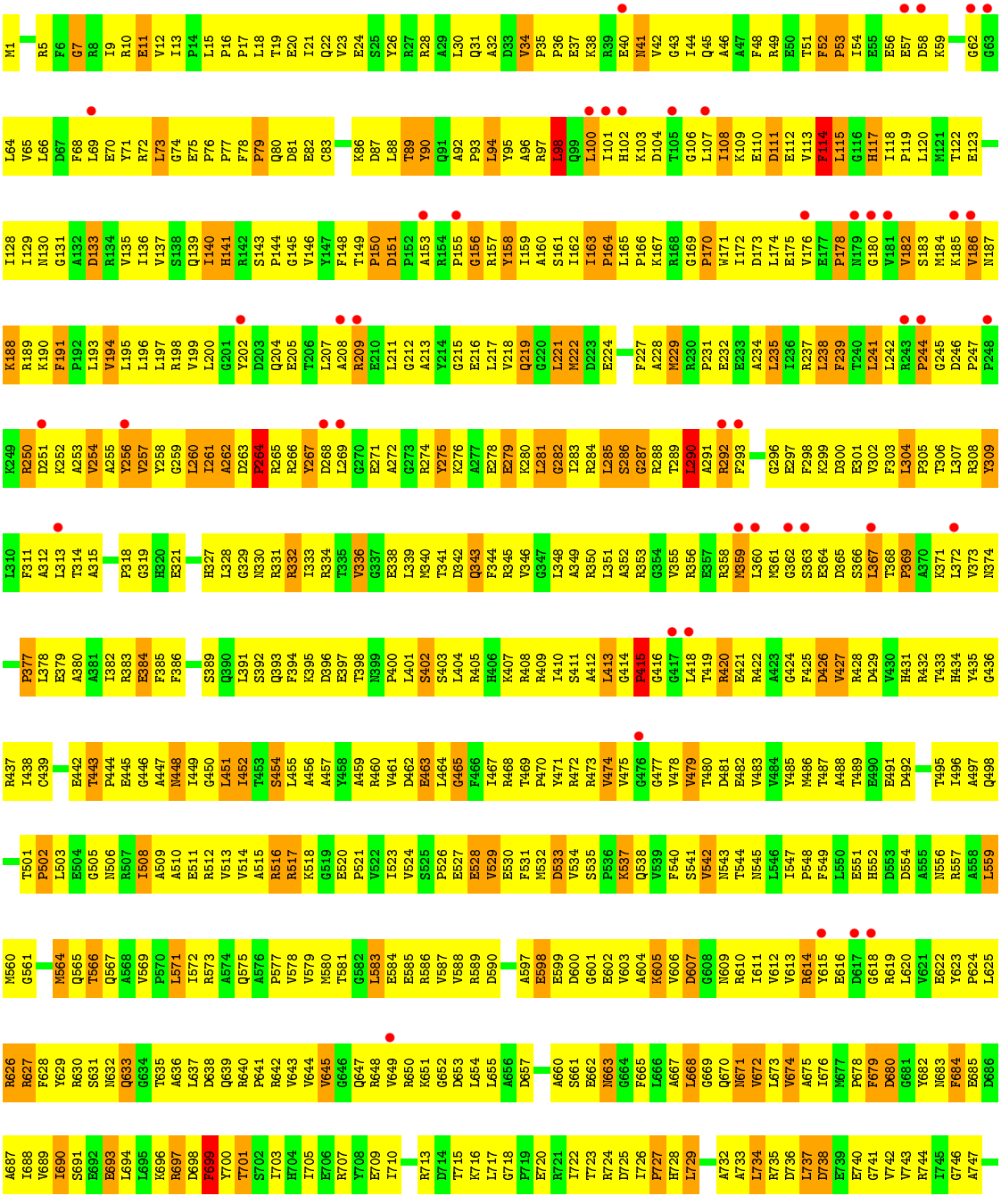


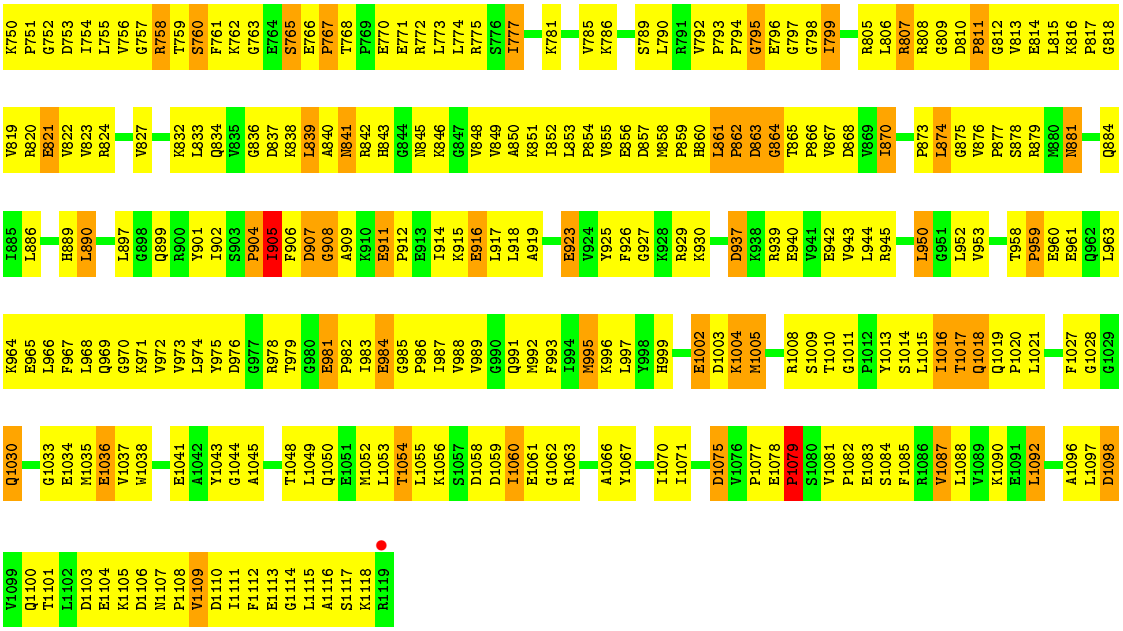


• Molecule 2: DNA-directed RNA polymerase subunit beta

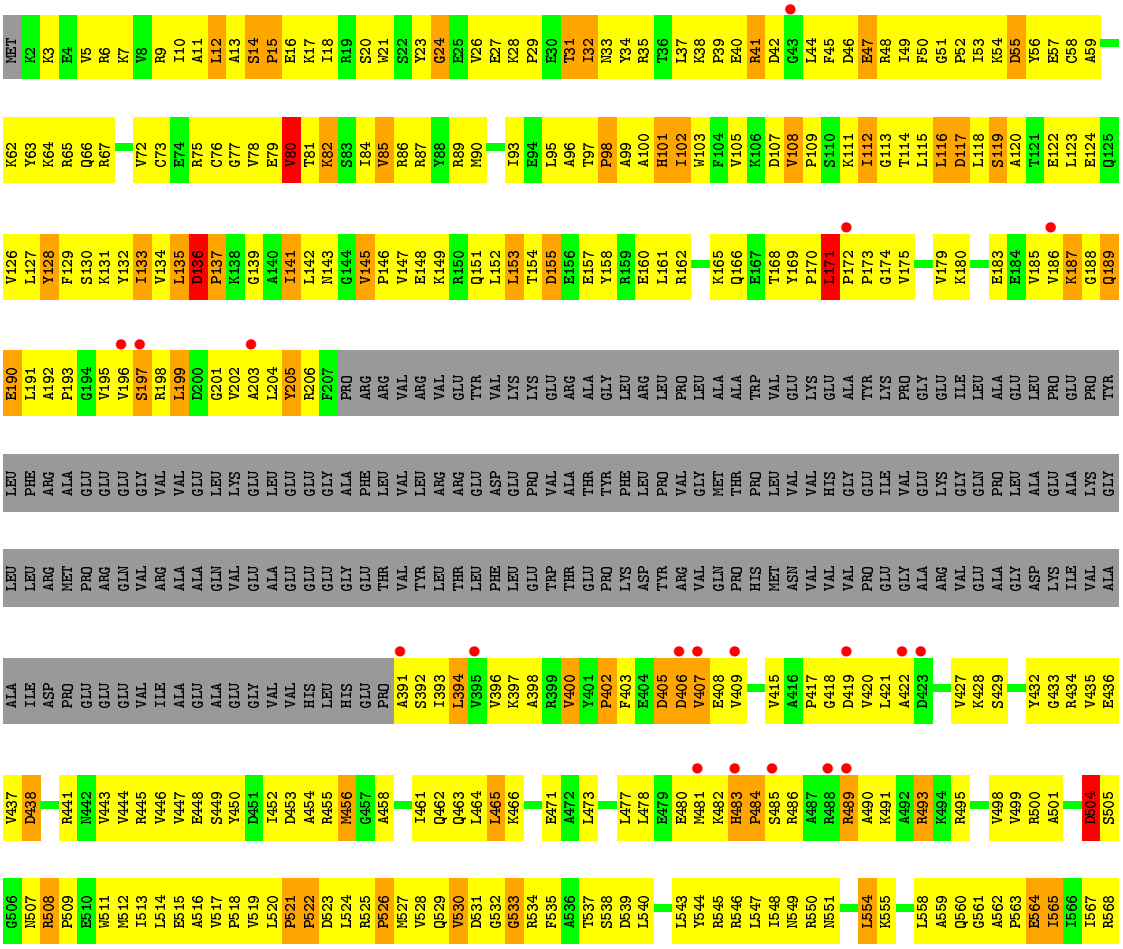
Chain M:

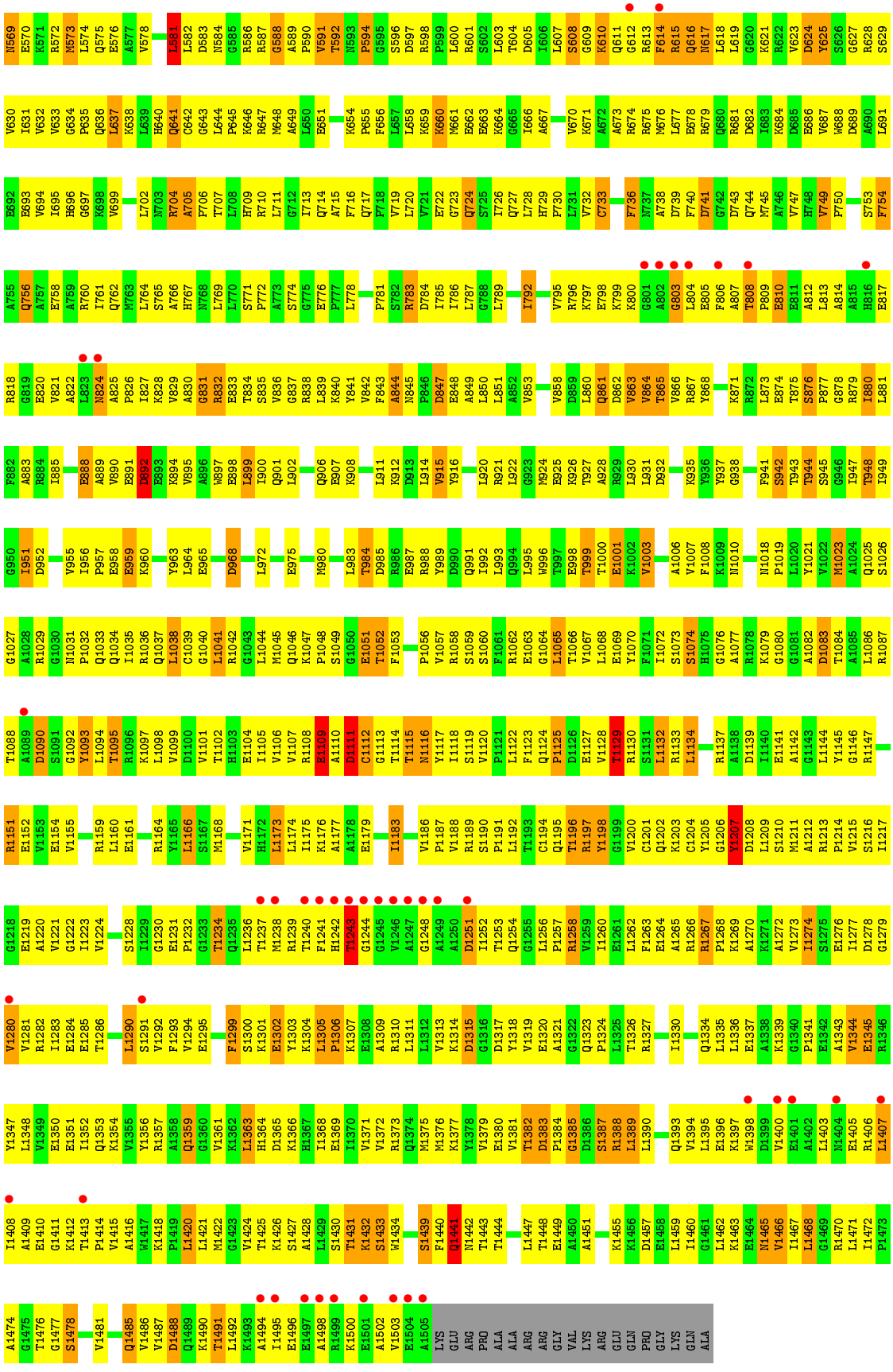






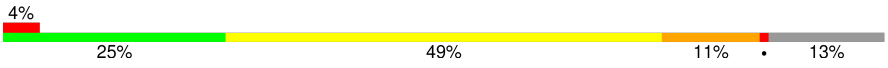
• Molecule 3: DNA-directed RNA polymerase subunit beta'





• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain N: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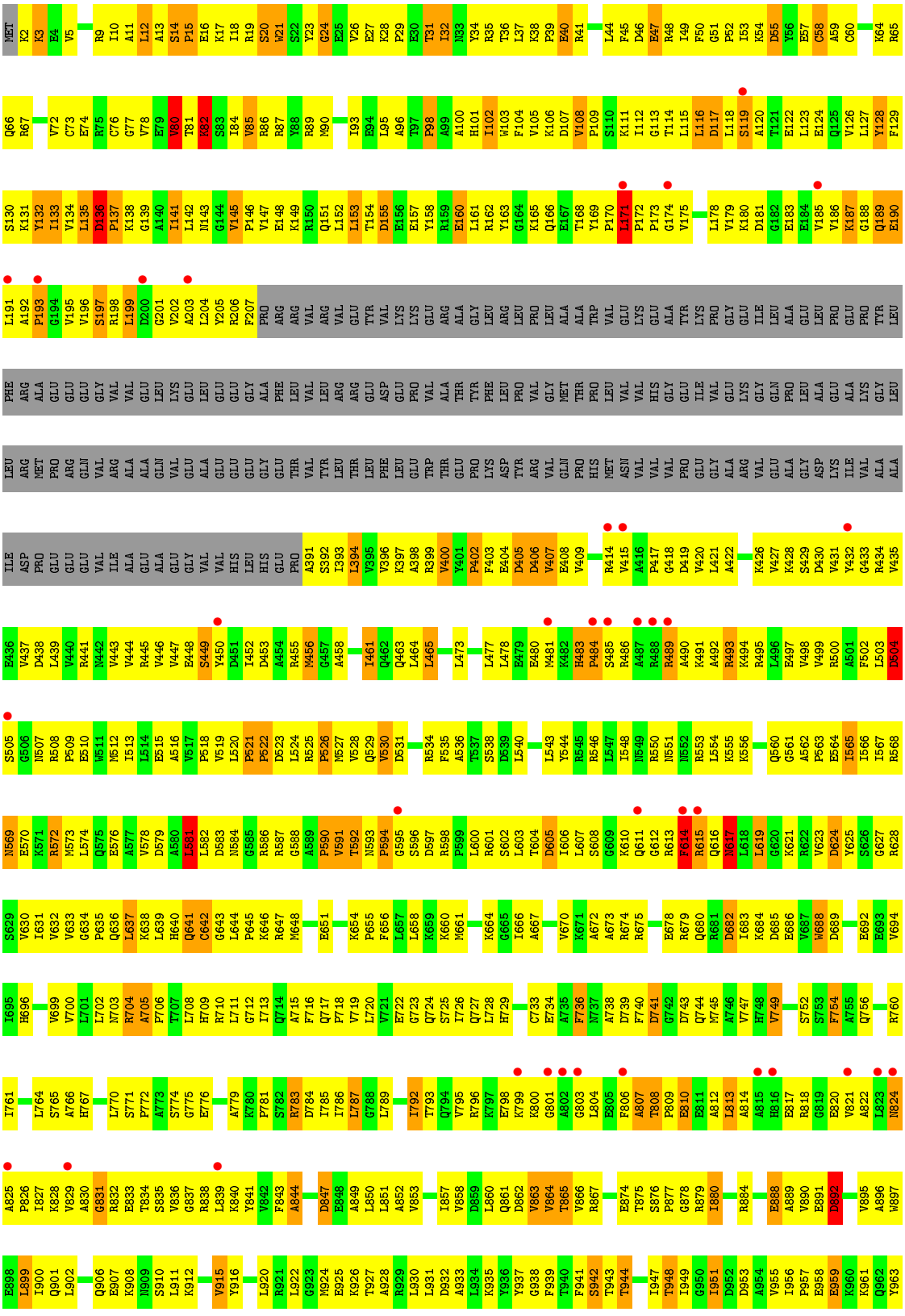
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Q66 R67 V72 C73 E74 R75 C76 G77 V78 E79 V80 T81 K82 S83 I84 V85 R86 R87 Y88 R89 M90 I93 E94 L95 A96 T97 P98 A99 A100 H101 I102 W103 F104 V105 K106 D107 V108 P109 S110 K111 I112 G113 T114 L115 L116 D117 L118 S119 A120 T121 E122 L123 E124 Q125 V126 L127 Y128 F129
S130 K131 Y132 I133 V134 L135 D136 P137 K138 G139 A140 I141 L142 N143 G144 V145 P146 V147 E148 K149 R150 Q151 L152 L153 T154 D155 E156 E157 Y158 R159 E160 L161 R162 Y163 G164 K165 Q166 E167 T168 Y169 P170 I171 P172 P173 G174 V175 L178 V179 K180 D181 G182 E183 E184 V185 V186 K187 G188 Q189 E190
L191 A192 P193 G194 V195 V196 S197 R198 L199 D200 G201 V202 A203 L204 Y205 R206 F207 PRO ARG ARG VAL ARG VAL GLU TYR VAL LYS LYS GLU ARG ALA GLY LEU ARG LEU PRO LEU ARG ALA ALA TRP VAL GLU LYS GLU ALA TYR LYS PRO GLY GLU ILE LEU ALA GLU LEU PRO GLU PRO TYR LEU
PHE ARG ALA GLU GLU GLU GLY VAL VAL GLU LEU LYS GLU LEU GLU GLU GLU GLY ALA PHE LEU VAL LEU ARG ARG ARG GLU ASP GLU PRO VAL ALA THR TYR PHE LEU PRO VAL GLY MET THR PRO LEU VAL VAL HIS GLY GLU ILE VAL GLU LYS GLY GLN PRO LEU ALA GLU GLY LYS GLY LEU
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S505 G506 N507 R508 P509 E510 W511 M512 I513 L514 E515 A516 V517 P518 V519 L520 P521 P522 D523 L524 R525 P526 M527 V528 Q529 V530 D531 R534 P535 A536 T537 S538 D539 L540 L543 Y544 R545 R546 L547 T548 N549 R550 N551 N552 R553 L554 K555 K556 Q560 G561 A562 P563 E564 I565 I566 I567 R568
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I695 H696 V699 V700 L701 L702 N703 R704 A705 P706 T707 L708 H709 R710 L711 G712 I713 Q714 A715 F716 Q717 P718 V719 L720 V721 E722 G723 Q724 S725 I726 Q727 L728 H729 C733 E734 A735 F736 N737 A738 D739 F740 D741 G742 D743 Q744 M745 A746 V747 H748 V749 S752 S753 F754 A755 Q756 R760
I761 L764 S765 A766 H767 A773 S774 G775 E776 A779 K780 P781 S782 R783 D784 I785 I786 L787 G788 L789 I792 T793 Q794 V795 R796 K797 E798 K799 K800 G801 A802 G803 L804 E805 F806 A807 T808 P809 E810 E811 A812 L813 A814 A815 E816 E817 R818 G819 E820 V821 A822 L823 N824
A825 P826 I827 K828 V829 A830 G831 R832 E833 T834 S835 V836 G837 R838 L839 K840 Y841 V842 F843 A844 D847 E848 A849 L850 L851 A852 V853 I857 V858 D859 L860 Q861 D862 V863 V864 T865 V866 R867 E874 T875 S876 P877 G878 R879 I880 R884 E888 A889 V890 E891 D892 V895 A896 W897
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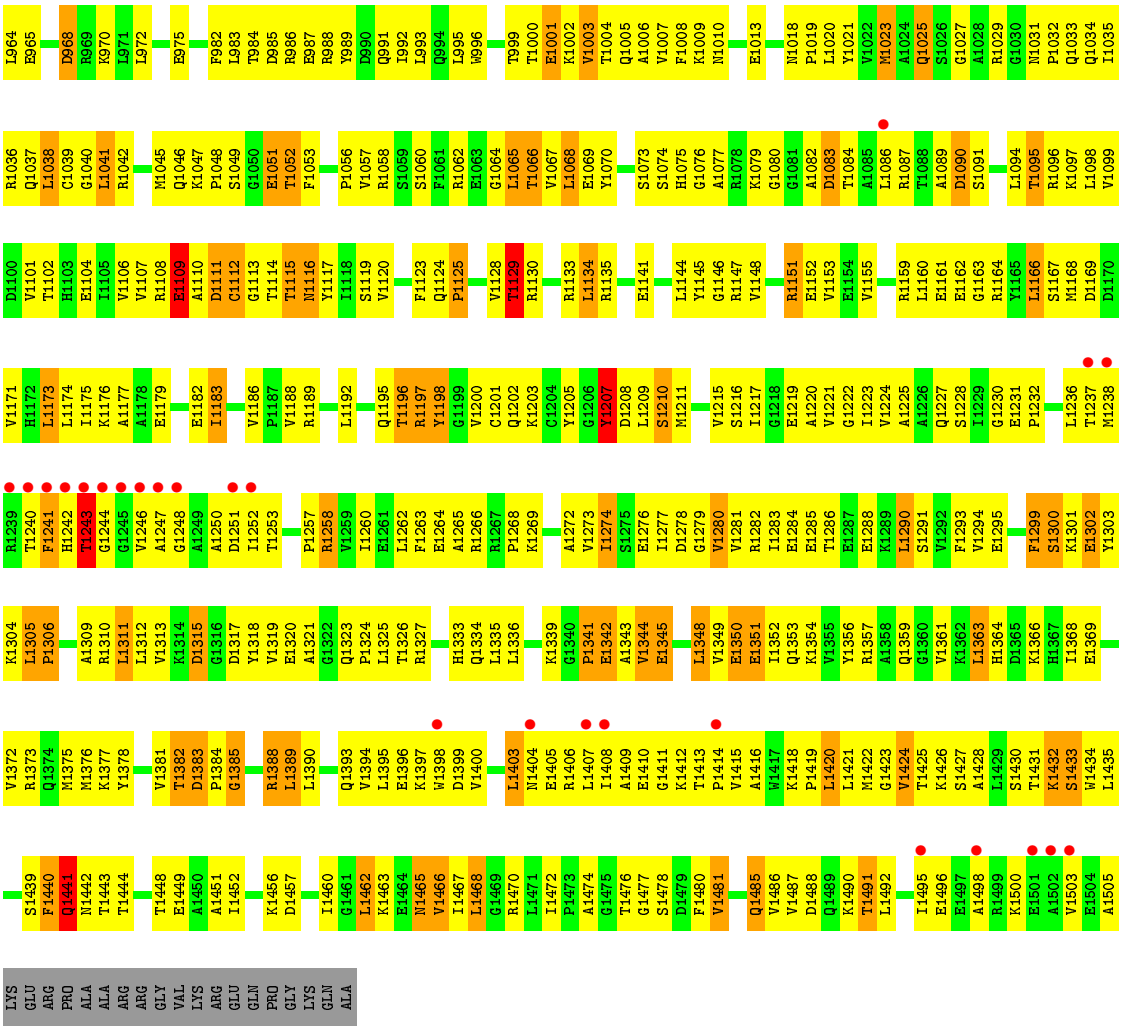
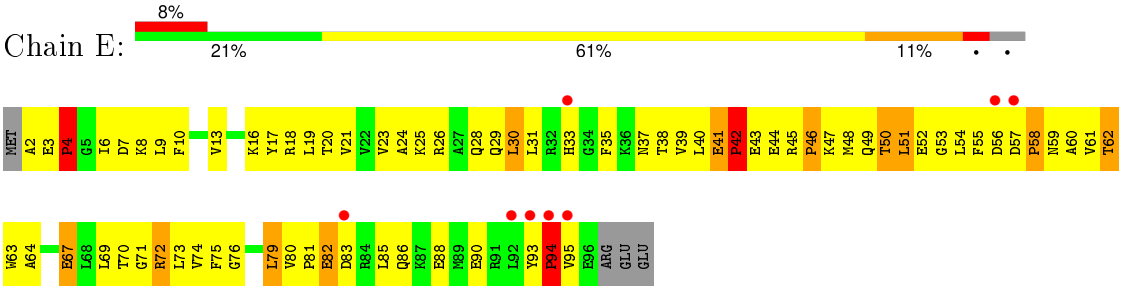
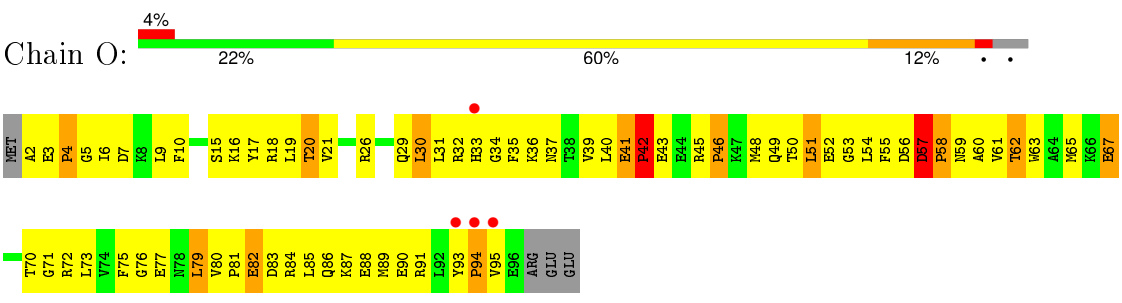


• Molecule 4: DNA-directed RNA polymerase subunit omega

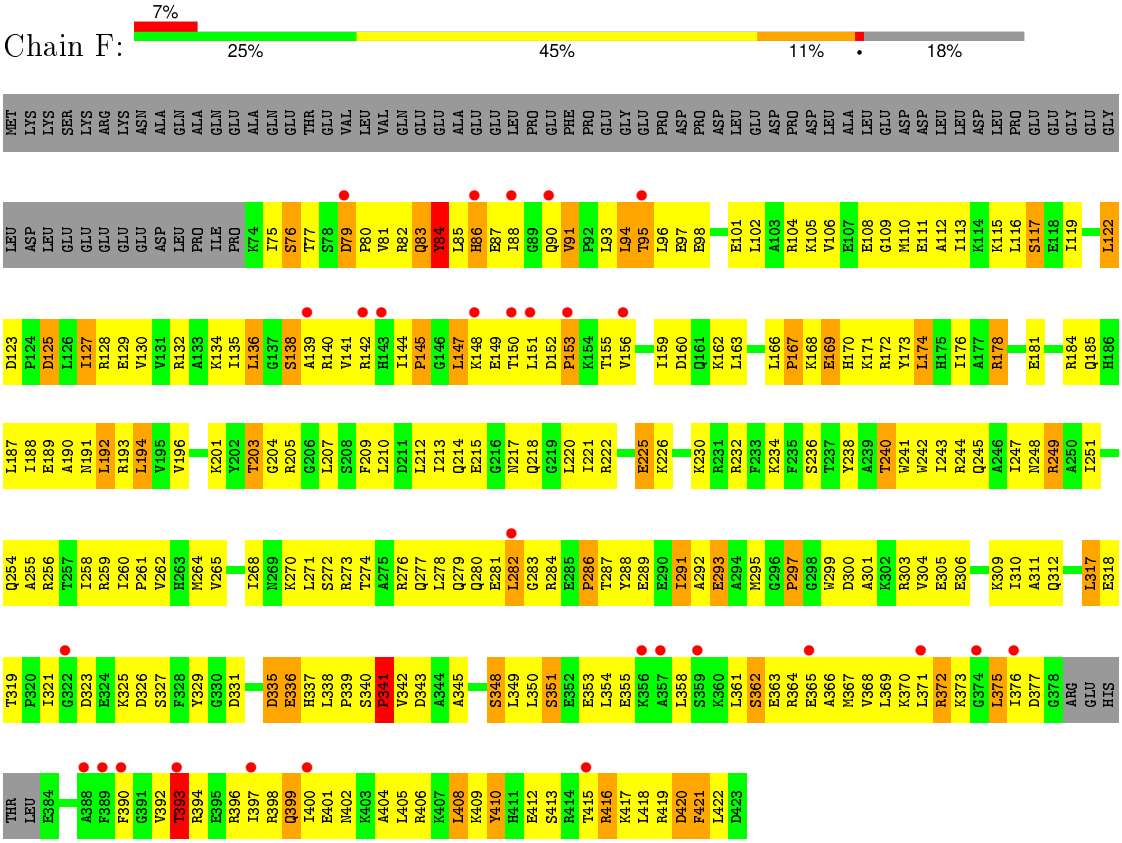


• Molecule 4: DNA-directed RNA polymerase subunit omega



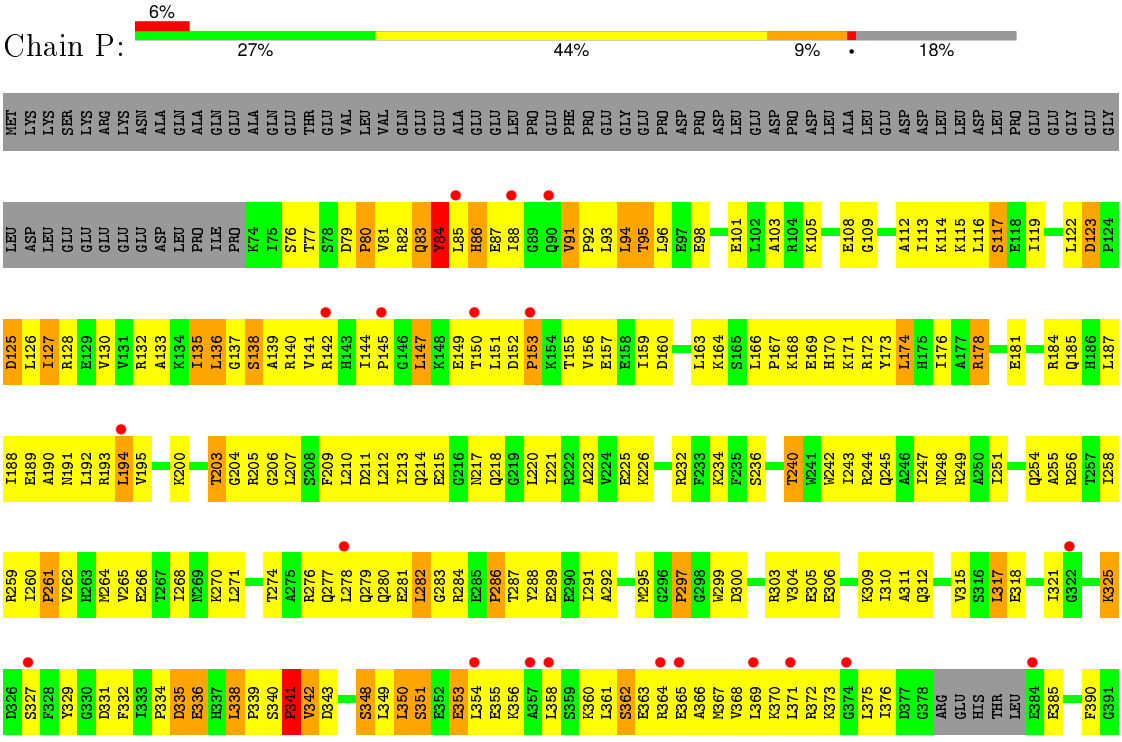
• Molecule 5: RNA polymerase sigma factor rpoD

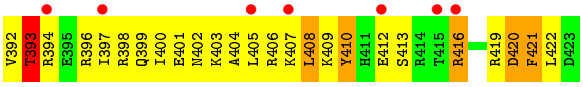
Chain F:



• Molecule 5: RNA polymerase sigma factor rpoD

Chain P:




V392
T393
R394
E395
R396
T397
R398
Q399
I400
E401
N402
K403
A404
L405
R406
K407
L408
K409
Y410
H411
E412
S413
R414
T415
R416
R419
D420
F421
L422
D423

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	235.00Å 235.00Å 254.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-2.70) 90.5 (39.96-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.270 0.237 , 0.260	Depositor DCC
R_{free} test set	18510 reflections (4.74%)	DCC
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 104.4	EDS
Estimated twinning fraction	0.166 for -h,-k,l 0.048 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 390896 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	57340	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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

5.1 Standard geometry

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

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	A	0.84	2/1838 (0.1%)	1.04	9/2498 (0.4%)
1	B	0.74	1/1838 (0.1%)	0.95	9/2498 (0.4%)
1	K	0.81	2/1838 (0.1%)	1.00	8/2498 (0.3%)
1	L	0.75	1/1838 (0.1%)	0.96	10/2498 (0.4%)
2	C	0.73	0/8997	0.94	14/12164 (0.1%)
2	M	0.73	0/8997	0.94	14/12164 (0.1%)
3	D	0.75	2/10582 (0.0%)	0.97	15/14294 (0.1%)
3	N	0.75	1/10582 (0.0%)	0.97	18/14294 (0.1%)
4	E	0.73	0/784	1.23	5/1057 (0.5%)
4	O	0.71	0/784	1.08	3/1057 (0.3%)
5	F	0.65	0/2812	0.85	3/3781 (0.1%)
5	P	0.65	0/2812	0.86	2/3781 (0.1%)
All	All	0.74	9/53702 (0.0%)	0.96	110/72584 (0.2%)

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
3	N	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	C-O	-11.04	1.02	1.23
1	K	26	GLU	C-O	-10.57	1.03	1.23
1	B	26	GLU	C-O	-10.23	1.03	1.23
1	L	26	GLU	C-O	-9.82	1.04	1.23
1	A	16	GLN	CB-CG	5.82	1.68	1.52

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	94	PRO	CA-N-CD	-18.30	85.89	111.50
1	B	138	LEU	CA-CB-CG	12.41	143.84	115.30
1	L	138	LEU	CA-CB-CG	12.19	143.33	115.30
4	O	94	PRO	CA-N-CD	-9.89	97.65	111.50
1	K	26	GLU	CA-C-N	9.51	143.72	117.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	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	A	1806	0	1861	184	0
1	B	1806	0	1861	197	0
1	K	1806	0	1861	212	0
1	L	1806	0	1861	198	0
2	C	8829	0	8933	1145	0
2	M	8829	0	8933	1073	0
3	D	10407	0	10633	1296	0
3	N	10407	0	10633	1283	0
4	E	770	0	784	121	0
4	O	770	0	784	113	0
5	F	2771	0	2844	316	0
5	P	2771	0	2844	312	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	30	0	31	18	0
7	N	30	0	31	18	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
9	A	141	0	0	28	0
9	B	149	0	0	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	704	0	0	215	0
9	D	927	0	0	239	0
9	E	82	0	0	29	0
9	F	305	0	0	77	0
9	K	152	0	0	41	0
9	L	148	0	0	34	0
9	M	680	0	0	180	0
9	N	864	0	0	235	0
9	O	84	0	0	26	0
9	P	260	0	0	71	0
All	All	57340	0	53894	6054	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 57.

The worst 5 of 6054 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)
3:D:610:LYS:HD3	7:D:1527:MXP:C15	1.49	1.41
3:N:610:LYS:HD3	7:N:1527:MXP:C15	1.55	1.37
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.27	1.15
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.27	1.13
3:D:610:LYS:HD3	7:D:1527:MXP:H15B	1.19	1.10

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
1	A	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	15 37
1	B	227/315 (72%)	195 (86%)	29 (13%)	3 (1%)	15 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	227/315 (72%)	201 (88%)	22 (10%)	4 (2%)	11 27
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	15 37
2	C	1117/1119 (100%)	905 (81%)	154 (14%)	58 (5%)	2 4
2	M	1117/1119 (100%)	904 (81%)	153 (14%)	60 (5%)	2 4
3	D	1317/1524 (86%)	1098 (83%)	170 (13%)	49 (4%)	4 9
3	N	1317/1524 (86%)	1089 (83%)	176 (13%)	52 (4%)	4 8
4	E	93/99 (94%)	77 (83%)	12 (13%)	4 (4%)	3 7
4	O	93/99 (94%)	77 (83%)	10 (11%)	6 (6%)	1 2
5	F	341/423 (81%)	285 (84%)	37 (11%)	19 (6%)	2 3
5	P	341/423 (81%)	287 (84%)	36 (11%)	18 (5%)	2 4
All	All	6644/7590 (88%)	5517 (83%)	848 (13%)	279 (4%)	3 7

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
2	C	7	GLY
2	C	178	PRO
2	C	231	PRO

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 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
1	A	202/273 (74%)	161 (80%)	41 (20%)	1 4
1	B	202/273 (74%)	163 (81%)	39 (19%)	2 4
1	K	202/273 (74%)	159 (79%)	43 (21%)	1 3
1	L	202/273 (74%)	166 (82%)	36 (18%)	2 5
2	C	941/941 (100%)	755 (80%)	186 (20%)	1 4
2	M	941/941 (100%)	757 (80%)	184 (20%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	1112/1279 (87%)	935 (84%)	177 (16%)	3 8
3	N	1112/1279 (87%)	934 (84%)	178 (16%)	3 8
4	E	84/88 (96%)	68 (81%)	16 (19%)	2 5
4	O	84/88 (96%)	68 (81%)	16 (19%)	2 5
5	F	295/370 (80%)	252 (85%)	43 (15%)	4 9
5	P	295/370 (80%)	254 (86%)	41 (14%)	4 10
All	All	5672/6448 (88%)	4672 (82%)	1000 (18%)	2 6

5 of 1000 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	57	ASP
1	L	112	ARG
3	N	1415	VAL
5	F	117	SER
1	K	20	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	86	HIS
1	L	128	HIS
3	N	1465	ASN
5	F	312	GLN
1	K	139	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	MXP	D	1527	-	26,30,30	2.82	11 (42%)	27,38,38	2.80	8 (29%)
7	MXP	N	1527	-	26,30,30	3.08	12 (46%)	27,38,38	3.01	11 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MXP	D	1527	-	-	0/25/28/28	0/1/1/1
7	MXP	N	1527	-	-	0/25/28/28	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1527	MXP	O5-C22	-5.06	1.27	1.34
7	D	1527	MXP	O5-C22	-4.22	1.28	1.34
7	D	1527	MXP	O5-C23	-2.92	1.38	1.45
7	N	1527	MXP	O5-C23	-2.54	1.39	1.45
7	N	1527	MXP	C21-N1	-2.07	1.34	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	1527	MXP	C9-C8-C7	-7.59	113.82	126.22
7	D	1527	MXP	C9-C8-C7	-6.82	115.06	126.22
7	D	1527	MXP	C8-C9-C10	-6.14	116.93	126.19
7	N	1527	MXP	C8-C9-C10	-5.95	117.22	126.19
7	N	1527	MXP	C19-C20-C21	-3.89	112.12	125.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1527	MXP	18	0
7	N	1527	MXP	18	0

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	A	229/315 (72%)	-0.08	6 (2%)	59	59	28, 50, 78, 101	0
1	B	229/315 (72%)	0.27	19 (8%)	14	11	36, 71, 86, 104	0
1	K	229/315 (72%)	-0.09	6 (2%)	59	59	25, 52, 81, 93	0
1	L	229/315 (72%)	0.30	16 (6%)	19	17	47, 73, 86, 104	0
2	C	1119/1119 (100%)	0.14	52 (4%)	36	35	14, 62, 88, 96	0
2	M	1119/1119 (100%)	0.10	46 (4%)	41	41	11, 60, 86, 101	0
3	D	1321/1524 (86%)	0.14	62 (4%)	35	34	10, 53, 85, 107	0
3	N	1321/1524 (86%)	0.12	61 (4%)	36	35	11, 54, 85, 109	0
4	E	95/99 (95%)	0.18	8 (8%)	14	11	30, 64, 90, 95	0
4	O	95/99 (95%)	0.07	4 (4%)	40	39	29, 61, 83, 100	0
5	F	345/423 (81%)	0.27	29 (8%)	14	11	27, 68, 89, 100	0
5	P	345/423 (81%)	0.29	27 (7%)	16	14	23, 68, 91, 103	0
All	All	6676/7590 (87%)	0.14	336 (5%)	32	31	10, 59, 87, 109	0

The worst 5 of 336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1241	PHE	9.5
3	N	1240	THR	8.2
3	N	1243	THR	7.5
3	D	1240	THR	7.3
1	B	6	LEU	6.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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
7	MXP	N	1527	30/30	0.95	0.20	0.04	17,30,38,40	0
7	MXP	D	1527	30/30	0.95	0.20	-0.04	13,20,27,34	0
6	ZN	D	1526	1/1	0.98	0.13	-0.47	48,48,48,48	0
6	ZN	N	1526	1/1	0.97	0.10	-1.06	66,66,66,66	0
6	ZN	N	1525	1/1	0.98	0.05	-2.12	58,58,58,58	0
6	ZN	D	1525	1/1	0.96	0.04	-2.55	62,62,62,62	0
8	MG	D	1528	1/1	0.97	0.06	-	35,35,35,35	0
8	MG	N	1528	1/1	0.95	0.11	-	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.