wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 09:06 PM EDT

PDB ID	:	5UAQ
Title	:	Escherichia coli RNA polymerase RpoB H526Y mutant
Authors	:	Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on	:	2016-12-19
Resolution	:	3.60 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 (1)) were used in the production of this report:

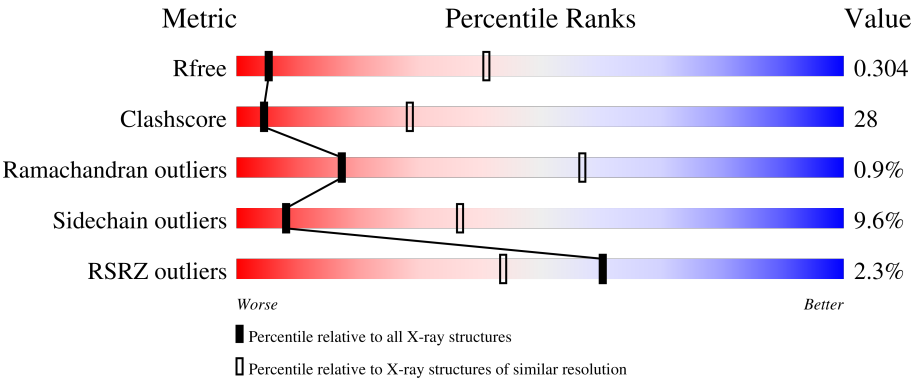
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	A	329	42% 42% 9% 6%
1	B	329	2% 29% 33% 34%
1	G	329	29% 31% 6% 32%
1	H	329	4% 27% 35% 34%
2	C	1342	2% 44% 47% 9%

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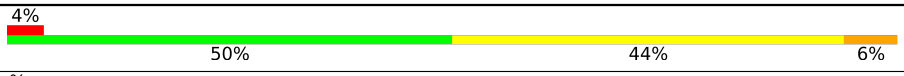
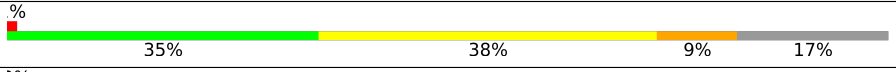
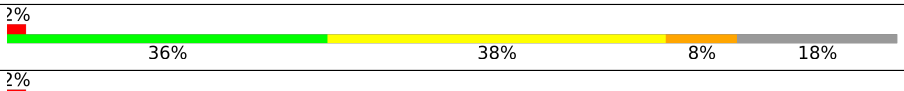
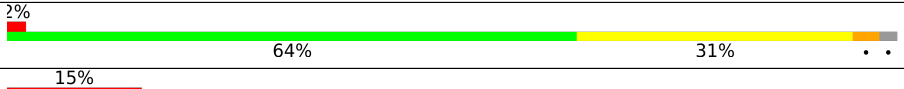
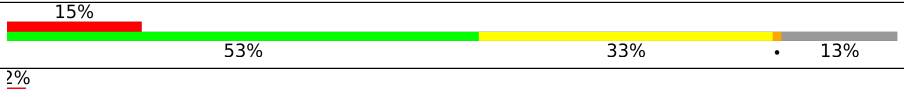
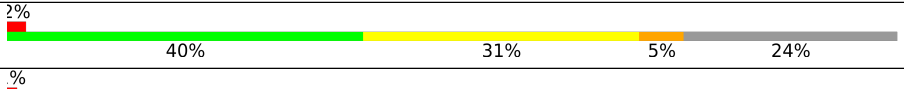
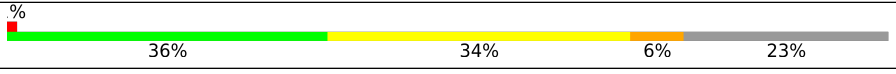
Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 55699 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	309	Total	C	N	O	S	0	0	0
			2403	1505	421	469	8			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1044	295	327	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10572	6634	1839	2056	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10568	6632	1838	2055	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	526	TYR	HIS	engineered mutation	UNP P0A8V2
I	526	TYR	HIS	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9029	5676	1620	1687	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	467	Total	C	N	O	S	0	0	0
			3806	2385	677	721	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

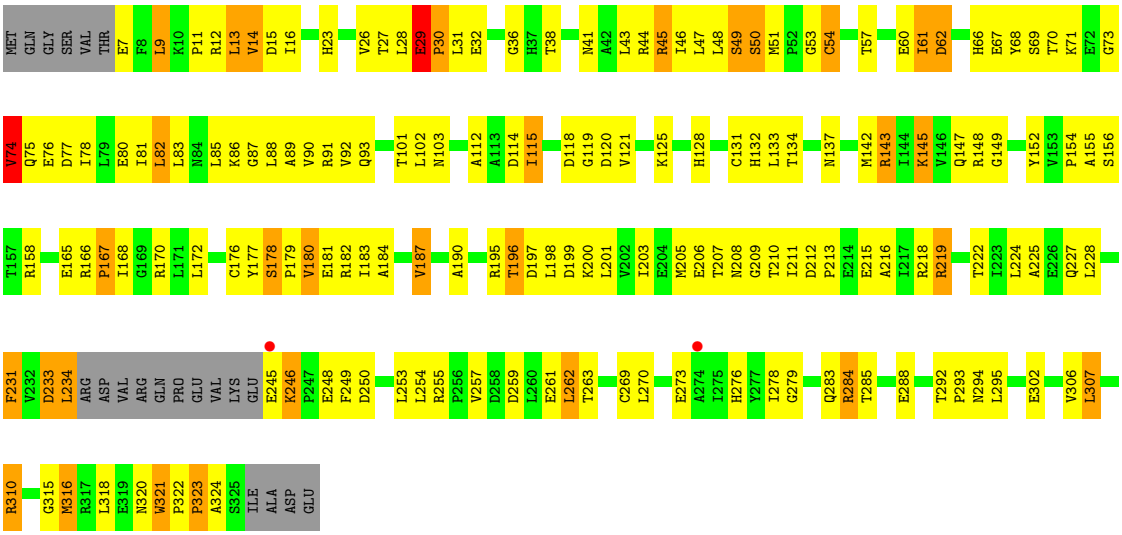
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	J	2	Total	Zn	0	0
			2	2		

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.

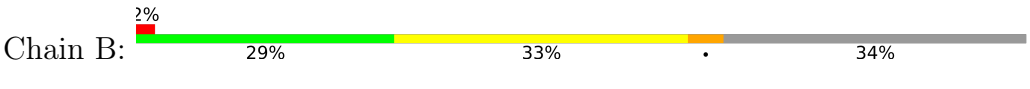
• Molecule 1: DNA-directed RNA polymerase subunit alpha

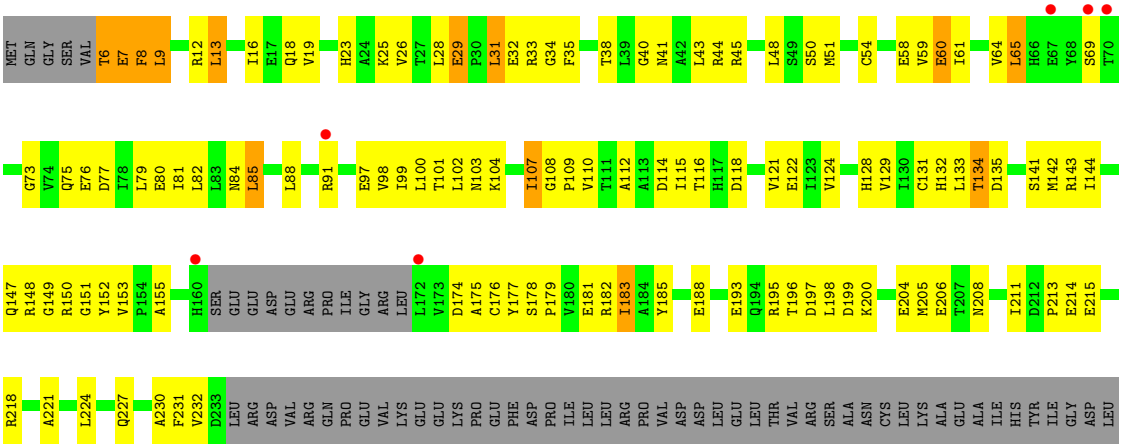
Chain A:

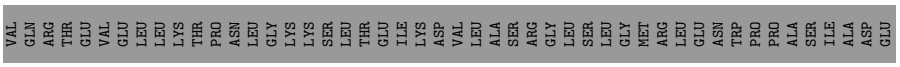


• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:

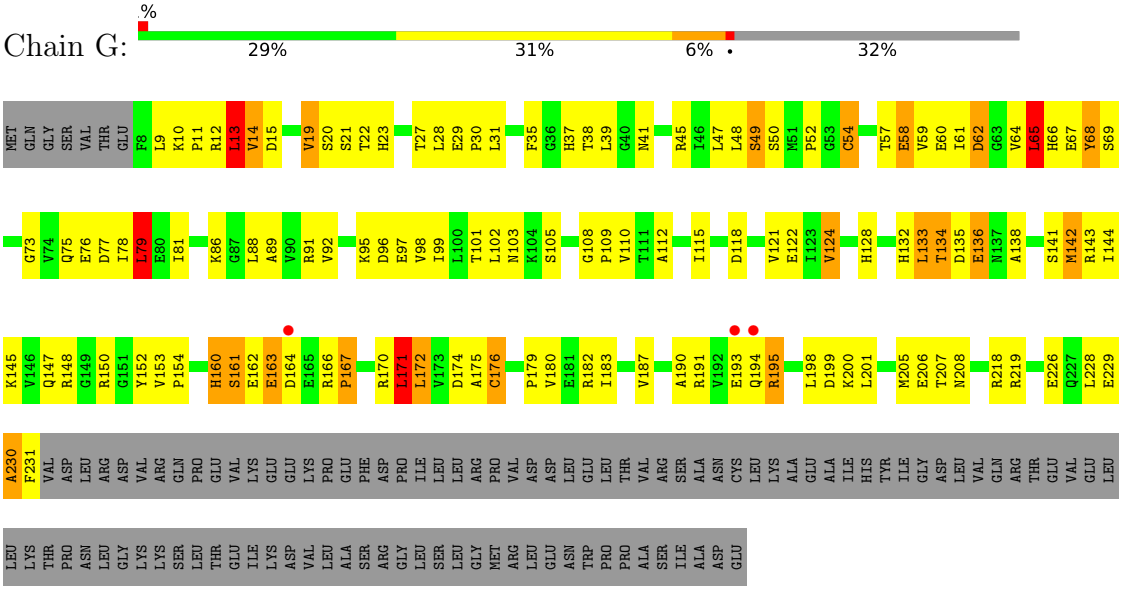






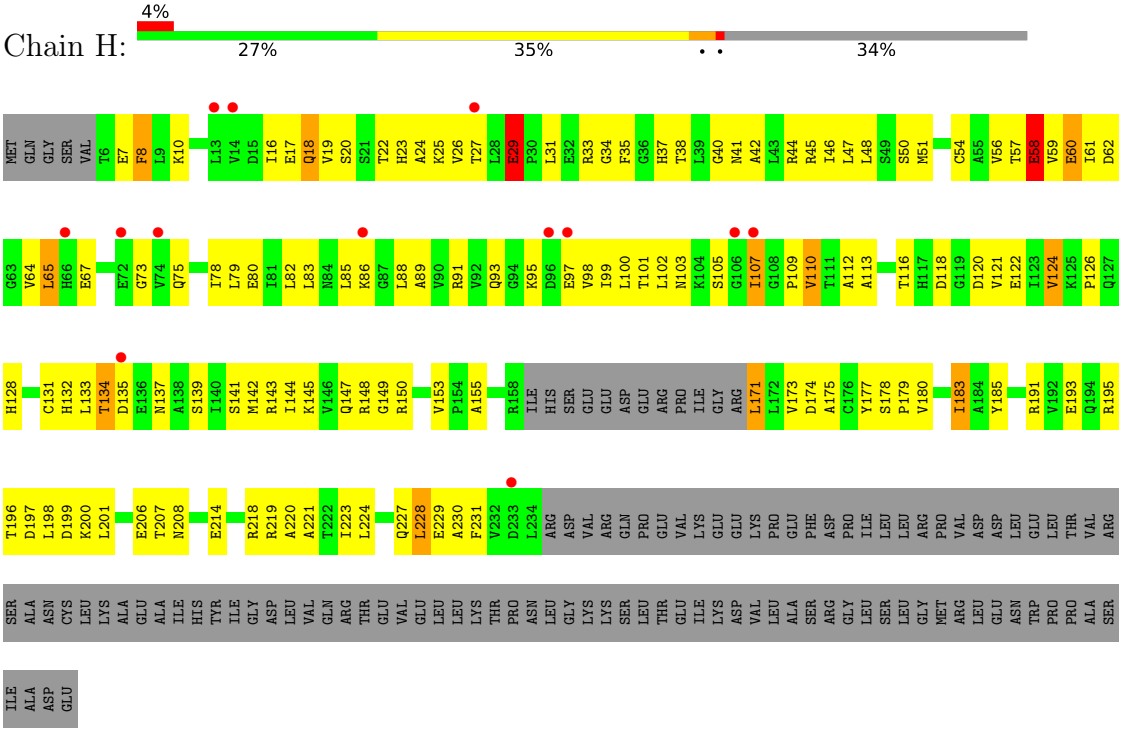
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



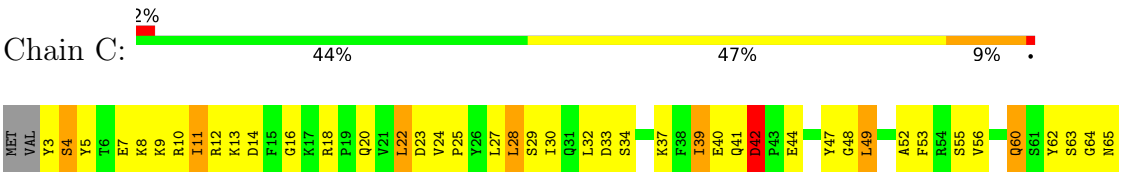
• Molecule 1: DNA-directed RNA polymerase subunit alpha

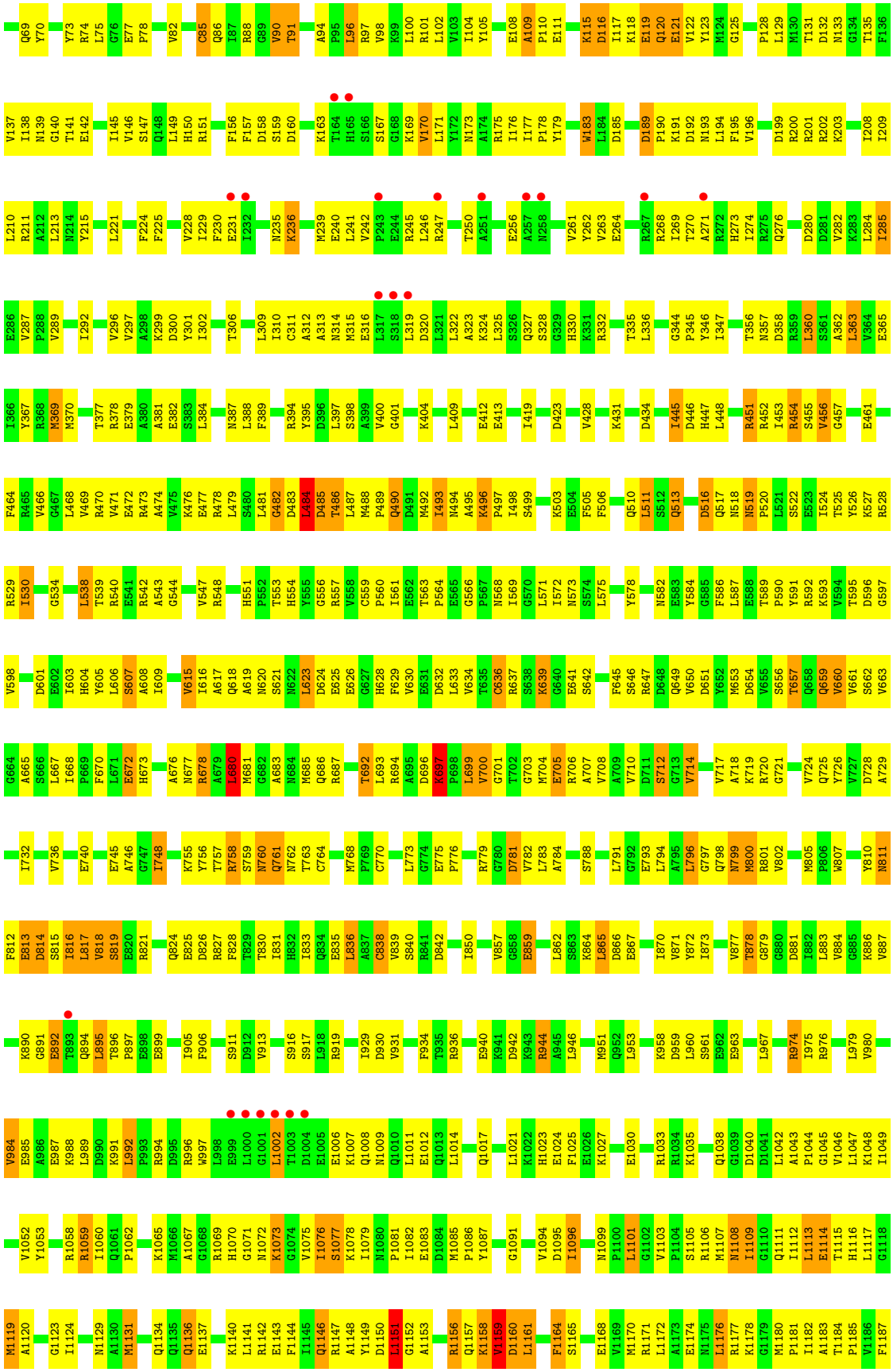
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

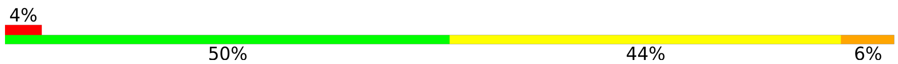
Chain C:

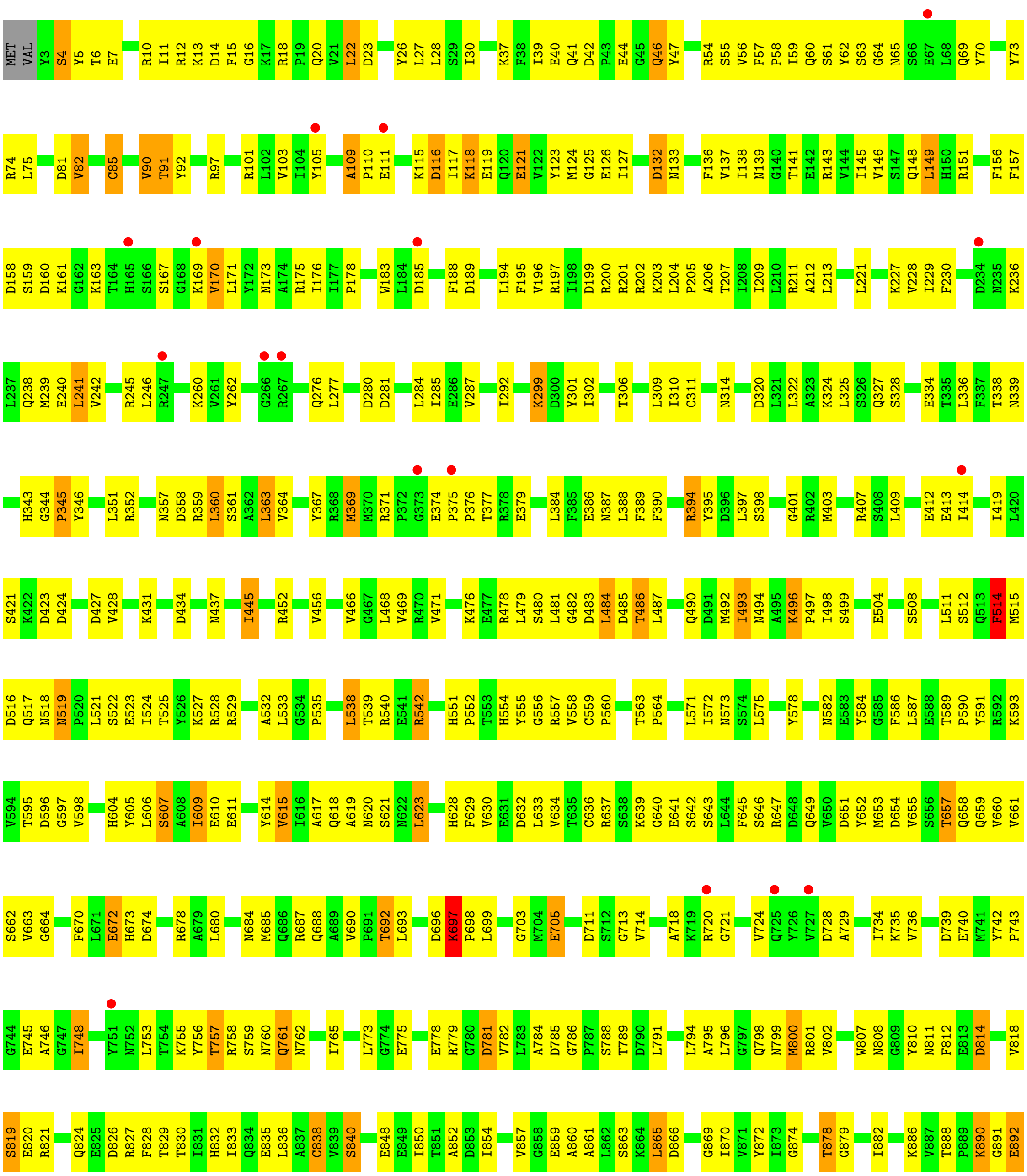


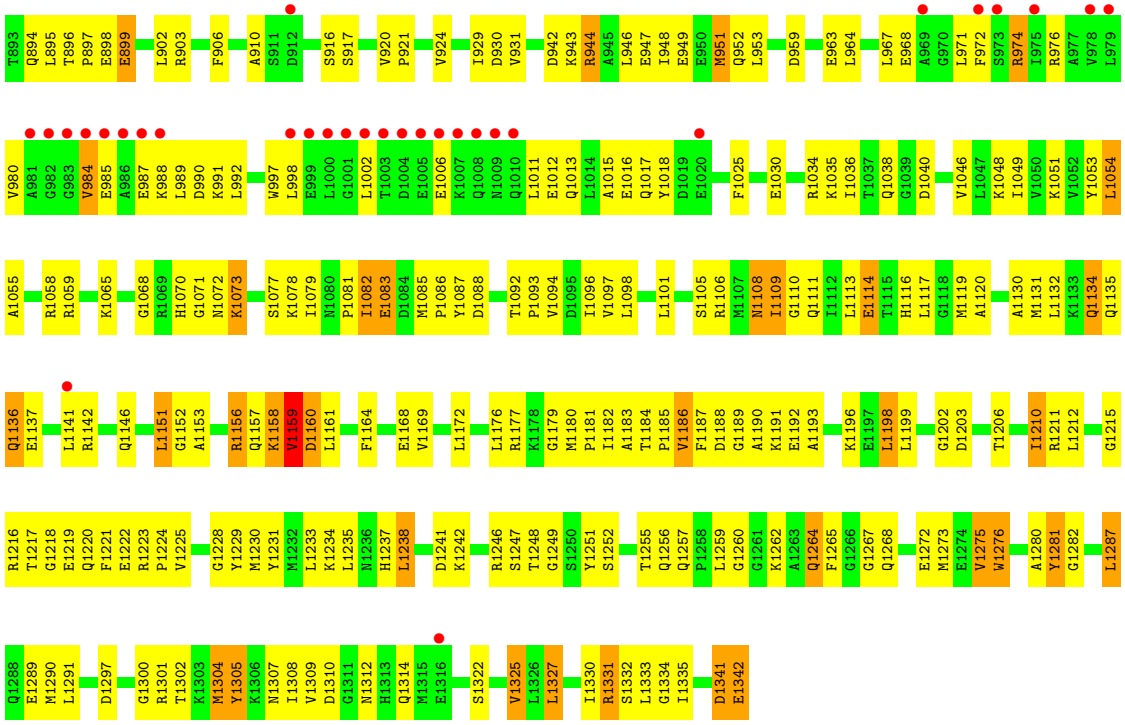


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I:

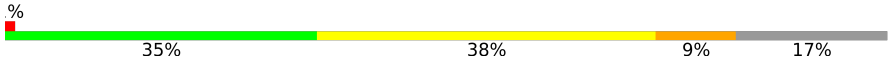


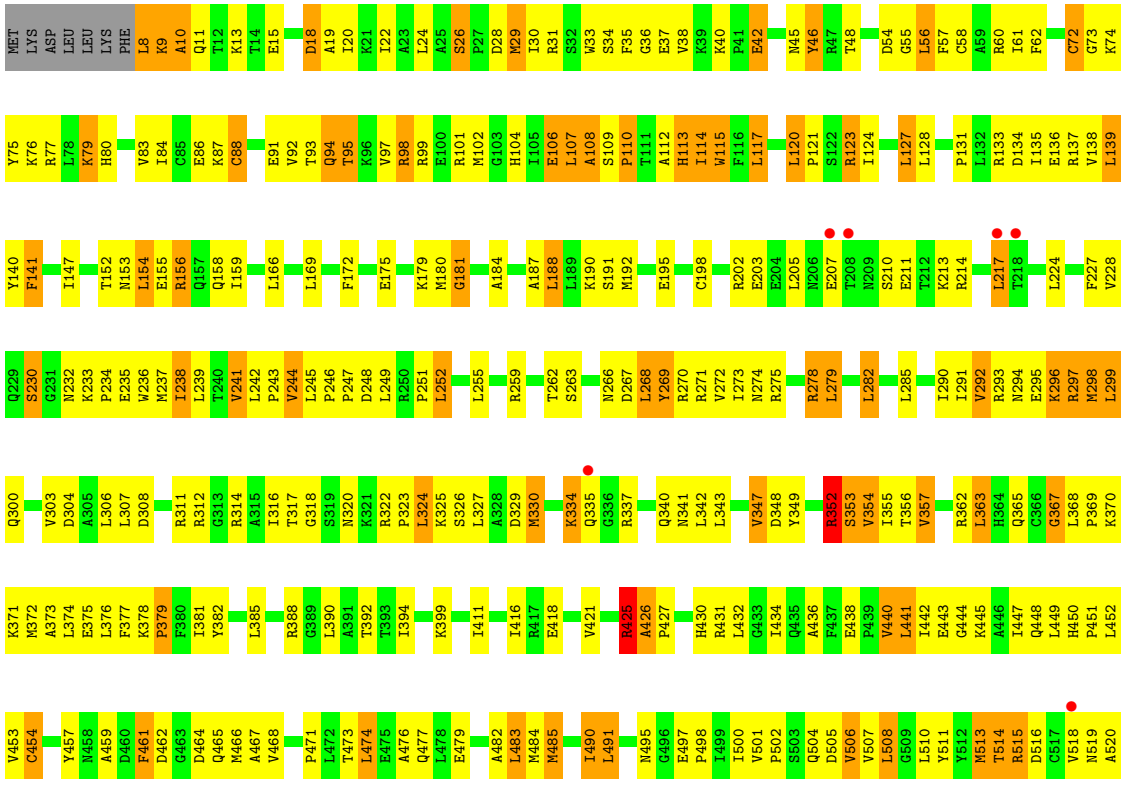


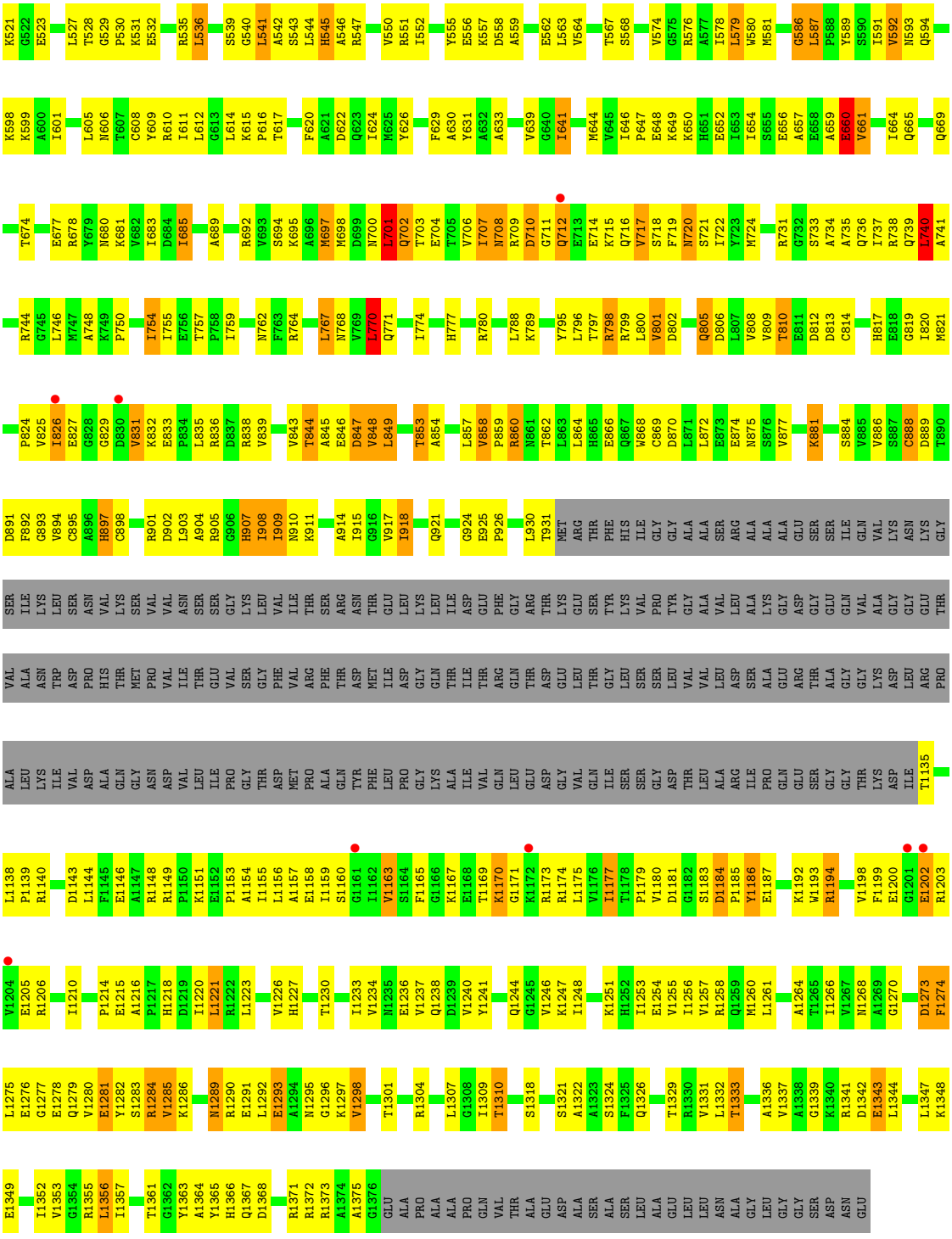


• Molecule 3: DNA-directed RNA polymerase subunit beta'

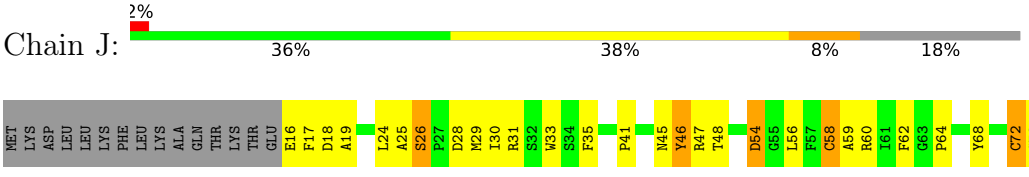
Chain D:

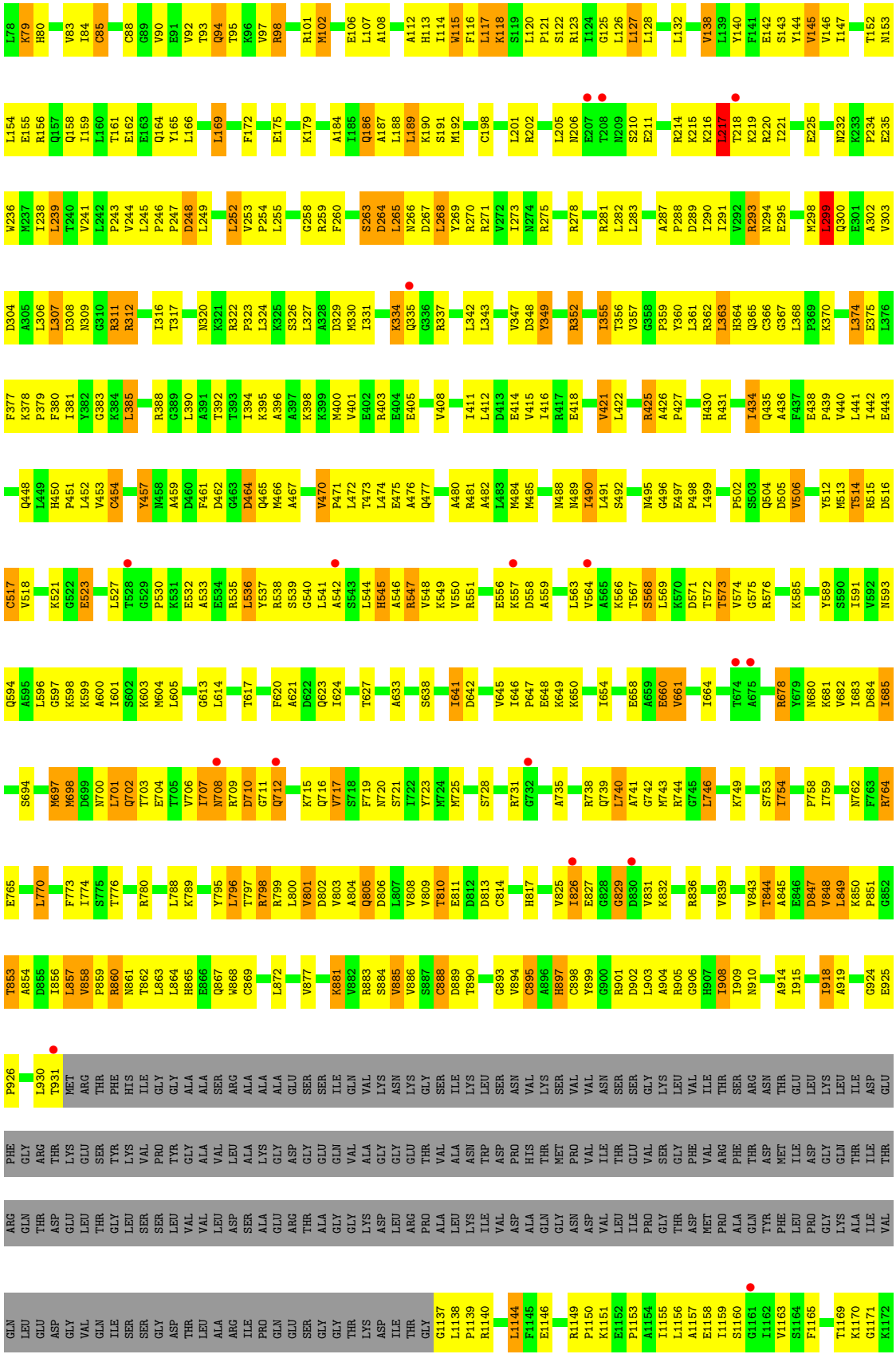


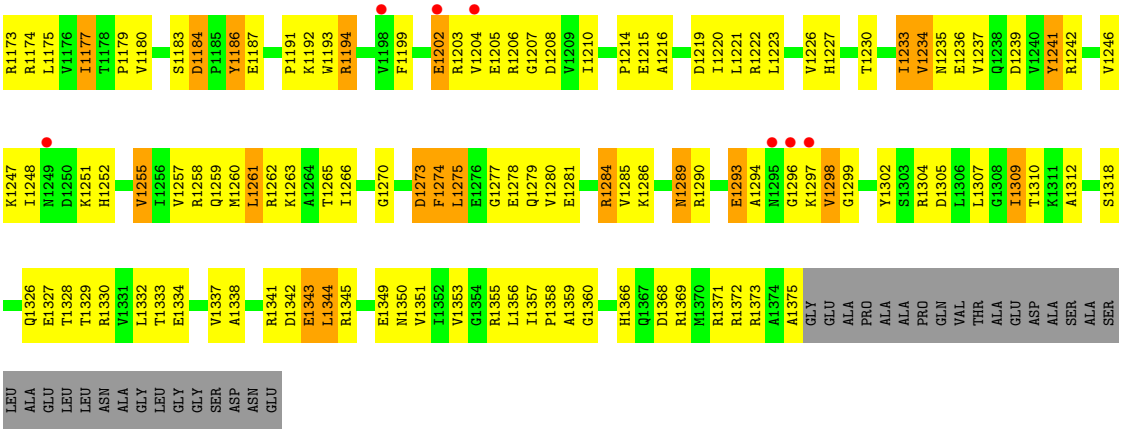




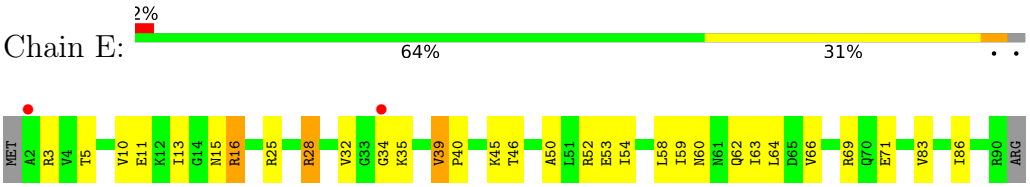
• Molecule 3: DNA-directed RNA polymerase subunit beta'



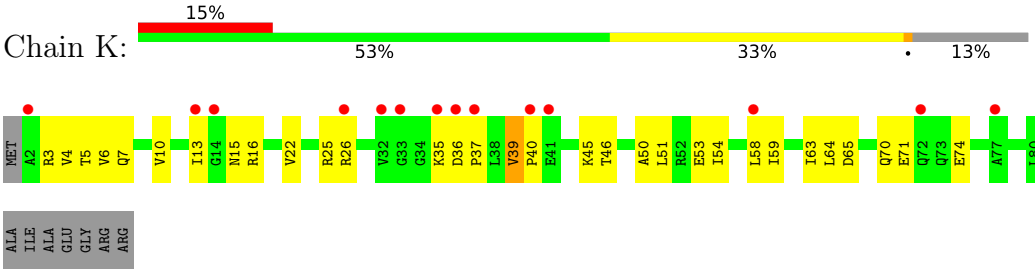

L78 K79 H80 V83 I84 C85 C88 G89 V90 E91 V92 T93 Q94 T95 K96 V97 R98 R101 M102 E106 L107 A108 A112 H113 I114 W115 F116 L117 K118 S119 L120 P121 S122 R123 I124 G125 L126 L127 L128 L132 V138 L139 Y140 F141 E142 S143 Y144 V145 V146 I147 T152 N153
L154 E155 R156 Q157 Q158 I159 L160 T161 E162 E163 Q164 Y165 L166 L169 F172 E175 K179 A184 I185 Q186 A187 L188 L189 K190 S191 M192 C198 L201 R202 L205 N206 E207 T208 N209 S210 E211 R214 K215 K216 L217 T218 K219 R220 I221 E225 N232 K233 P234 E235
W236 M237 I238 L239 T240 V241 L242 P243 V244 L245 P246 P247 D248 L249 L252 V253 P254 L255 G258 R259 F260 S263 D264 L265 N266 D267 L268 Y269 R270 R271 V272 I273 N274 R275 R278 R281 L282 L283 A287 P288 D289 I290 I291 V292 R293 N294 E295 M298 L299 Q300 E301 A302 V303
D304 A305 L306 L307 D308 N309 G310 R311 R312 I316 T317 N320 K321 R322 P323 L324 K325 S326 L327 A328 D329 M330 I331 K334 Q335 G336 R337 L342 L343 V347 D348 Y349 R352 I355 T356 V357 G358 P359 Y360 L361 R362 L363 H364 Q365 C366 G367 L368 P369 K370 L374 E375 L376
F377 K378 P379 F380 I381 Y382 G383 K384 L385 R388 G389 L390 A391 T392 T393 I394 K395 A396 A397 K398 K399 M400 V401 E402 R403 E404 E405 V408 I411 L412 D413 E414 V415 I416 R417 E418 V421 L422 R425 A426 P427 H430 R431 I434 Q435 A436 F437 E438 P439 V440 L441 I442 E443
Q448 L449 H450 P451 L452 V453 C454 Y457 N458 A459 D460 F461 D462 G463 D464 Q465 M466 A467 V470 P471 L472 T473 L474 E475 A476 Q477 A480 R481 A482 L483 M484 M485 N488 N489 I490 L491 S492 N495 G496 E497 P498 I499 P502 S503 Q504 D505 V506 K585 Y512 M513 T514 R515 D516
C517 V518 K521 G522 E523 L527 T528 G529 P530 K531 E532 A533 E534 R535 L536 Y537 R538 S539 G540 L541 A542 S543 L544 H545 A546 R547 V548 K549 V550 R551 E556 K557 D558 A559 L563 V564 A565 K566 T567 S568 L569 K570 D571 T572 T573 V574 G575 R576 K585 Y589 S590 I591 V592 N593
Q594 A595 L596 G597 K598 K599 A600 I601 S602 K603 M604 L605 G613 L614 T617 F620 A621 D622 Q623 I624 T627 A633 S638 I641 D642 V645 I646 P647 E648 K649 K650 I654 E658 A659 E660 V661 I664 T674 A675 R678 Y679 N680 K681 V682 I683 D684 I685
S694 M697 M698 D699 N700 L701 Q702 T703 E704 T705 V706 I707 N708 R709 D710 G711 Q712 K715 Q716 V717 S718 F719 N720 S721 I722 Y723 M724 M725 S728 R731 G732 A735 R738 Q739 L740 A741 G742 M743 R744 G745 L746 K749 S753 I754 P758 I759 N762 F763 R764
E765 L770 F773 I774 S775 T776 R780 L788 K789 Y795 L796 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 L807 V808 V809 T810 E811 D812 D813 C814 H817 V825 I826 E827 G828 G829 D830 V831 K832 R836 V839 V843 T844 A845 E846 D847 V848 L849 K850 P851 G852
T853 A854 D855 I856 L857 V858 P859 R860 N861 T862 L863 L864 H865 E866 Q867 W868 C869 L872 V877 K881 V882 R883 S884 V885 V886 S887 C888 D889 T890 G893 V894 C895 A896 H897 C898 Y899 G900 R901 D902 L903 A904 R905 G906 H907 I908 I909 N910 A914 I915 I918 A919 G924 E925
P926 L930 T931
MET ARG THR PHE HIS ILE GLY GLY ALA ALA SER ARG ALA ALA ALA GLU GLU SER SER ILE GLN VAL ALA LYS GLY LYS LYS GLY GLU THR PRO ALA LEU LYS ILE VAL ASP PRO HIS THR MET PRO VAL ILE THR GLU VAL LYS SER ASN VAL ASP VAL ASN SER SER GLY LYS LEU VAL PHE THR SER ARG ASN THR MET ILE ASP LEU GLU LEU LYS LEU ILE ASP
PHE GLY ARG THR LYS GLU SER TYR LYS VAL PRO TYR GLY ALA VAL LEU ASP ALA LYS GLY ASP GLY GLU GLN VAL ALA LYS GLY GLY GLU VAL SER GLY PHE VAL ARG PHE THR ASP MET ILE ASP GLY GLN THR ILE THR
ARG GLN THR ASP GLU LEU THR GLY LYS ASP LEU ARG PRO ALA LEU LYS ILE VAL ASP ALA GLN GLY ASN ASP VAL LEU ILE PRO GLY LYS ALA ILE VAL
GLN LEU GLU ASP GLY VAL THR LYS ASP ILE THR GLY G1137 L1138 P1139 R1140 L1144 F1145 E1146 R1149 P1150 K1151 E1152 P1153 A1154 I1155 L1156 A1157 E1158 I1159 S1160 G1161 I1162 V1163 S1164 F1165 T1169 K1170 G1171 K1172



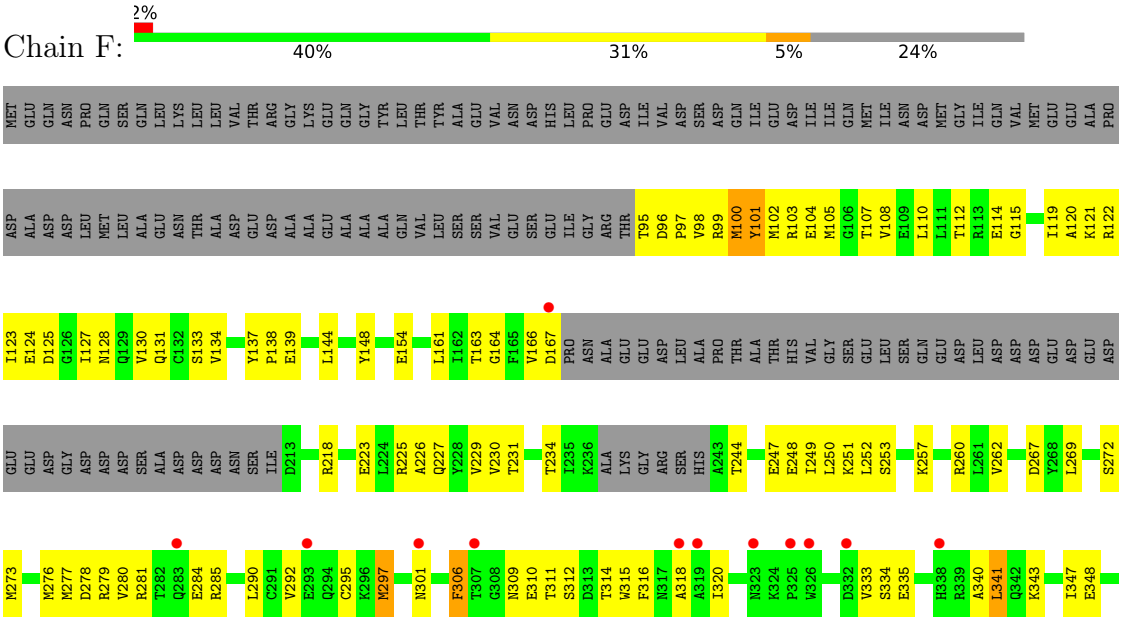
• Molecule 4: DNA-directed RNA polymerase subunit omega

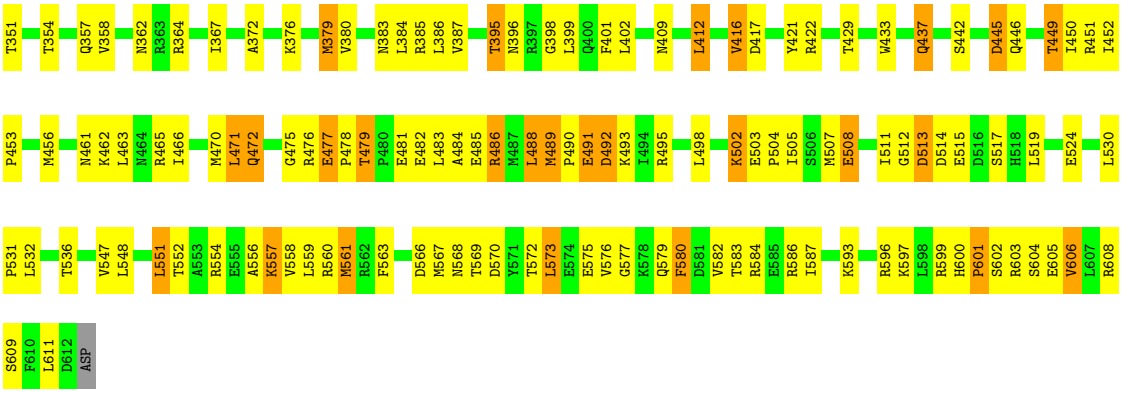


• Molecule 4: DNA-directed RNA polymerase subunit omega



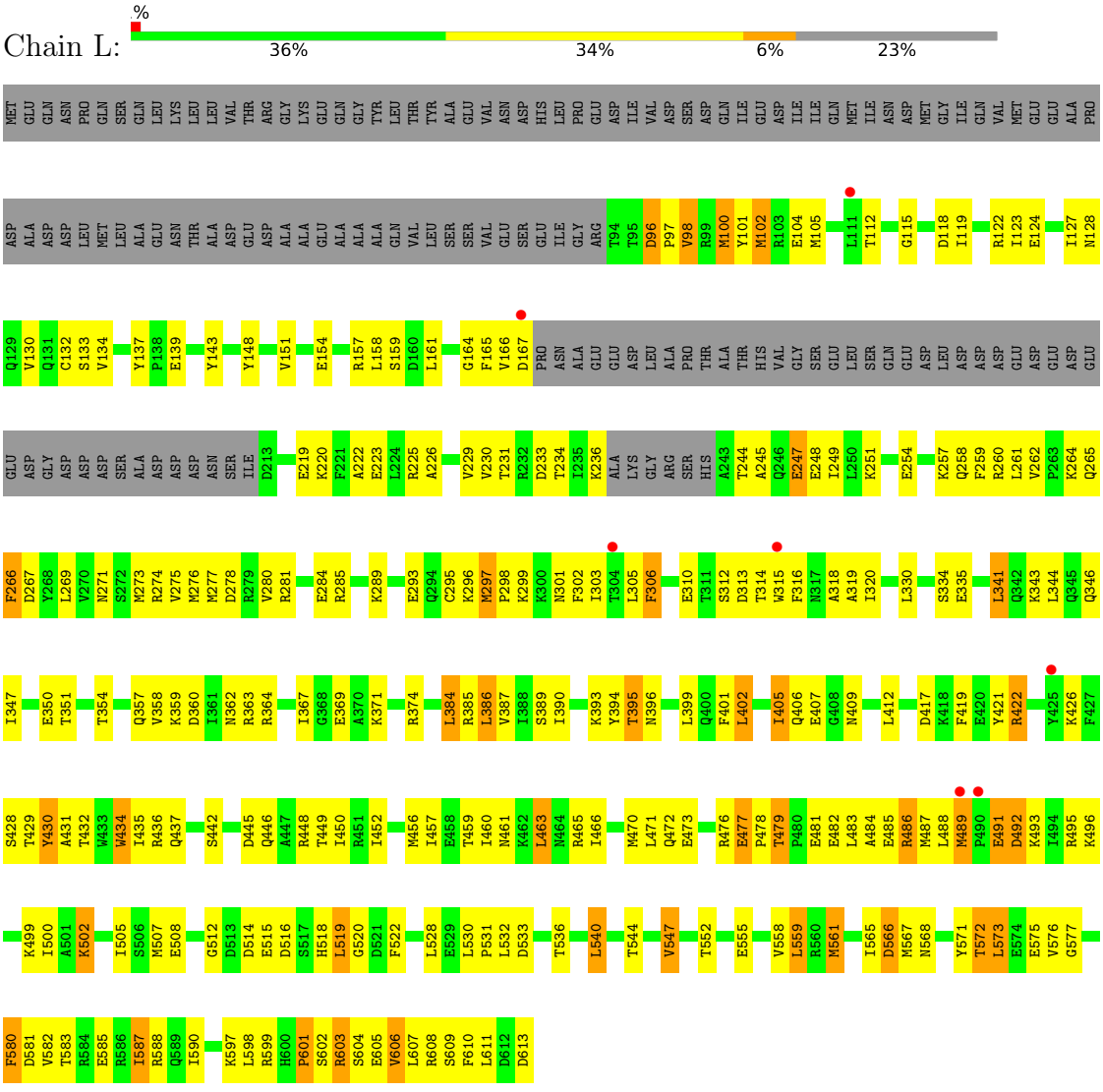
• Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	185.36Å 206.28Å 308.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.60 29.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.90-3.60) 93.7 (29.90-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.246 , 0.305 0.246 , 0.304	Depositor DCC
R_{free} test set	1932 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å^2)	142.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 91.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	55699	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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	A	0.84	4/2435 (0.2%)	1.07	12/3300 (0.4%)
1	B	0.75	1/1692 (0.1%)	1.01	5/2293 (0.2%)
1	G	0.58	0/1751	1.05	9/2373 (0.4%)
1	H	0.59	0/1686	0.91	4/2285 (0.2%)
2	C	1.17	37/10741 (0.3%)	1.21	65/14492 (0.4%)
2	I	0.80	7/10737 (0.1%)	0.97	15/14487 (0.1%)
3	D	1.21	60/9246 (0.6%)	1.24	74/12478 (0.6%)
3	J	1.02	27/9168 (0.3%)	1.13	52/12374 (0.4%)
4	E	0.65	0/693	0.83	0/935
4	K	0.38	0/629	0.61	0/847
5	F	0.82	2/3857 (0.1%)	1.05	10/5184 (0.2%)
5	L	0.77	3/3872 (0.1%)	0.99	12/5205 (0.2%)
All	All	0.98	141/56507 (0.2%)	1.10	258/76253 (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	A	0	2
1	G	0	1
2	C	0	11
2	I	0	2
3	D	0	12
3	J	0	9
5	F	0	1
5	L	0	1
All	All	0	39

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	811	ASN	CB-CG	-9.14	1.30	1.51
1	A	131	CYS	CB-SG	-8.93	1.67	1.82
3	J	145	VAL	CB-CG2	-8.81	1.34	1.52
2	C	636	CYS	CB-SG	-8.52	1.67	1.82
3	J	72	CYS	CB-SG	-7.87	1.68	1.82

The worst 5 of 258 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1287	LEU	CB-CG-CD2	-14.16	86.92	111.00
3	D	376	LEU	CB-CG-CD2	-10.83	92.59	111.00
3	D	114	ILE	CG1-CB-CG2	-10.71	87.84	111.40
2	C	796	LEU	CB-CG-CD2	-9.94	94.10	111.00
3	D	188	LEU	CB-CG-CD2	-9.88	94.20	111.00

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	TRP	Peptide
1	A	49	SER	Mainchain
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
2	C	473	ARG	Mainchain

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	2403	0	2453	197	0
1	B	1672	0	1693	112	0
1	G	1730	0	1756	145	0
1	H	1667	0	1689	123	1
2	C	10572	0	10584	657	3
2	I	10568	0	10578	602	0
3	D	9107	0	9308	612	0
3	J	9029	0	9225	587	0
4	E	691	0	695	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	26	0
5	F	3806	0	3873	199	2
5	L	3821	0	3884	190	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	55699	0	56372	3190	3

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 28.

The worst 5 of 3190 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)
1:A:27:THR:O	1:A:28:LEU:HD12	1.10	1.23
2:I:27:LEU:O	2:I:528:ARG:NH1	1.78	1.17
1:A:27:THR:O	1:A:28:LEU:CD1	1.93	1.17
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.36	1.08
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.16	1.08

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:ASP:OD1	5:F:554:ARG:NH2[4_455]	1.99	0.21
2:C:44:GLU:OE1	5:F:596:ARG:NH1[4_455]	2.05	0.15
2:C:940:GLU:OE1	1:H:139:SER:OG[4_455]	2.05	0.15

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	305/329 (93%)	271 (89%)	25 (8%)	9 (3%)	4 33
1	B	213/329 (65%)	191 (90%)	20 (9%)	2 (1%)	17 57
1	G	222/329 (68%)	182 (82%)	28 (13%)	12 (5%)	2 19
1	H	213/329 (65%)	193 (91%)	20 (9%)	0	100 100
2	C	1338/1342 (100%)	1225 (92%)	103 (8%)	10 (1%)	22 61
2	I	1338/1342 (100%)	1226 (92%)	100 (8%)	12 (1%)	17 57
3	D	1162/1407 (83%)	1074 (92%)	79 (7%)	9 (1%)	19 59
3	J	1151/1407 (82%)	1064 (92%)	82 (7%)	5 (0%)	34 71
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100 100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100 100
5	F	461/613 (75%)	422 (92%)	37 (8%)	2 (0%)	34 71
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	47 79
All	All	7030/8222 (86%)	6424 (91%)	544 (8%)	62 (1%)	17 57

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	30	PRO
1	A	324	ALA
1	B	232	VAL
2	C	345	PRO

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
1	A	268/286 (94%)	249 (93%)	19 (7%)	14 48
1	B	184/286 (64%)	166 (90%)	18 (10%)	8 36
1	G	191/286 (67%)	179 (94%)	12 (6%)	18 53
1	H	183/286 (64%)	165 (90%)	18 (10%)	8 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	1155/1157 (100%)	1046 (91%)	109 (9%)	8 38
2	I	1154/1157 (100%)	1046 (91%)	108 (9%)	8 38
3	D	975/1168 (84%)	875 (90%)	100 (10%)	7 34
3	J	967/1168 (83%)	869 (90%)	98 (10%)	7 34
4	E	72/75 (96%)	64 (89%)	8 (11%)	6 31
4	K	67/75 (89%)	63 (94%)	4 (6%)	19 54
5	F	416/540 (77%)	373 (90%)	43 (10%)	7 34
5	L	418/540 (77%)	372 (89%)	46 (11%)	6 31
All	All	6050/7024 (86%)	5467 (90%)	583 (10%)	8 37

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	506	VAL
5	L	561	MET
3	J	661	VAL
3	J	490	ILE
3	J	1255	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	294	ASN
4	K	7	GLN
3	J	365	GLN
3	J	910	ASN
5	L	455	HIS

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 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	A	309/329 (93%)	-0.31	2 (0%) 89 81	99, 147, 225, 245	0
1	B	217/329 (65%)	-0.01	6 (2%) 53 37	112, 194, 254, 272	0
1	G	224/329 (68%)	-0.07	3 (1%) 77 63	163, 206, 241, 270	0
1	H	217/329 (65%)	0.07	13 (5%) 21 12	146, 213, 252, 285	0
2	C	1340/1342 (99%)	-0.35	21 (1%) 72 57	74, 121, 234, 285	0
2	I	1340/1342 (99%)	-0.16	48 (3%) 42 28	86, 159, 261, 388	0
3	D	1166/1407 (82%)	-0.30	14 (1%) 79 66	72, 112, 215, 264	0
3	J	1155/1407 (82%)	-0.22	24 (2%) 63 48	86, 138, 229, 274	0
4	E	89/91 (97%)	-0.02	2 (2%) 62 45	147, 183, 216, 241	0
4	K	79/91 (86%)	0.79	14 (17%) 1 1	202, 277, 319, 350	0
5	F	467/613 (76%)	-0.23	12 (2%) 56 40	93, 165, 290, 340	0
5	L	469/613 (76%)	-0.29	7 (1%) 73 60	116, 178, 288, 353	0
All	All	7072/8222 (86%)	-0.22	166 (2%) 60 44	72, 147, 251, 388	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.1
3	D	335	GLN	6.4
2	I	1001	GLY	5.5
1	B	160	HIS	5.0
2	I	1000	LEU	5.0

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 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
7	ZN	D	1502	1/1	0.81	0.13	134,134,134,134	0
6	MG	J	1501	1/1	0.92	0.35	94,94,94,94	0
6	MG	D	1501	1/1	0.94	0.54	87,87,87,87	0
7	ZN	J	1503	1/1	0.95	0.09	97,97,97,97	0
7	ZN	J	1502	1/1	0.97	0.02	131,131,131,131	0
7	ZN	D	1503	1/1	0.99	0.06	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.