wwPDB X-ray Structure Validation Summary Report (i)

Feb 2, 2017 – 02:16 PM EST

PDB ID	:	5TBZ
Title	:	E. Coli RNA Polymerase complexed with NusG
Authors	:	Liu, B.; Steitz, T.A.
Deposited on	:	2016-09-13
Resolution	:	7.00 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:

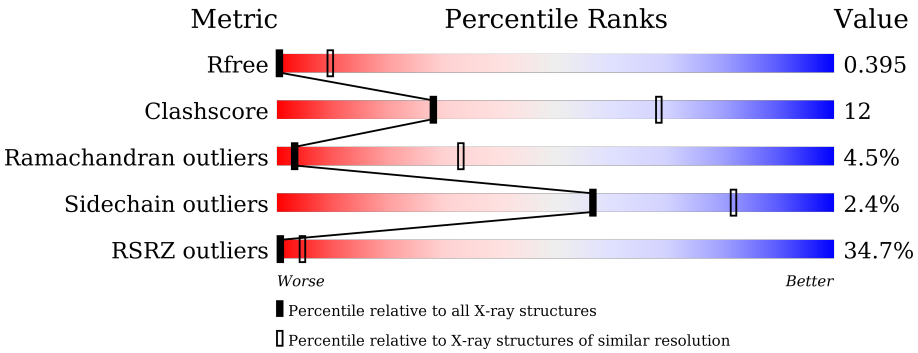
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 7.00 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.



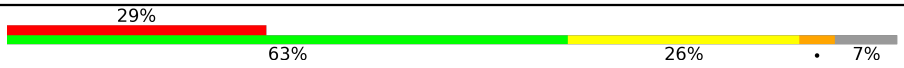
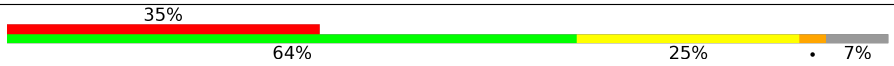
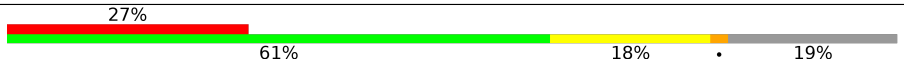
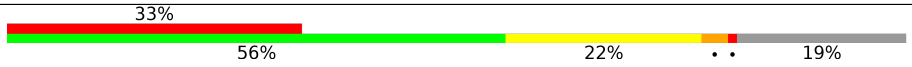
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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	242	26% 73% 18% • 7%
1	B	242	47% 69% 18% • 11%
1	F	242	23% 72% 20% • 7%
1	G	242	38% 71% 17% • 11%
2	C	1342	32% 77% 20% ••
2	H	1342	34% 75% 21% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1407	
3	I	1407	
4	J	181	
4	K	181	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50147 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	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	B	215	Total	C	N	O	S	0	0	0
			1657	1034	291	326	6			
1	F	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	G	216	Total	C	N	O	S	0	0	0
			1667	1040	294	327	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP P0A7Z6
A	-5	HIS	-	expression tag	UNP P0A7Z6
A	-4	HIS	-	expression tag	UNP P0A7Z6
A	-3	HIS	-	expression tag	UNP P0A7Z6
A	-2	HIS	-	expression tag	UNP P0A7Z6
A	-1	HIS	-	expression tag	UNP P0A7Z6
A	0	HIS	-	expression tag	UNP P0A7Z6
B	-6	ALA	-	expression tag	UNP P0A7Z6
B	-5	HIS	-	expression tag	UNP P0A7Z6
B	-4	HIS	-	expression tag	UNP P0A7Z6
B	-3	HIS	-	expression tag	UNP P0A7Z6
B	-2	HIS	-	expression tag	UNP P0A7Z6
B	-1	HIS	-	expression tag	UNP P0A7Z6
B	0	HIS	-	expression tag	UNP P0A7Z6
F	-6	ALA	-	expression tag	UNP P0A7Z6
F	-5	HIS	-	expression tag	UNP P0A7Z6
F	-4	HIS	-	expression tag	UNP P0A7Z6
F	-3	HIS	-	expression tag	UNP P0A7Z6
F	-2	HIS	-	expression tag	UNP P0A7Z6
F	-1	HIS	-	expression tag	UNP P0A7Z6
F	0	HIS	-	expression tag	UNP P0A7Z6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	ALA	-	expression tag	UNP P0A7Z6
G	-5	HIS	-	expression tag	UNP P0A7Z6
G	-4	HIS	-	expression tag	UNP P0A7Z6
G	-3	HIS	-	expression tag	UNP P0A7Z6
G	-2	HIS	-	expression tag	UNP P0A7Z6
G	-1	HIS	-	expression tag	UNP P0A7Z6
G	0	HIS	-	expression tag	UNP P0A7Z6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			
2	H	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1302	Total	C	N	O	S	0	0	0
			10085	6326	1800	1911	48			
3	I	1306	Total	C	N	O	S	0	0	0
			10126	6353	1809	1916	48			

- Molecule 4 is a protein called Transcription termination/antitermination protein NusG.

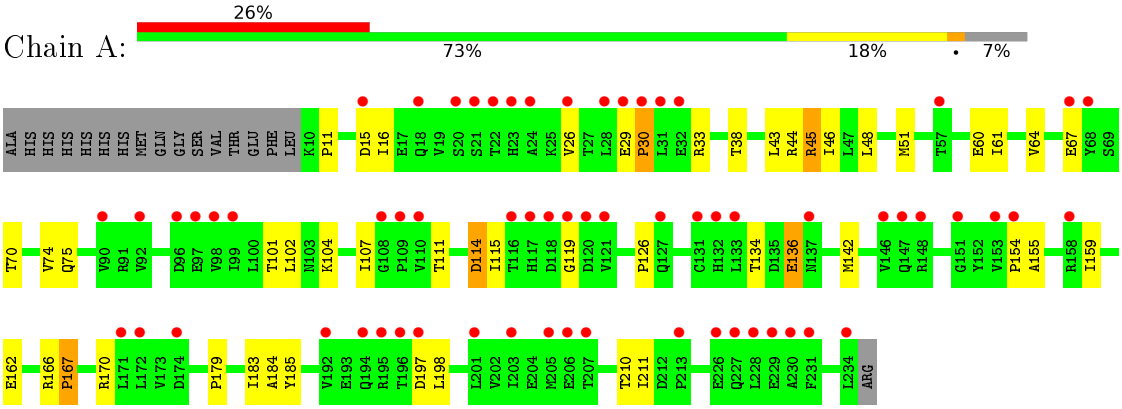
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			
4	K	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			

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.

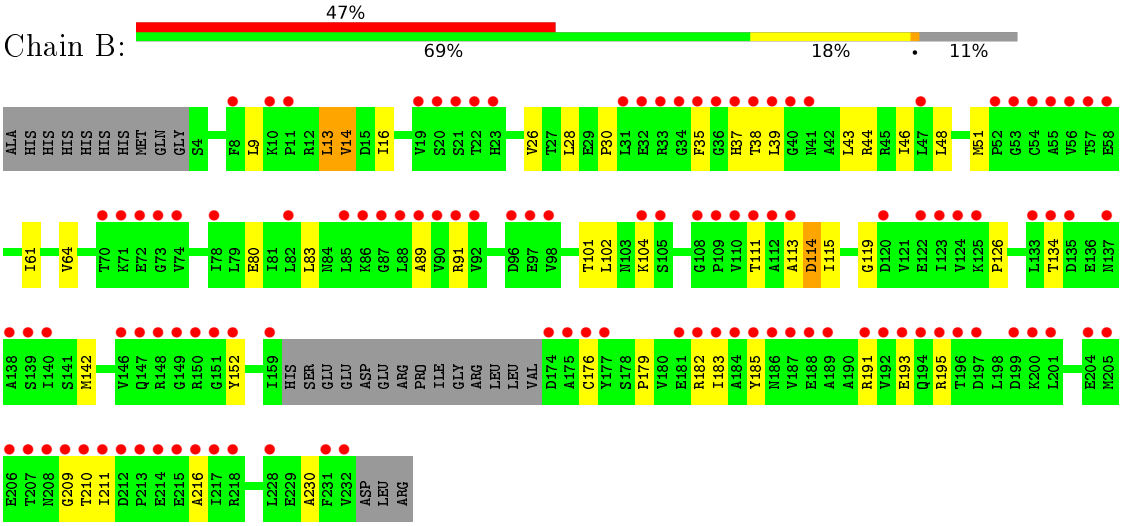
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



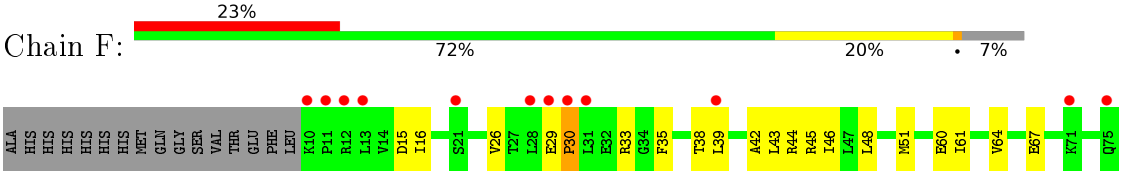
- Molecule 1: DNA-directed RNA polymerase subunit alpha

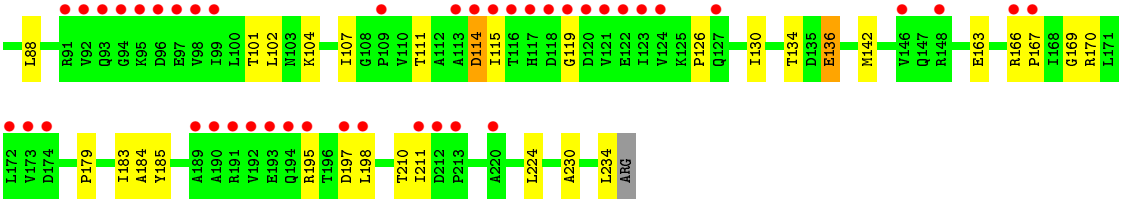
Chain B:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

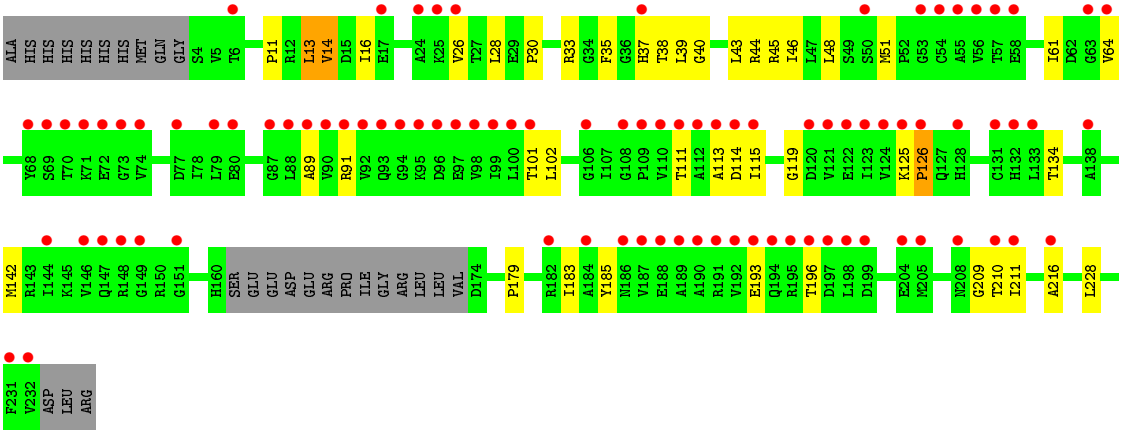
Chain F:





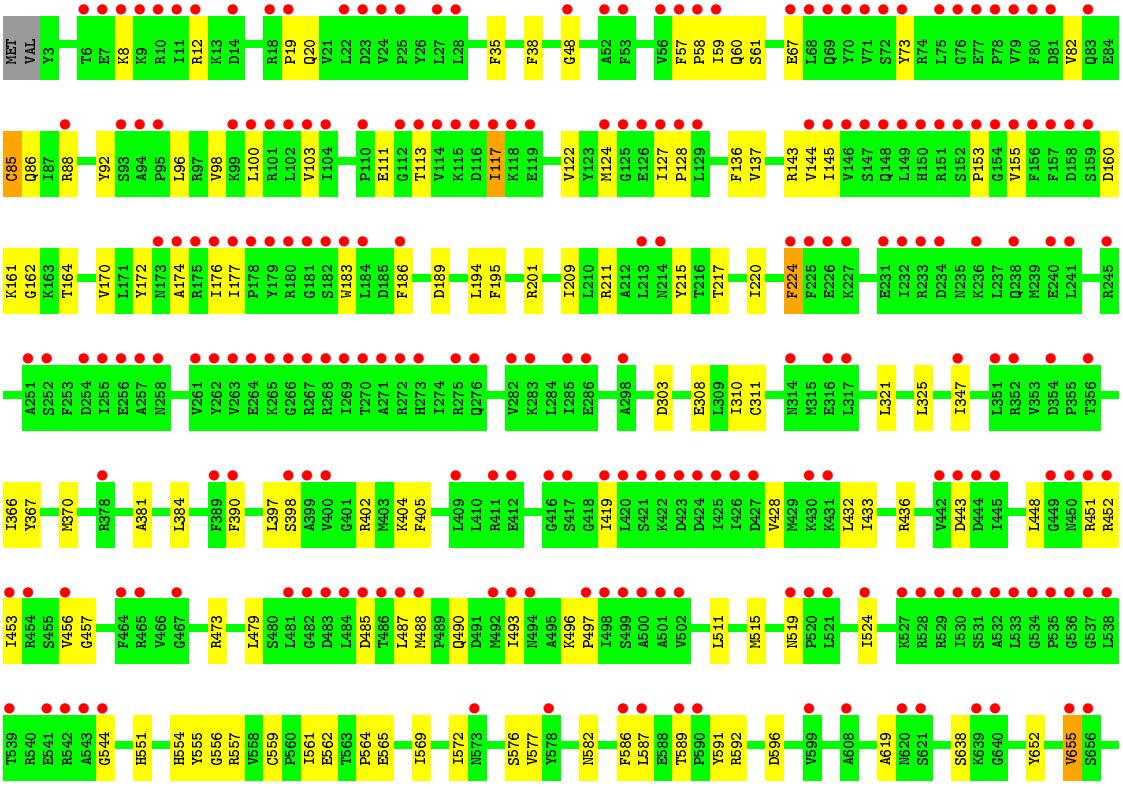
• Molecule 1: DNA-directed RNA polymerase subunit alpha

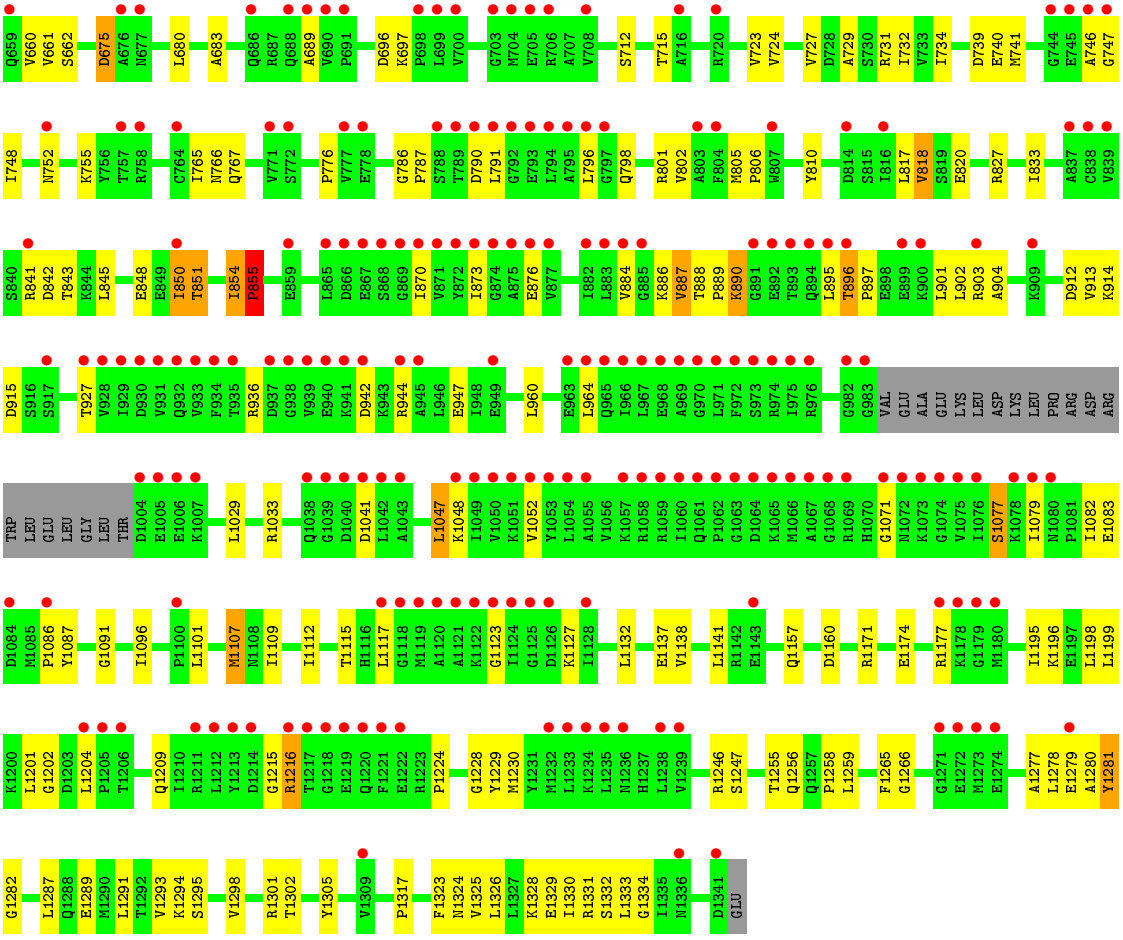
Chain G:



• Molecule 2: DNA-directed RNA polymerase subunit beta

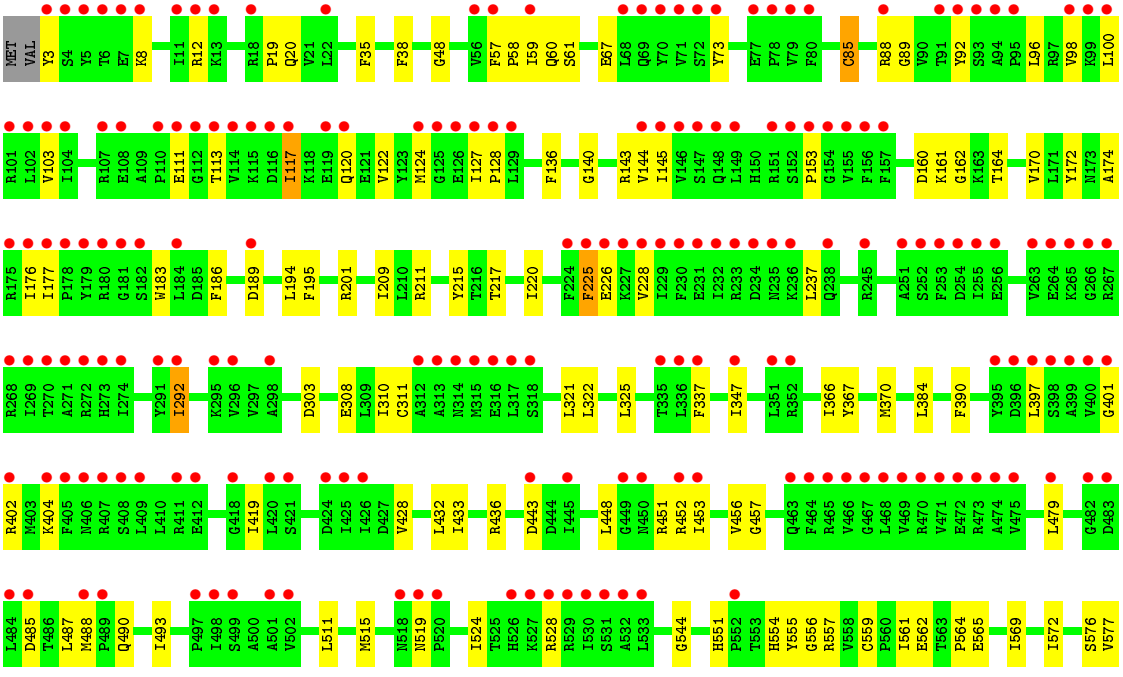
Chain C:

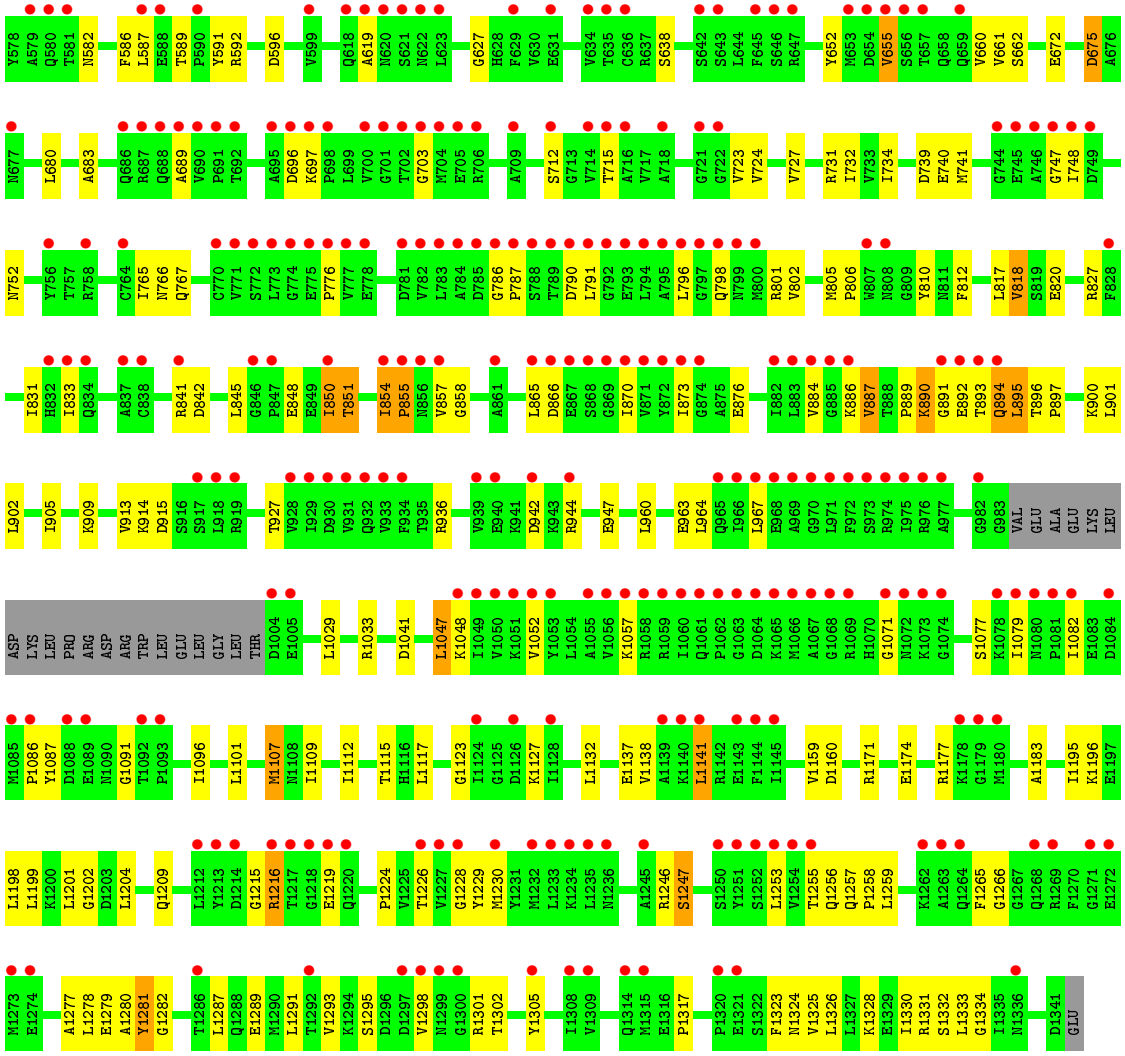




- Molecule 2: DNA-directed RNA polymerase subunit beta

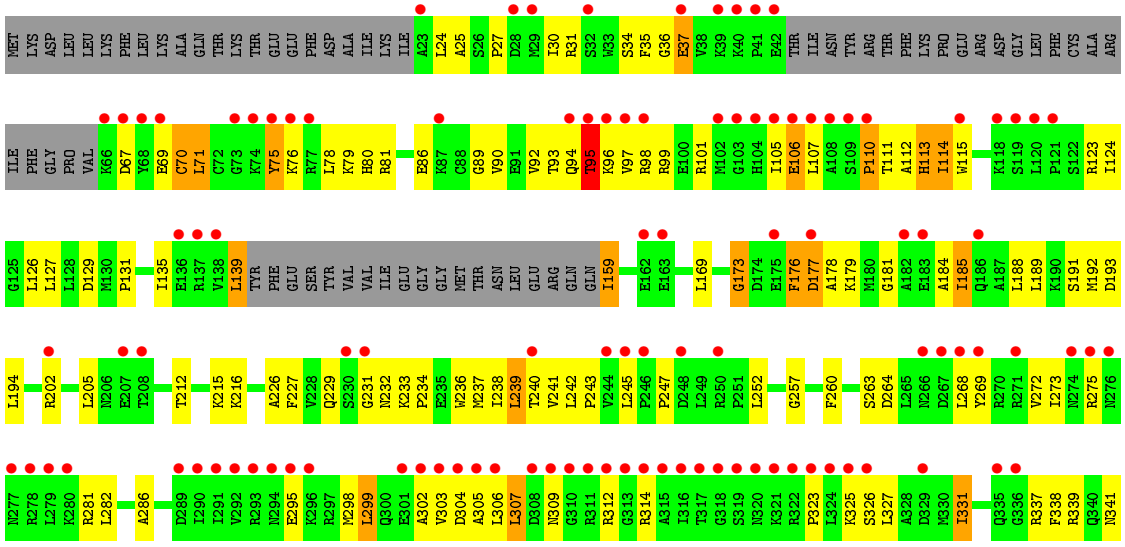
Chain H:

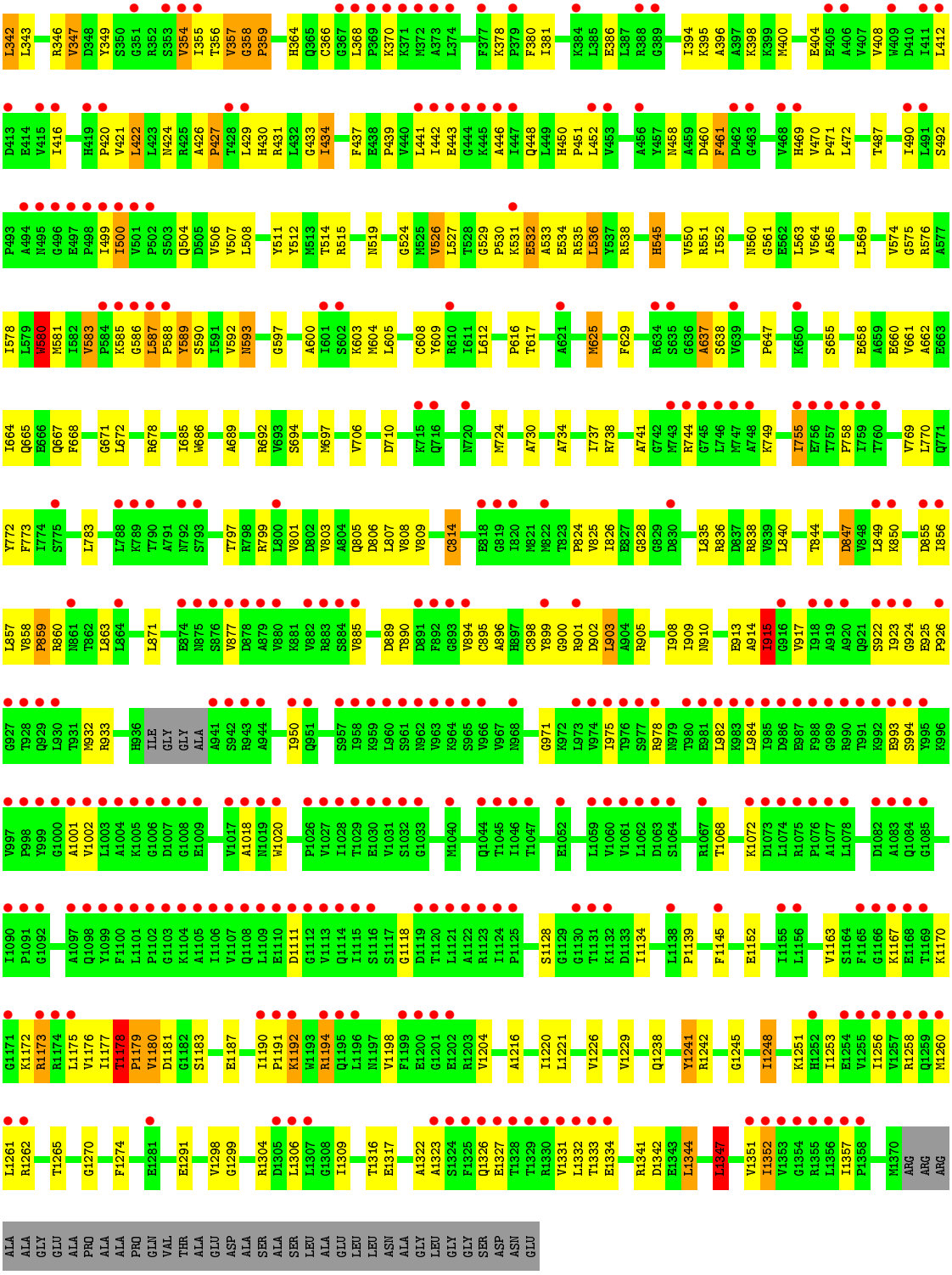




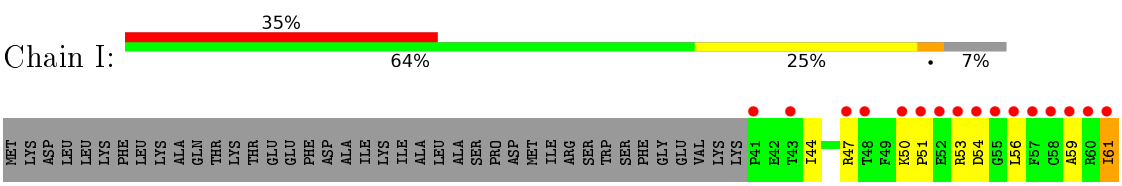
• Molecule 3: DNA-directed RNA polymerase subunit beta'

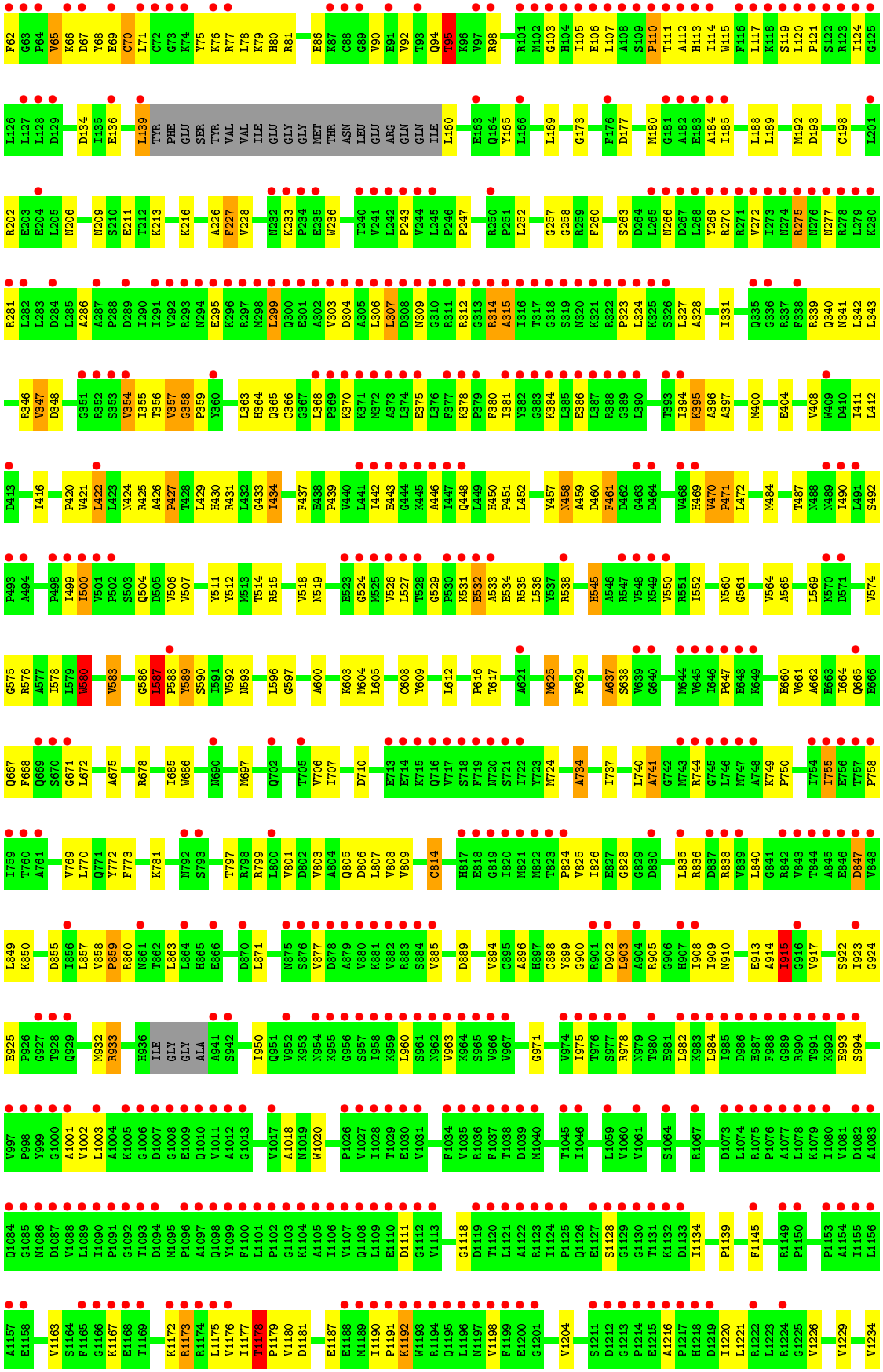
Chain D:

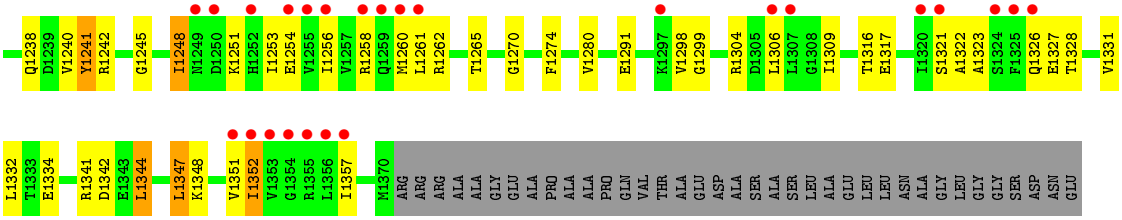


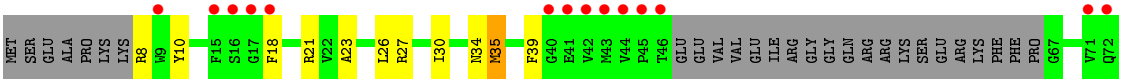


• Molecule 3: DNA-directed RNA polymerase subunit beta'




F62 G63 P64 V65 K66 D67 Y68 E69 C70 L71 C72 G73 K74 Y75 K76 R77 L78 K79 H80 R81 E86 K87 C88 G89 V90 E91 V92 T93 Q94 T95 K96 V97 R98 R101 M102 G103 H104 I105 E106 L107 A108 S109 P110 T111 A112 H113 I114 W115 F116 L117 K118 S119 L120 P121 S122 R123 I124 G125
L126 L127 L128 D129 D134 I135 E136 L139 TYR PHE GLU SER TYR VAL VAL ILE GLU GLY GLY MET THR ASN LEU GLU ARG GLN GLN ILE L160 E163 Q164 Y165 L166 L169 G173 F176 D177 M180 G181 A182 E183 A184 I185 L188 L189 N192 D193 C198 L201
R202 E203 E204 L205 N206 N209 S210 E211 T212 K213 K216 A226 F227 V228 N232 K233 P234 E235 W236 T240 V241 L242 P243 V244 L245 P246 P247 R250 P251 L252 G257 G258 R259 F260 S263 D264 L265 N266 D267 L268 Y269 R270 R271 V272 I273 N274 R275 N276 N277 R278 L279 K280
R281 L282 I283 D284 L285 A286 A287 P288 D289 I290 I291 V292 R293 N294 E295 K296 R297 M298 L299 Q300 E301 A302 V303 D304 A305 L306 L307 D308 N309 G310 R311 R312 G313 R314 A315 T316 T317 G318 S319 N320 K321 R322 P323 L324 K325 S326 L327 A328 I331 Q335 G336 R337 F338 R339 Q340 N341 L342 L343
R346 V347 D348 G351 R352 S353 V354 I355 T356 V357 G358 P359 Y360 L363 H364 Q365 C366 G367 L368 P369 K370 K371 M372 A373 L374 E375 L376 F377 K378 P379 F380 I381 Y382 G383 K384 I385 E386 L387 R388 G389 L390 T393 I394 K395 A396 A397 M400 E404 V408 W409 D410 I411 L412
D413 I416 P420 V421 L422 L423 M424 R425 A426 P427 T428 L429 H430 R431 L432 G433 T434 F437 E438 P439 V440 L441 I442 E443 G444 K445 A446 I447 Q448 L449 H450 P451 L452 Y457 N458 A459 D460 F461 D462 G463 D464 V468 H469 V470 P471 L472 M484 T487 N488 N489 L491 S492
P493 A494 P498 I499 I500 V501 P502 S503 Q504 D505 V506 V507 Y511 Y512 N513 T514 R515 V518 N519 E523 G524 M525 V526 L527 T528 G529 P530 K531 E532 A533 E534 R535 L536 V537 R538 H545 A546 R547 V548 K549 V550 R551 I552 N560 G561 V564 A565 L569 K570 D571 V574
G575 R576 A577 I578 L579 W580 V583 G586 L587 P588 Y589 S590 I591 V592 N593 L596 G597 A600 K603 M604 L605 C608 Y609 L612 P616 T617 A621 M625 F629 A637 S638 V639 G640 M644 V645 I646 P647 E648 K649 E660 V661 A662 E663 I664 Q665 E666
Q667 F668 Q669 S670 G671 L672 A675 R678 I685 W686 N690 M697 Q702 T705 V706 I707 D710 E713 E714 K715 Q716 V717 S718 F719 N720 S721 I722 Y723 M724 A734 I737 L740 A741 G742 M743 R744 G745 L746 M747 A748 K749 P750 I754 I755 E756 T757 P758
I759 T760 A761 V769 L770 Q771 Y772 F773 K781 N792 S793 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 L807 V808 V809 C814 H817 E818 G819 I820 M821 M822 T823 P824 V825 I826 E827 G828 G829 D830 L835 R836 D837 R838 V839 L840 G841 R842 V843 T844 A845 E846 D847 V848
L849 K850 D855 I856 L857 V858 P859 R860 N861 T862 L863 L864 H865 E866 D870 L871 N875 S876 V877 D878 A879 V880 K881 V882 R883 S884 V885 D889 V894 C895 A896 H897 C898 Y899 G900 R901 D902 L903 A904 R905 G906 H907 I908 I909 N910 E913 A914 I915 G916 V917 S922 I923 G924
E925 P926 G927 T928 Q929 M932 R933 H936 ILE GLY GLY ALA A941 S942 I950 Q951 V952 K953 N954 K955 G956 S957 I958 K959 L960 S961 N962 V963 K964 S965 V966 V967 G971 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 P988 G989 R990 T991 K992 E993 S994
V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 Q1010 V1011 A1012 G1013 V1017 A1018 N1019 W1020 P1026 V1027 I1028 T1029 E1030 V1031 F1034 V1035 R1036 F1037 T1038 D1039 M1040 T1045 I1046 L1059 V1060 V1061 S1064 R1067 D1073 L1074 R1075 P1076 A1077 L1078 K1079 I1080 V1081 D1082 A1083
Q1084 G1085 N1086 D1087 V1088 L1089 I1090 P1091 G1092 T1093 D1094 M1095 P1096 A1097 Q1098 Y1099 F1100 L1101 P1102 G1103 K1104 A1105 I1106 V1107 Q1108 L1109 E1110 D1111 G1112 V1113 G1118 D1119 T1120 L1121 A1122 R1123 I1124 P1125 Q1126 E1127 S1128 G1129 G1130 T1131 K1132 D1133 I1134 P1139 F1145 R1149 P1150 P1153 A1154 I1155 L1156
A1157 E1158 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1172 R1173 R1174 L1175 V1176 I1177 T1178 P1179 V1180 D1181 E1187 E1188 M1189 I1190 P1191 K1192 W1193 R1194 Q1195 L1196 N1197 V1198 F1199 E1200 G1201 V1204 S1211 D1212 G1213 P1214 E1215 A1216 P1217 H1218 D1219 I1220 L1221 R1222 L1223 R1224 G1225 V1226 V1229 V1234



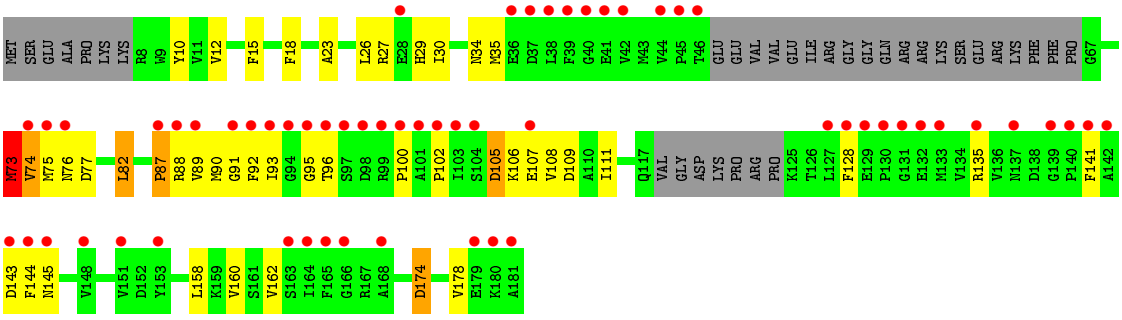


• Molecule 4: Transcription termination/antitermination protein NusG

Chain J:

• Molecule 4: Transcription termination/antitermination protein NusG

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.16Å 313.78Å 162.79Å 90.00° 130.23° 90.00°	Depositor
Resolution (Å)	162.19 – 7.00 49.91 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (162.19-7.00) 93.3 (49.91-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 6.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.330 , 0.395 0.330 , 0.395	Depositor DCC
R_{free} test set	707 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	314.0	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 500.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.185 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	50147	wwPDB-VP
Average B, all atoms (Å^2)	330.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

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	0.45	0/1761	0.72	0/2387
1	B	0.46	0/1676	0.71	0/2271
1	F	0.45	0/1761	0.74	0/2387
1	G	0.47	0/1687	0.70	0/2286
2	C	0.43	0/10569	0.67	0/14258
2	H	0.43	0/10569	0.67	0/14258
3	D	0.44	0/10233	0.76	5/13816 (0.0%)
3	I	0.44	0/10277	0.74	1/13877 (0.0%)
4	J	0.50	0/1188	0.70	0/1603
4	K	0.50	0/1188	0.74	1/1603 (0.1%)
All	All	0.44	0/50909	0.71	7/68746 (0.0%)

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	C	0	2
2	H	0	2
3	D	0	1
3	I	0	1
4	K	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1194	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	D	239	LEU	CA-CB-CG	5.33	127.56	115.30
3	D	173	GLY	N-CA-C	5.30	126.36	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	117	LEU	CA-CB-CG	5.29	127.46	115.30
4	K	73	MET	C-N-CA	5.27	134.87	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	PHE	Peptide
2	C	855	PRO	Peptide
3	D	1178	THR	Peptide
2	H	57	PHE	Peptide
2	H	855	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1740	0	1767	40	0
1	B	1657	0	1686	40	0
1	F	1740	0	1767	38	0
1	G	1667	0	1693	35	0
2	C	10401	0	10414	216	0
2	H	10401	0	10414	232	0
3	D	10085	0	10303	380	2
3	I	10126	0	10341	316	0
4	J	1165	0	1145	26	0
4	K	1165	0	1145	30	0
All	All	50147	0	50675	1182	2

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 12.

The worst 5 of 1182 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:I:1001:ALA:HA	3:I:1020:TRP:HE1	1.12	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:29:HIS:HB3	4:K:82:LEU:HG	1.35	1.06
3:D:226:ALA:HB1	3:D:227:PHE:HA	1.31	1.06
3:D:1001:ALA:HA	3:D:1020:TRP:HE1	1.12	1.06
3:D:247:PRO:HB3	3:I:53:ARG:HH12	1.18	1.06

All (2) 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)
3:D:184:ALA:O	3:D:191:SER:OG[2_957]	2.03	0.17
3:D:1183:SER:OG	3:D:1183:SER:OG[2_957]	2.12	0.08

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	223/242 (92%)	182 (82%)	29 (13%)	12 (5%)	2	29
1	B	211/242 (87%)	175 (83%)	27 (13%)	9 (4%)	3	34
1	F	223/242 (92%)	183 (82%)	28 (13%)	12 (5%)	2	29
1	G	212/242 (88%)	177 (84%)	26 (12%)	9 (4%)	3	34
2	C	1316/1342 (98%)	1108 (84%)	172 (13%)	36 (3%)	6	45
2	H	1316/1342 (98%)	1110 (84%)	168 (13%)	38 (3%)	6	43
3	D	1294/1407 (92%)	1023 (79%)	190 (15%)	81 (6%)	2	25
3	I	1300/1407 (92%)	1024 (79%)	197 (15%)	79 (6%)	2	26
4	J	141/181 (78%)	123 (87%)	15 (11%)	3 (2%)	9	50
4	K	141/181 (78%)	117 (83%)	18 (13%)	6 (4%)	3	34
All	All	6377/6828 (93%)	5222 (82%)	870 (14%)	285 (4%)	3	33

5 of 285 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	67	GLU
1	A	114	ASP
1	A	155	ALA
1	B	114	ASP

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	193/208 (93%)	191 (99%)	2 (1%)	82	92
1	B	184/208 (88%)	182 (99%)	2 (1%)	80	91
1	F	193/208 (93%)	192 (100%)	1 (0%)	92	96
1	G	185/208 (89%)	183 (99%)	2 (1%)	80	91
2	C	1137/1157 (98%)	1121 (99%)	16 (1%)	74	89
2	H	1137/1157 (98%)	1120 (98%)	17 (2%)	72	88
3	D	1087/1168 (93%)	1048 (96%)	39 (4%)	42	74
3	I	1091/1168 (93%)	1054 (97%)	37 (3%)	44	75
4	J	128/158 (81%)	122 (95%)	6 (5%)	32	68
4	K	128/158 (81%)	121 (94%)	7 (6%)	27	63
All	All	5463/5798 (94%)	5334 (98%)	129 (2%)	57	82

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1347	LEU
2	H	1041	ASP
4	J	109	ASP
1	G	14	VAL
2	H	443	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	777	HIS
1	G	41	ASN
3	I	495	ASN
3	D	1249	ASN
3	D	1366	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	225/242 (92%)	1.34	64 (28%) 1 5	267, 330, 380, 416	0
1	B	215/242 (88%)	2.69	114 (53%) 0 3	266, 335, 388, 430	0
1	F	225/242 (92%)	1.26	55 (24%) 1 6	248, 320, 383, 403	0
1	G	216/242 (89%)	2.10	91 (42%) 0 4	279, 337, 380, 412	0
2	C	1319/1342 (98%)	1.62	431 (32%) 1 5	232, 313, 384, 510	0
2	H	1319/1342 (98%)	1.75	450 (34%) 0 4	231, 315, 383, 482	0
3	D	1302/1407 (92%)	1.65	415 (31%) 1 5	230, 326, 424, 473	0
3	I	1306/1407 (92%)	2.06	498 (38%) 0 4	231, 332, 431, 492	0
4	J	147/181 (81%)	1.64	49 (33%) 0 5	300, 384, 446, 483	0
4	K	147/181 (81%)	2.13	59 (40%) 0 4	324, 413, 469, 491	0
All	All	6421/6828 (94%)	1.78	2226 (34%) 0 4	230, 324, 419, 510	0

The worst 5 of 2226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	314	ARG	18.1
3	I	989	GLY	17.0
2	H	788	SER	16.3
3	I	315	ALA	15.7
3	D	315	ALA	15.4

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.