wwPDB X-ray Structure Validation Summary Report (i)

Sep 24, 2023 – 06:38 AM EDT

PDB ID	:	5UAG
Title	:	Escherichia coli RNA polymerase mutant - RpoB D516V
Authors	:	Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on	:	2016-12-19
Resolution	:	3.40 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:

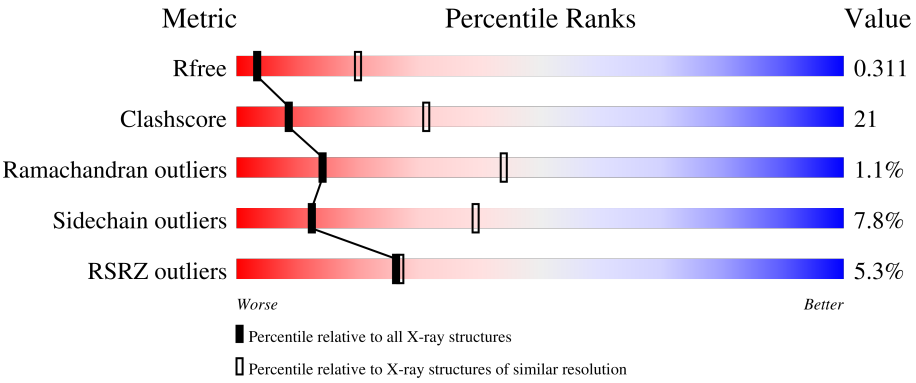
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	320	% 39% 30% 27%
1	B	320	7% 32% 32% 32%
1	G	320	3% 36% 30% 29%
1	H	320	7% 32% 32% 32%
2	C	1342	4% 57% 39%

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Mol	Chain	Length	Quality of chain
2	I	1342	7% 58% 38%
3	D	1407	2% 47% 31% 17%
3	J	1407	4% 45% 33% 18%
4	E	90	3% 60% 30% 9%
4	K	90	22% 54% 27% 7% 12%
5	F	613	4% 45% 28% 24%
5	L	613	4% 45% 28% 23%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 55066 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	233	Total	C	N	O	S	0	0	0
			1812	1127	323	356	6			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	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
			10569	6632	1841	2053	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10565	6630	1840	2052	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2
I	516	VAL	ASP	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	1167	Total	C	N	O	S	0	0	0
			9065	5700	1622	1697	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	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	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	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	2	Total	Mg	0	0
			2	2		
6	I	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).

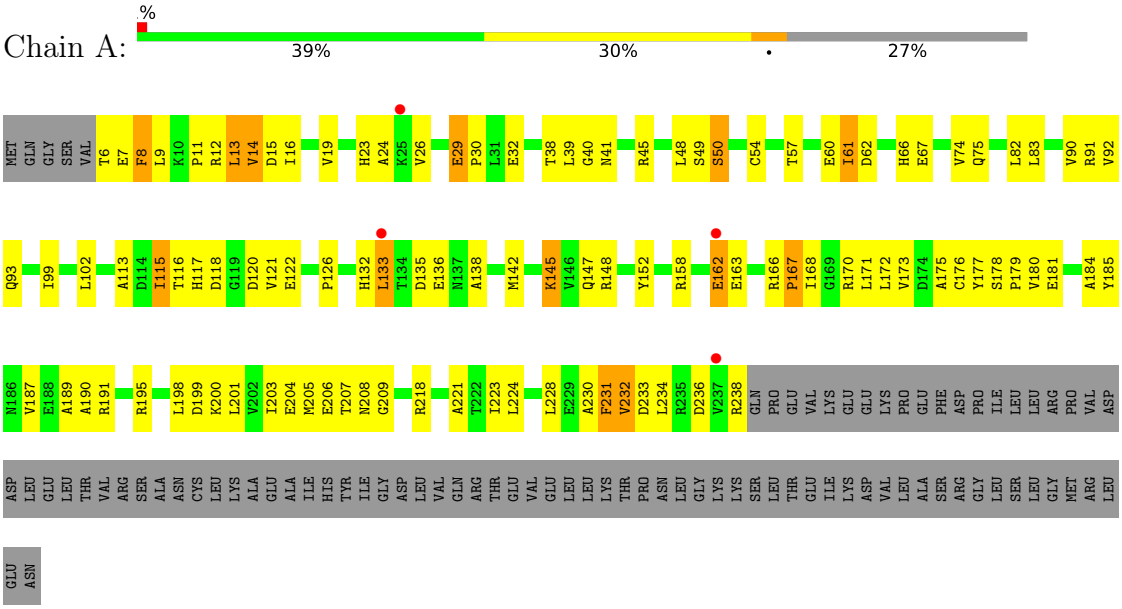
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	J	2	Total	Zn	0	0
			2	2		

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.

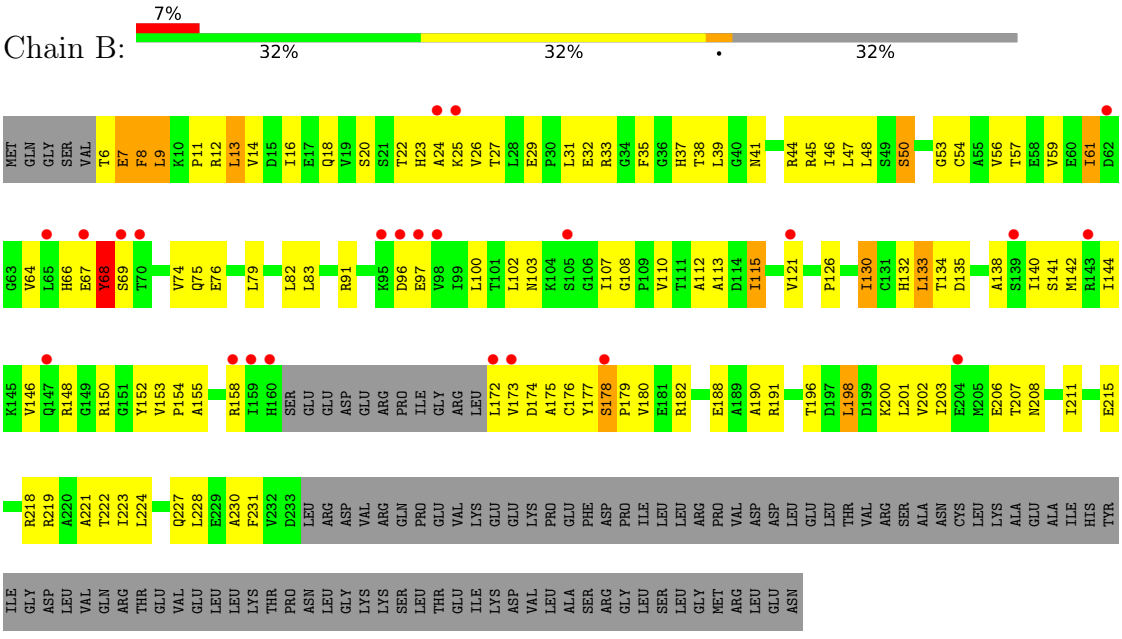
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



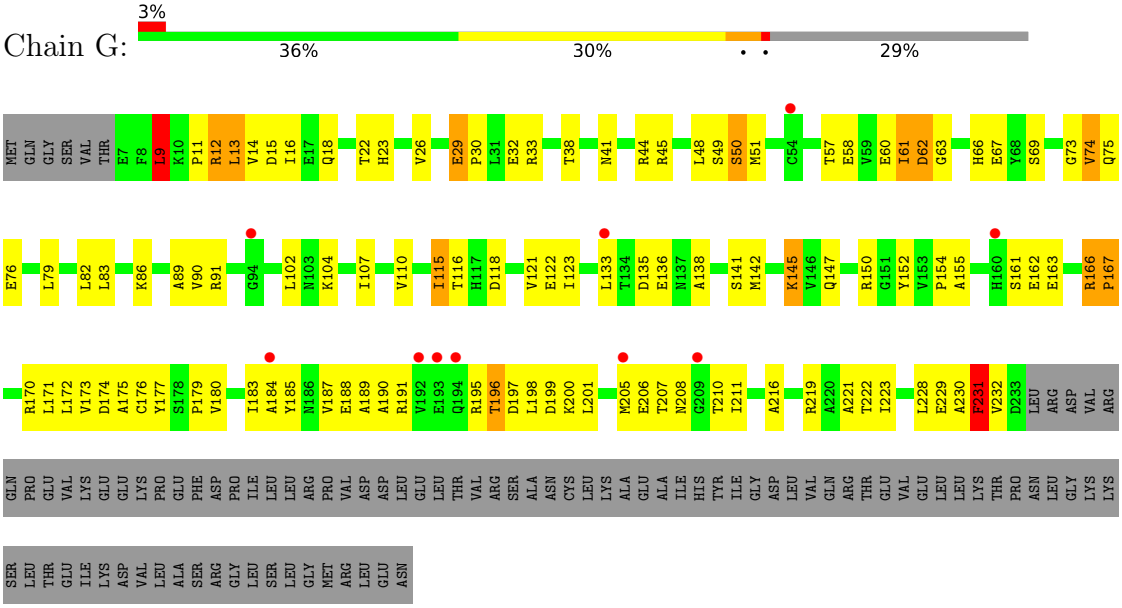
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



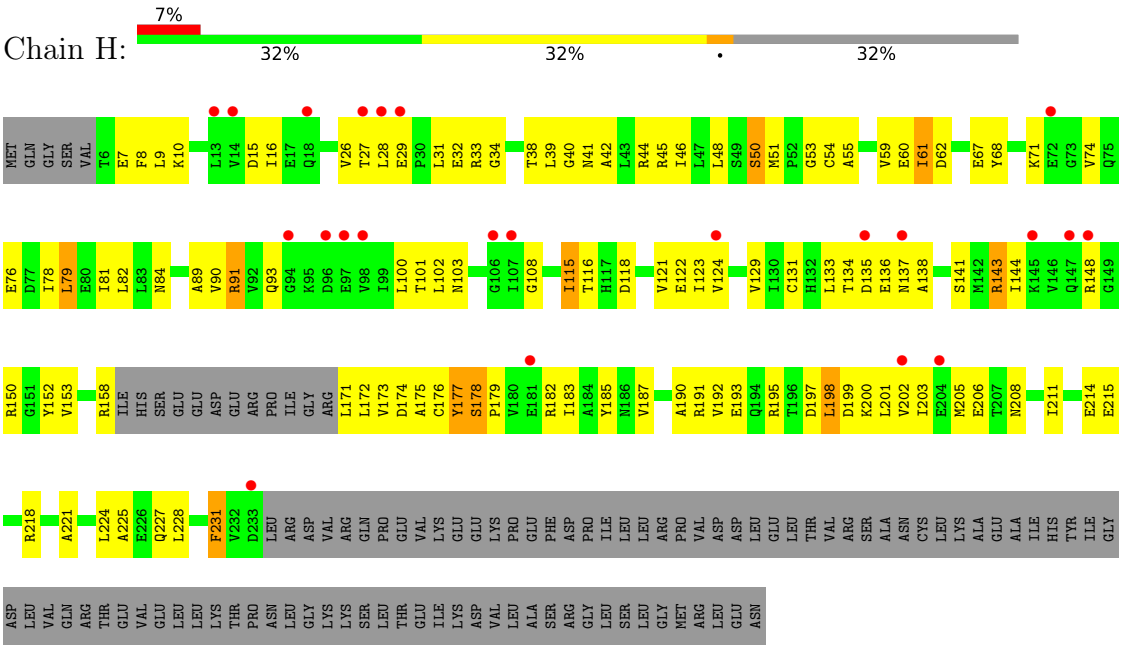
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



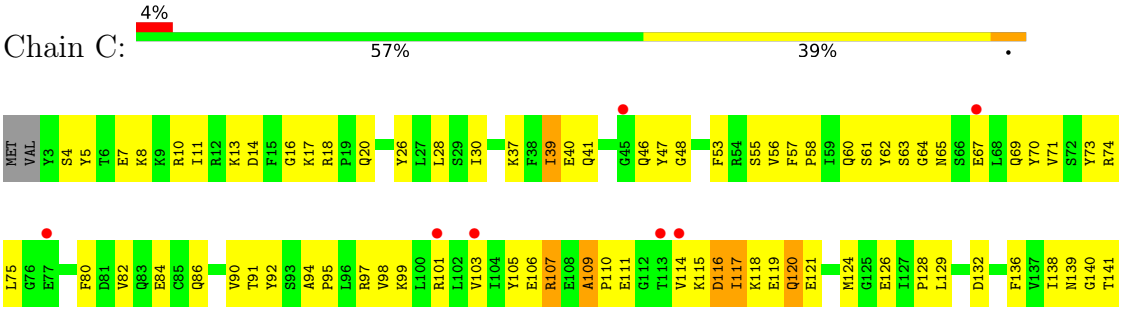
• Molecule 1: DNA-directed RNA polymerase subunit alpha

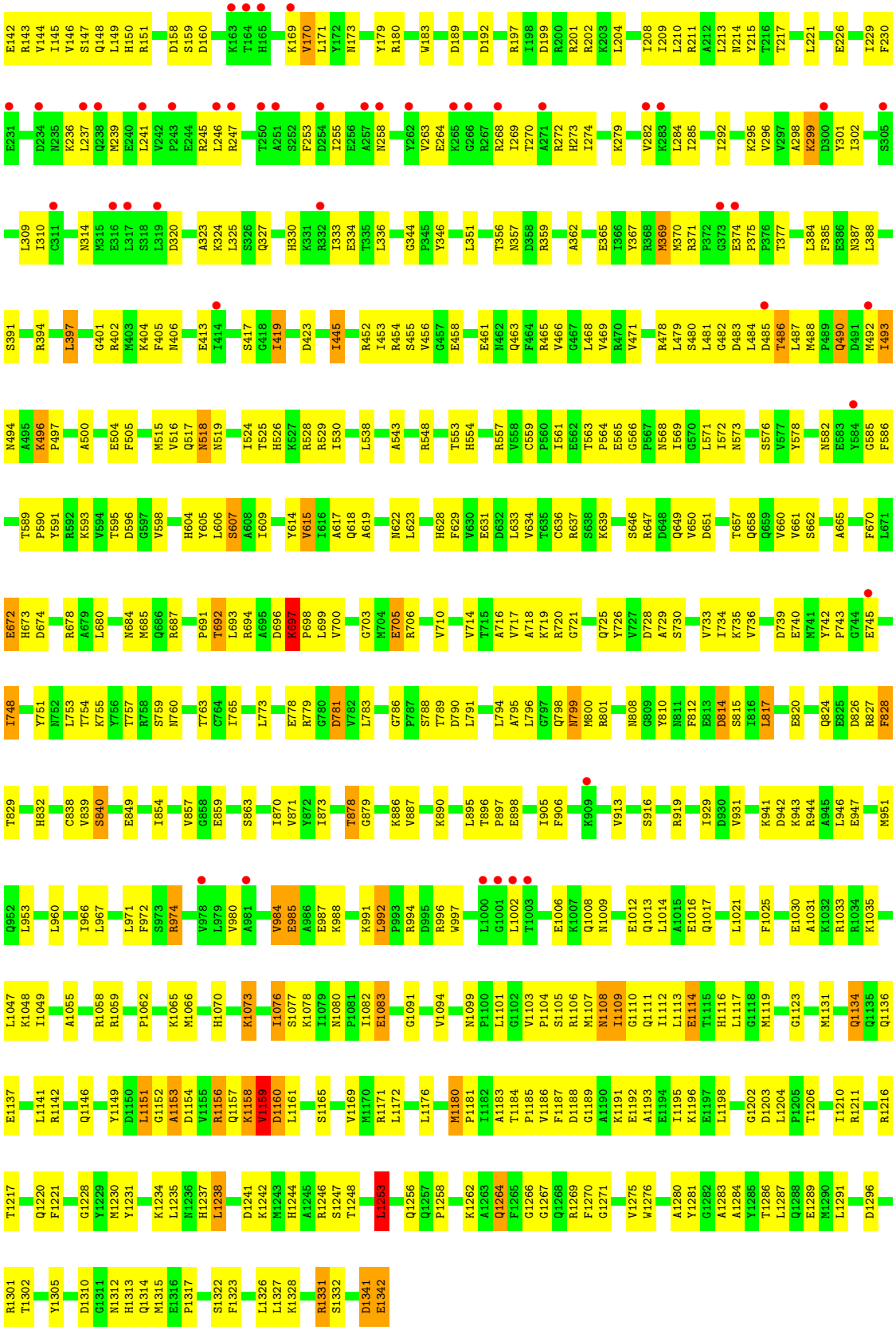
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

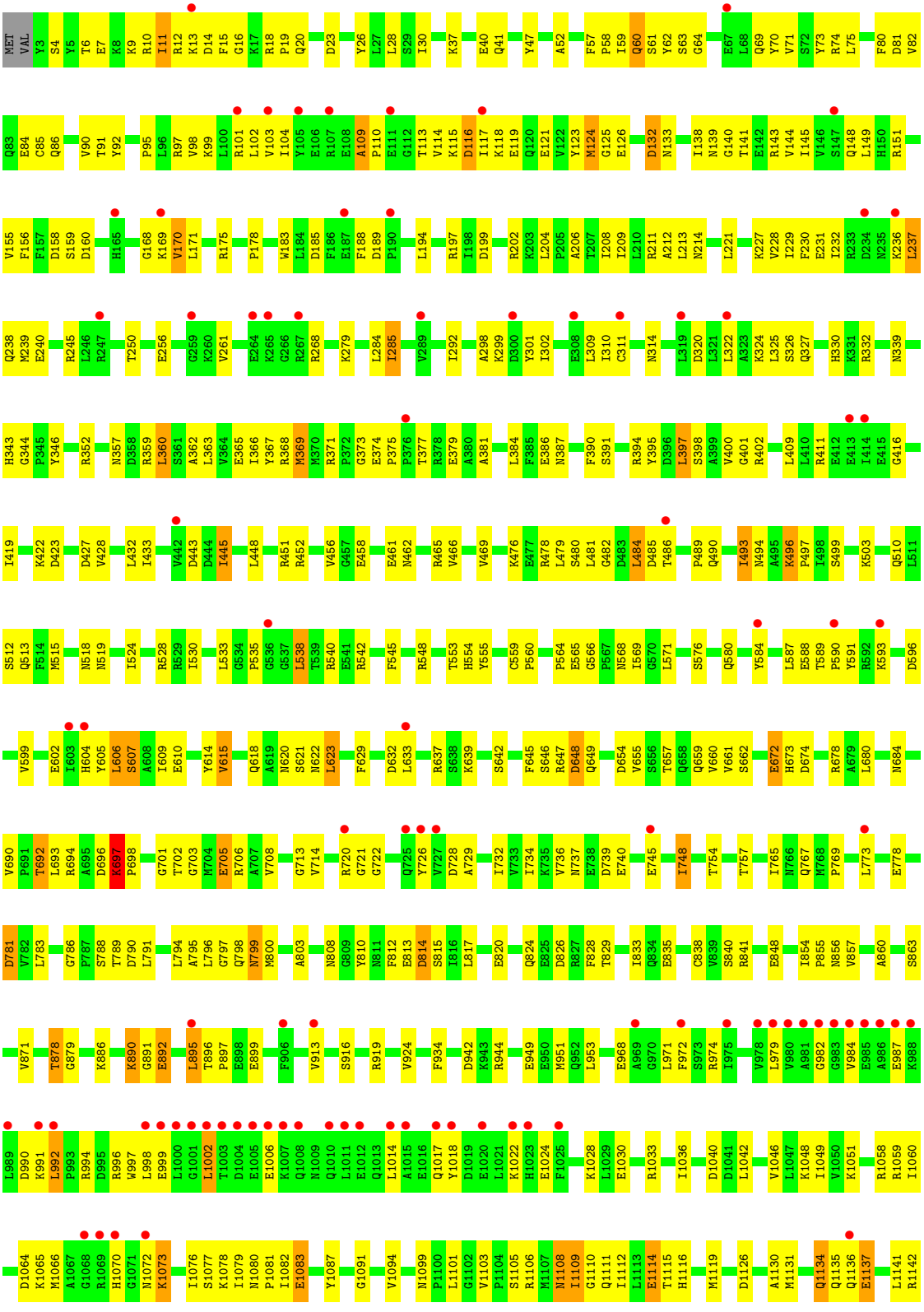


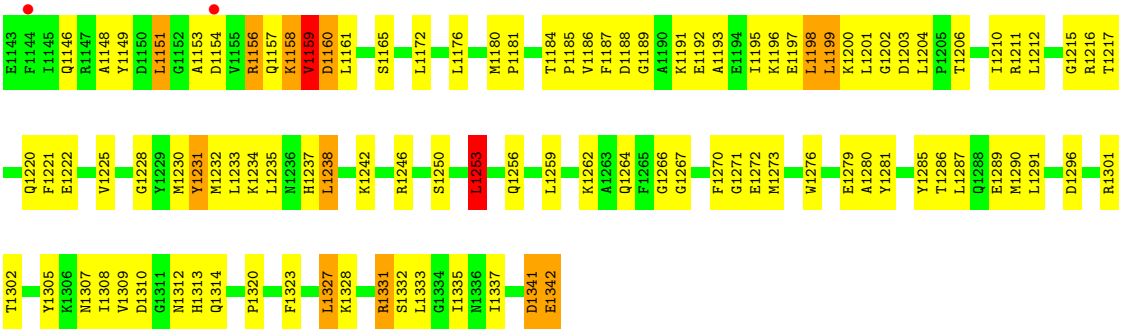


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I:

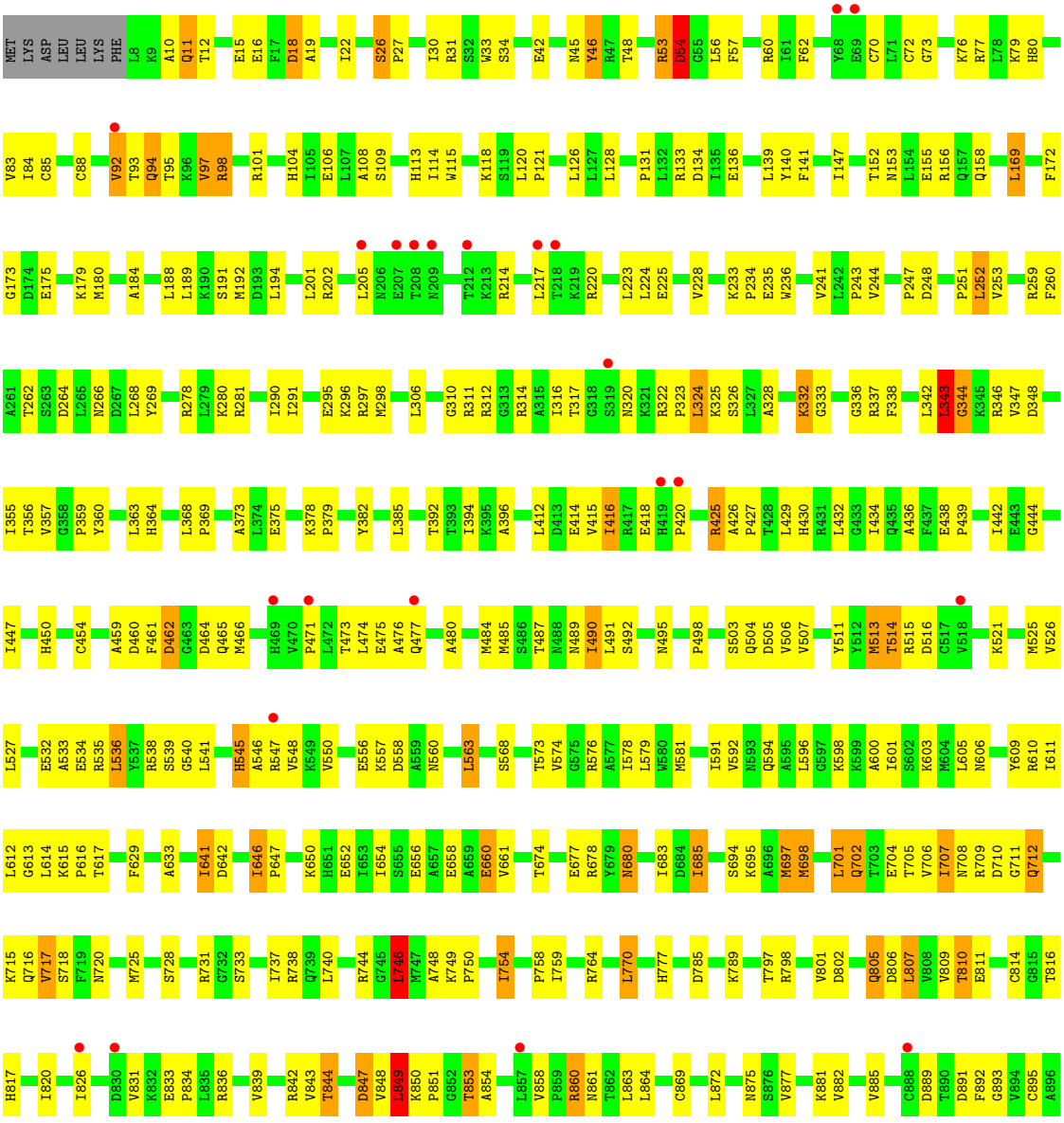

7%
58%
38%

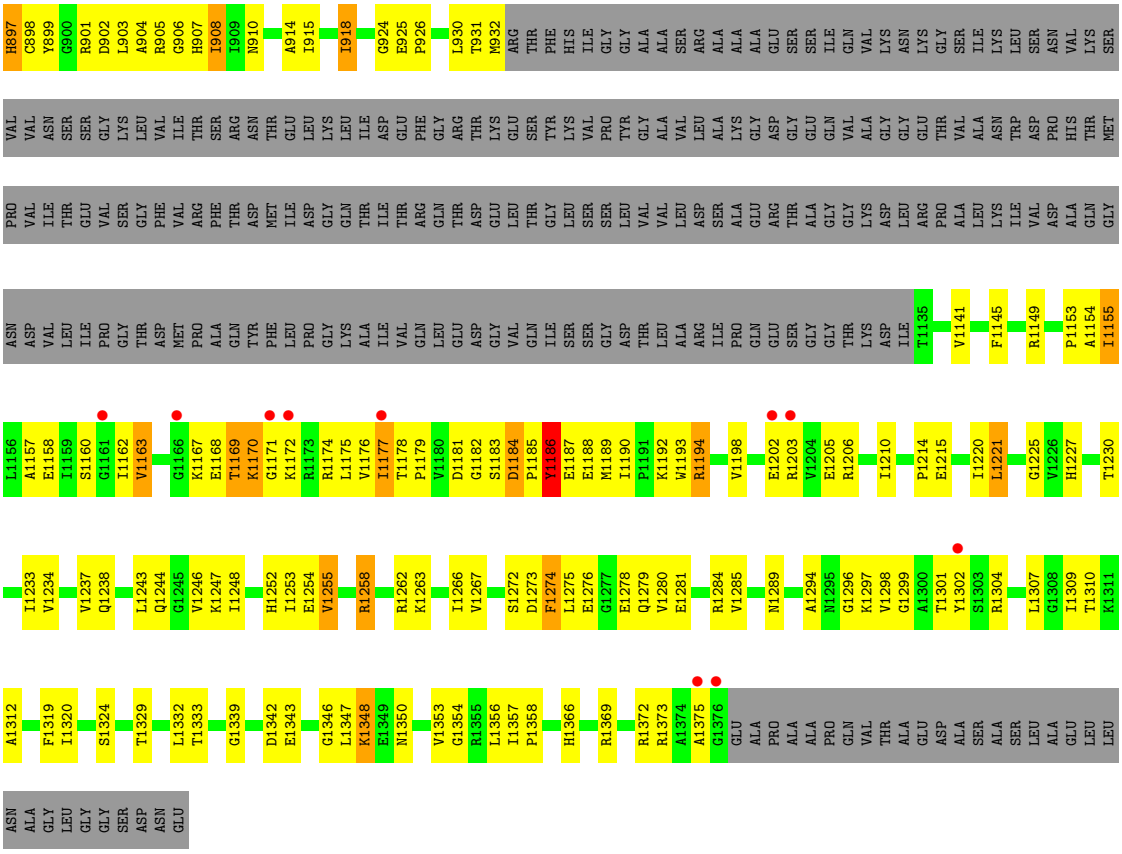

MET VAL Y3 S4 Y5 T6 E7 K8 K9 R10 I11 R12 K13 D14 F15 G16 K17 R18 P19 Q20 D23 Y26 L27 L28 S29 I30 K37 E40 Q41 Y47 A52 F57 P58 I59 Q60 S61 Y62 S63 G64 E67 L68 Q69 Y70 V71 S72 Y73 R74 L75 F80 D81 V82
Q83 E84 C85 Q86 V90 T91 Y92 P95 L96 R97 V98 K99 L100 R101 L102 V103 I104 Y105 E106 R107 E108 A109 P110 E111 G112 T113 V114 K115 D116 I117 K118 E119 Q120 E121 V122 Y123 M124 G125 E126 D132 N133 I138 N139 G140 T141 E142 R143 V144 I145 V146 S147 Q148 L149 H150 R151
V155 F156 F157 D158 S159 D160 H165 G168 K169 V170 L171 R175 P178 W183 L184 D185 F186 E187 F188 D189 P190 L194 R197 I198 D199 R202 K203 L204 P205 A206 T207 I208 I209 L210 R211 A212 L213 N214 L221 K227 V228 I229 F230 E231 I232 R233 D234 N235 K236 L237
Q238 M239 E240 R245 L246 R247 T250 E256 G259 K260 V261 E264 K265 G266 R267 R268 K279 L284 I285 V289 I292 A298 K299 D300 Y301 I302 E308 L309 I310 C311 N314 L319 D320 L321 L322 A323 K324 L325 S326 Q327 H330 K331 R332 N339
H343 G344 P345 Y346 R352 N357 D358 R359 L360 S361 A362 L363 V364 E365 I366 Y367 R368 M369 M370 R371 P372 G373 E374 P375 P376 T377 R378 E379 A380 A381 L384 F385 E386 N387 F390 S391 R394 Y395 D396 L397 S398 A399 V400 G401 R402 L409 L410 R411 E412 E413 I414 E415 G416
I419 K422 D423 D427 V428 L432 I433 V442 D443 D444 I445 L448 R451 R452 V456 G457 E458 E461 N462 R465 V466 V469 K476 E477 R478 L479 S480 L481 G482 D483 L484 D485 T486 P489 Q490 I493 N494 A495 K496 P497 I498 S499 K503 Q510 L511
S512 Q513 F514 M515 N518 N519 I524 R528 R529 I530 L533 G534 P535 G536 G537 L538 T539 R540 E541 R542 F545 R548 T553 H554 Y555 C559 P560 P564 E565 G566 P567 N568 I569 G570 L571 S576 Q580 Y584 L587 E588 T589 P590 Y591 R592 K593 D596
V599 E602 I603 H604 Y605 L606 S607 A608 I609 E610 Y614 V615 Q618 A619 N620 S621 N622 L623 F629 D632 L633 R637 S638 K639 S642 F645 S646 R647 D648 Q649 D654 V655 S656 T657 Q658 Q659 V660 V661 S662 E672 H673 D674 R678 A679 L680 N684
V690 P691 T692 L693 R694 A695 D696 K697 P698 G701 T702 G703 M704 E705 R706 A707 V708 G713 V714 R720 G721 G722 Q725 Y726 V727 D728 A729 I732 V733 I734 K735 V736 N737 E738 D739 E740 E745 I748 T754 T757 I765 N766 Q767 M768 P769 L773 E778
D781 V782 L783 G786 P787 S788 T789 D790 L791 L794 A795 L796 G797 Q798 N799 M800 A803 N808 G809 Y810 N811 F812 E813 D814 S815 I816 L817 E820 Q824 E825 D826 R827 F828 T829 I833 Q834 E835 C838 V839 S840 R841 E848 I854 P855 N856 V857 A860 S863
V871 T878 G879 K886 K890 Q891 E892 L895 T896 P897 E898 E899 F906 V913 S916 R919 V924 F934 D942 K943 R944 E949 E950 M951 Q952 L953 E968 A969 G970 L971 F972 S973 R974 I975 V978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988
L989 D990 K991 L992 P993 R994 D995 R996 W997 L998 E999 L1000 G1001 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012 Q1013 L1014 A1015 E1016 Q1017 Y1018 D1019 E1020 L1021 K1022 H1023 E1024 F1025 K1028 L1029 E1030 R1033 I1036 D1040 D1041 L1042 V1046 L1047 K1048 I1049 V1050 K1051 R1058 R1059 I1060
D1064 K1065 M1066 A1067 G1068 R1069 H1070 G1071 N1072 K1073 I1076 S1077 K1078 I1079 N1080 P1081 I1082 E1083 Y1087 G1091 V1094 N1099 P1100 L1101 G1102 V1103 P1104 S1105 R1106 M1107 N1108 I1109 G1110 Q1111 I1112 L1113 E1114 T1115 H1116 M1119 D1126 A1130 M1131 Q1134 Q1135 Q1136 E1137 L1141 R1142



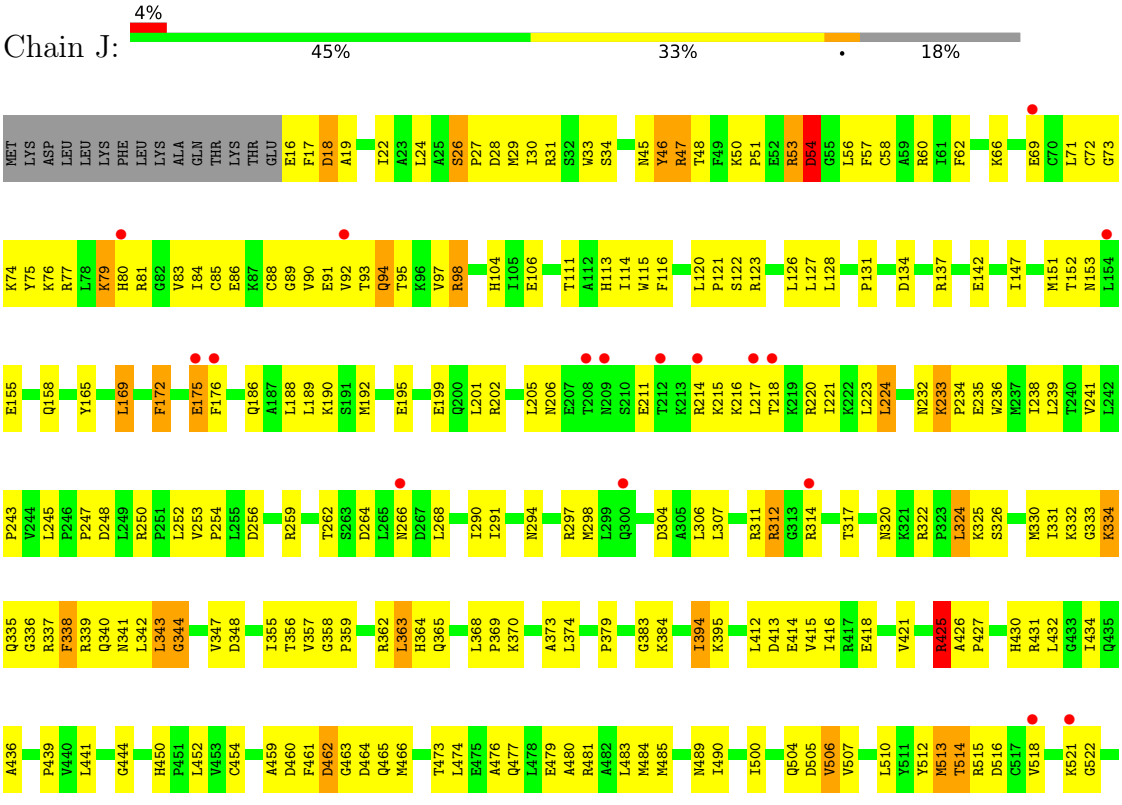
• Molecule 3: DNA-directed RNA polymerase subunit beta'

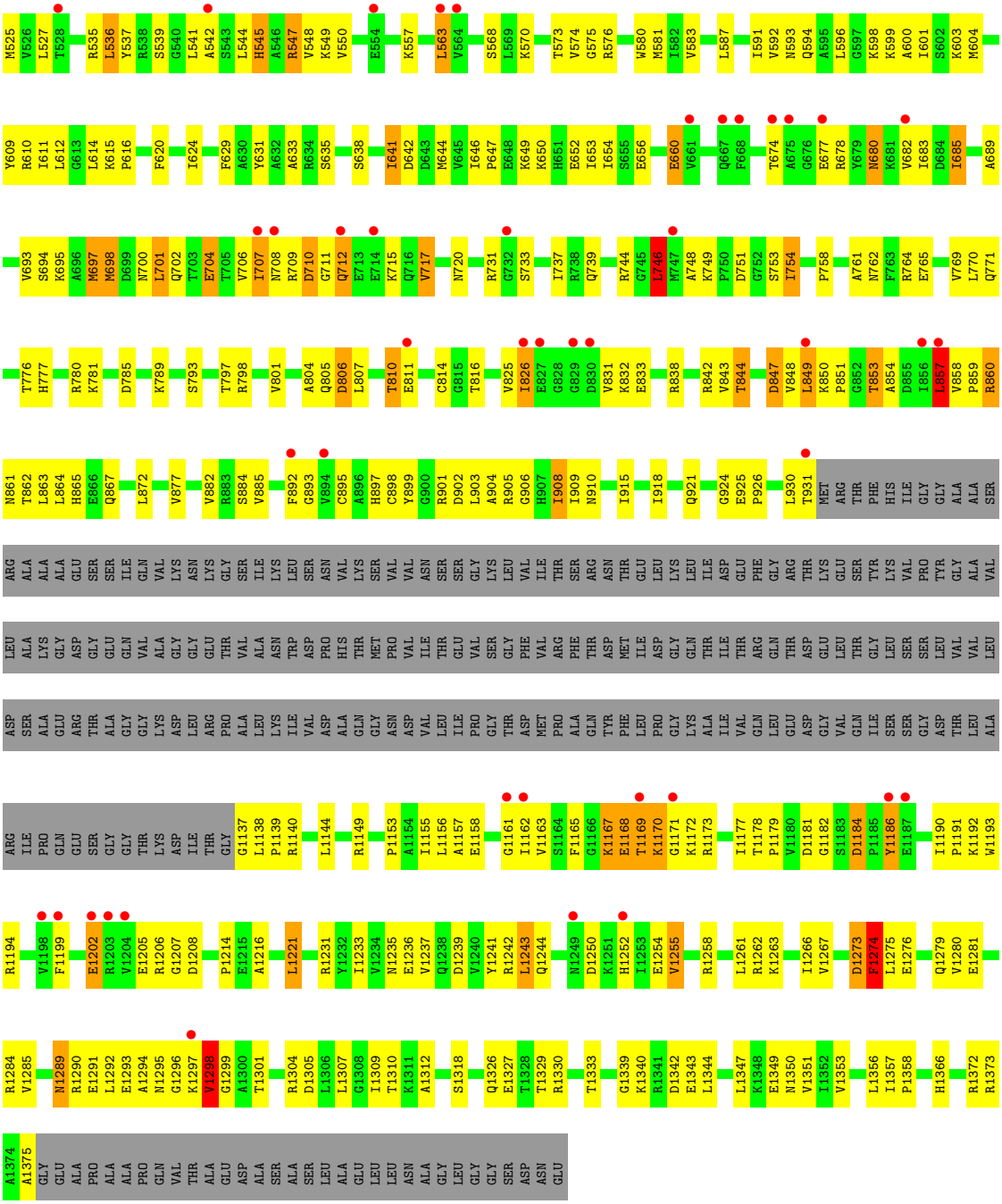
Chain D:



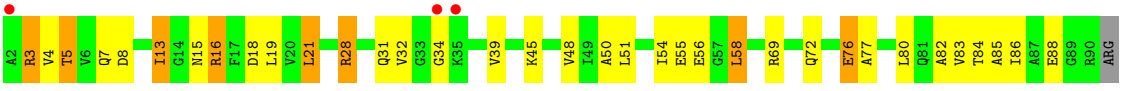


• Molecule 3: DNA-directed RNA polymerase subunit beta'

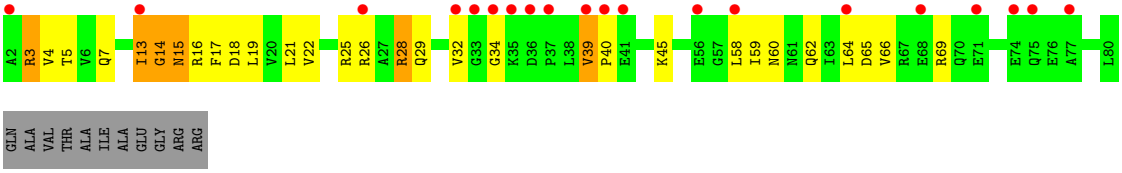




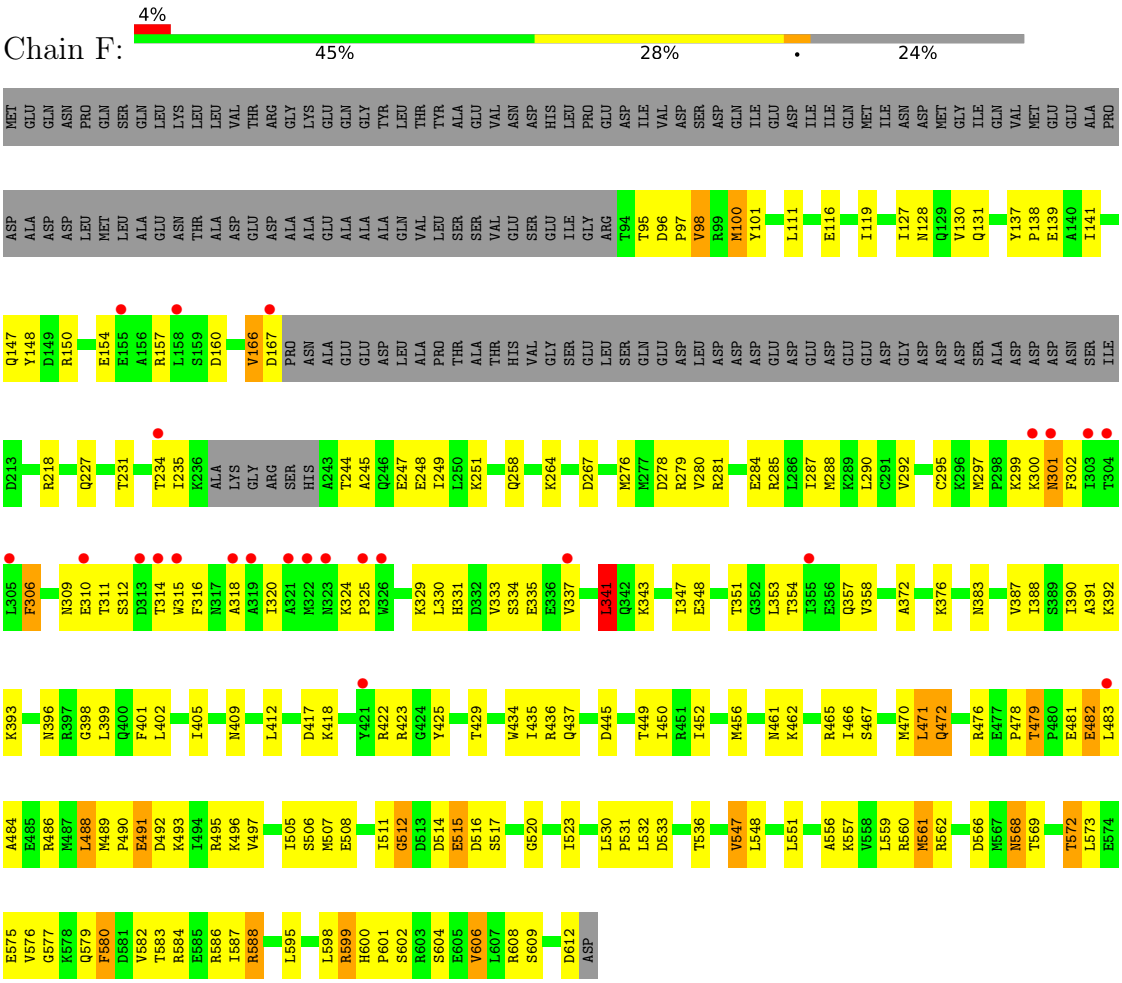
• Molecule 4: DNA-directed RNA polymerase subunit omega



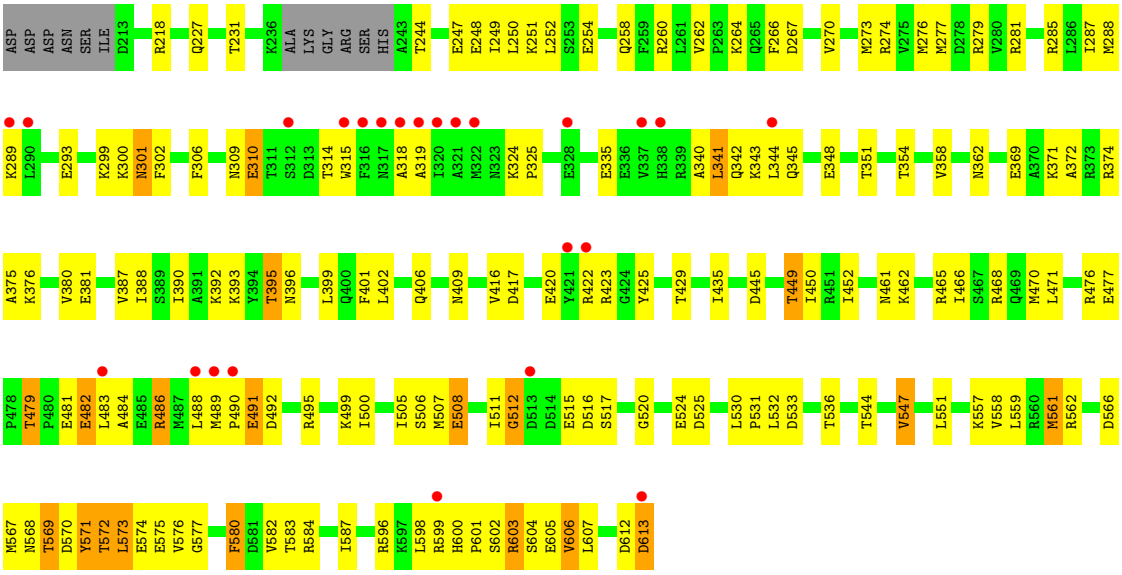
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD


ASP ASP ASP ASN SER ILE D213 R218 Q227 T231 K236 ALA LYS GLY ARG SER HIS A243 T244 E247 E248 I249 L250 K251 L252 S253 E254 Q258 F259 R260 L261 V262 P263 K264 Q265 F266 D267 V270 M273 R274 V275 M276 M277 D278 R279 V280 R281 R285 L286 I287 M288
K289 L290 E293 K299 K300 N301 F302 F306 N309 E310 T311 S312 D313 T314 W315 F316 N317 A318 A319 I320 A321 M322 N323 K324 P325 E328 E335 E336 V337 H338 R339 A340 L341 Q342 K343 L344 Q345 E348 T351 T354 V358 N362 E369 A370 K371 A372 R373 R374
A375 K376 V380 E381 V387 I388 S389 I390 A391 K392 K393 Y394 T395 N396 L399 Q400 F401 L402 Q406 N409 V416 D417 E420 Y421 R422 R423 G424 Y425 T429 I435 D445 T449 I450 R451 I452 N461 K462 R465 I466 S467 R468 Q469 M470 L471 R476 E477
P478 T479 P480 E481 E482 L483 A484 E485 R486 M487 L488 M489 P490 E491 D492 R495 K499 I500 I505 S506 M507 E508 I511 G512 D513 D514 E515 D516 S517 G520 E524 D525 L530 P531 L532 D533 T536 T544 V547 L551 K557 V558 L559 R560 M561 R562 D566
M567 N568 T569 D570 Y571 T572 L573 E574 E575 V576 G577 F580 D581 V582 T583 R584 I587 R596 K597 L598 R599 H600 P601 S602 R603 S604 E605 V606 L607 D612 D613

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	184.83Å 205.04Å 307.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.40 29.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.99-3.40) 89.0 (29.99-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.277 , 0.311 0.277 , 0.311	Depositor DCC
R_{free} test set	1977 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å^2)	135.9	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 85.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	55066	wwPDB-VP
Average B, all atoms (Å^2)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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	0.46	1/1834 (0.1%)	0.85	0/2485
1	B	0.45	0/1697	1.00	3/2300 (0.1%)
1	G	0.52	1/1777 (0.1%)	0.93	5/2408 (0.2%)
1	H	0.44	0/1681	0.98	3/2278 (0.1%)
2	C	0.44	0/10738	0.83	7/14488 (0.0%)
2	I	0.42	1/10734 (0.0%)	0.81	12/14483 (0.1%)
3	D	0.45	0/9205	0.84	12/12430 (0.1%)
3	J	0.45	0/9140	0.88	22/12341 (0.2%)
4	E	0.43	0/693	0.76	1/935 (0.1%)
4	K	0.43	0/629	0.81	2/847 (0.2%)
5	F	0.42	0/3864	0.83	5/5194 (0.1%)
5	L	0.43	0/3872	0.83	3/5205 (0.1%)
All	All	0.44	3/55864 (0.0%)	0.85	75/75394 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	C	0	4
2	I	0	2
3	D	0	2
3	J	0	3
4	E	0	1
5	L	0	1
All	All	0	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	29	GLU	C-N	9.36	1.52	1.34
2	I	373	GLY	C-N	7.20	1.50	1.34
1	A	29	GLU	C-N	6.31	1.46	1.34

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	425	ARG	NE-CZ-NH2	14.52	127.56	120.30
3	J	425	ARG	NE-CZ-NH1	-13.50	113.55	120.30
3	J	343	LEU	CB-CG-CD1	-11.67	91.16	111.00
1	G	12	ARG	NE-CZ-NH1	-10.66	114.97	120.30
3	D	343	LEU	CB-CG-CD2	-10.37	93.37	111.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
2	C	658	GLN	Sidechain
2	C	985	GLU	Mainchain
3	D	1184	ASP	Peptide

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	1812	0	1839	111	0
1	B	1677	0	1703	127	0
1	G	1755	0	1773	105	0
1	H	1662	0	1687	111	0
2	C	10569	0	10587	439	0
2	I	10565	0	10581	437	0
3	D	9065	0	9210	430	0
3	J	9001	0	9165	461	0
4	E	691	0	695	26	0
4	K	627	0	634	26	0
5	F	3813	0	3880	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	3821	0	3884	149	0
6	D	2	0	0	0	0
6	I	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	55066	0	55638	2292	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 21.

The worst 5 of 2292 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)
2:I:1271:GLY:HA2	3:J:343:LEU:HD11	1.25	1.18
2:C:1269:ARG:HG2	3:D:343:LEU:HD12	1.24	1.11
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.35	1.08
3:D:1167:LYS:HZ3	3:D:1170:LYS:HB2	1.18	1.06
3:J:54:ASP:OD2	3:J:60:ARG:NH1	1.89	1.03

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	231/320 (72%)	201 (87%)	25 (11%)	5 (2%)	6 29
1	B	213/320 (67%)	186 (87%)	24 (11%)	3 (1%)	11 37
1	G	225/320 (70%)	193 (86%)	26 (12%)	6 (3%)	5 26
1	H	212/320 (66%)	189 (89%)	19 (9%)	4 (2%)	8 31
2	C	1338/1342 (100%)	1229 (92%)	99 (7%)	10 (1%)	22 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	I	1338/1342 (100%)	1227 (92%)	100 (8%)	11 (1%)	19 51
3	D	1163/1407 (83%)	1067 (92%)	86 (7%)	10 (1%)	17 49
3	J	1151/1407 (82%)	1054 (92%)	81 (7%)	16 (1%)	11 37
4	E	87/90 (97%)	82 (94%)	5 (6%)	0	100 100
4	K	77/90 (86%)	72 (94%)	3 (4%)	2 (3%)	5 26
5	F	462/613 (75%)	421 (91%)	36 (8%)	5 (1%)	14 44
5	L	463/613 (76%)	422 (91%)	39 (8%)	2 (0%)	34 67
All	All	6960/8184 (85%)	6343 (91%)	543 (8%)	74 (1%)	14 44

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	232	VAL
2	C	170	VAL
2	C	484	LEU
2	C	1137	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
1	A	201/279 (72%)	192 (96%)	9 (4%)	27 58
1	B	186/279 (67%)	173 (93%)	13 (7%)	15 44
1	G	193/279 (69%)	182 (94%)	11 (6%)	20 50
1	H	183/279 (66%)	172 (94%)	11 (6%)	19 49
2	C	1155/1157 (100%)	1066 (92%)	89 (8%)	13 40
2	I	1154/1157 (100%)	1063 (92%)	91 (8%)	12 39
3	D	962/1168 (82%)	885 (92%)	77 (8%)	12 38
3	J	960/1168 (82%)	881 (92%)	79 (8%)	11 37
4	E	72/74 (97%)	64 (89%)	8 (11%)	6 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	67/74 (90%)	63 (94%)	4 (6%)	19 49
5	F	417/540 (77%)	381 (91%)	36 (9%)	10 35
5	L	418/540 (77%)	382 (91%)	36 (9%)	10 35
All	All	5968/6994 (85%)	5504 (92%)	464 (8%)	12 39

5 of 464 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	606	VAL
5	L	445	ASP
2	I	604	HIS
5	L	395	THR
3	J	844	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	1108	ASN
3	J	465	GLN
2	I	1116	HIS
3	J	206	ASN
3	J	910	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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	233/320 (72%)	-0.03	4 (1%) 70 68	105, 144, 198, 236	0
1	B	217/320 (67%)	0.49	23 (10%) 6 7	121, 192, 243, 265	0
1	G	227/320 (70%)	0.25	10 (4%) 34 34	162, 195, 234, 271	0
1	H	216/320 (67%)	0.61	23 (10%) 6 7	175, 215, 240, 264	0
2	C	1340/1342 (99%)	0.07	52 (3%) 39 38	78, 133, 242, 297	0
2	I	1340/1342 (99%)	0.33	93 (6%) 16 18	104, 171, 269, 334	0
3	D	1167/1407 (82%)	0.09	32 (2%) 54 53	83, 120, 204, 261	0
3	J	1155/1407 (82%)	0.24	60 (5%) 27 27	99, 146, 228, 277	0
4	E	89/90 (98%)	-0.03	3 (3%) 45 44	118, 156, 179, 198	0
4	K	79/90 (87%)	1.24	20 (25%) 0 0	211, 251, 298, 305	0
5	F	468/613 (76%)	0.17	24 (5%) 28 28	115, 167, 295, 326	0
5	L	469/613 (76%)	0.20	25 (5%) 26 27	130, 181, 301, 320	0
All	All	7000/8184 (85%)	0.21	369 (5%) 26 27	78, 156, 252, 334	0

The worst 5 of 369 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	7.7
2	C	319	LEU	7.0
2	I	1005	GLU	6.7
2	I	1000	LEU	6.6
2	I	999	GLU	6.5

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	2003	1/1	0.70	0.20	189,189,189,189	0
6	MG	D	2001	1/1	0.71	0.27	189,189,189,189	0
7	ZN	D	2004	1/1	0.74	0.29	189,189,189,189	0
6	MG	D	2002	1/1	0.78	0.29	189,189,189,189	0
6	MG	I	1401	1/1	0.85	0.30	189,189,189,189	0
6	MG	J	2001	1/1	0.85	0.29	189,189,189,189	0
7	ZN	J	2003	1/1	0.88	0.22	189,189,189,189	0
7	ZN	J	2002	1/1	0.94	0.13	310,310,310,310	0

6.5 Other polymers (i)

There are no such residues in this entry.