wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 06:32 am BST

PDB ID	:	4XLQ
Title	:	Crystal structure of T.aquaticus transcription initiation complex containing upstream fork (-11 base-paired) promoter
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2015-01-13
Resolution	:	4.60 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 following versions of software and data (see references (1)) were used in the production of this report:

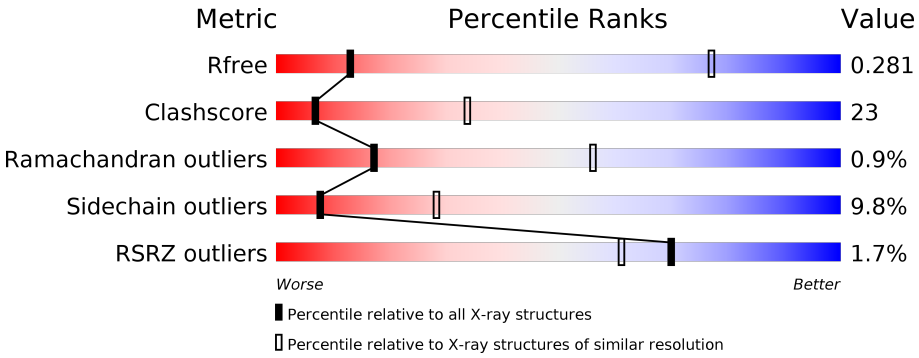
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.60 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	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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 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	314	40% 28% 28%
1	B	314	33% 34% 5% 28%
1	G	314	5% 36% 31% 5% 28%
1	H	314	35% 32% 5% 28%
2	C	1119	45% 48% 6%
2	I	1119	46% 47% 6%

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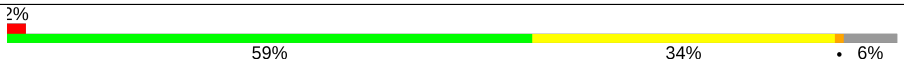
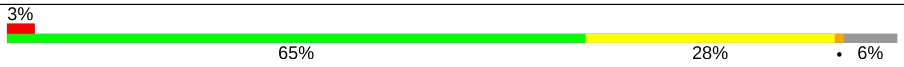
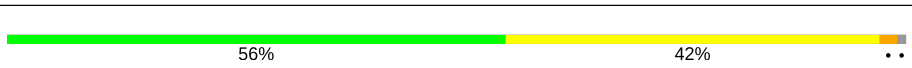
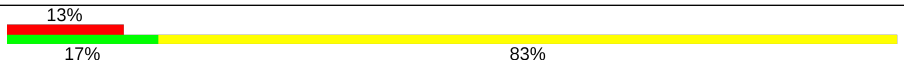
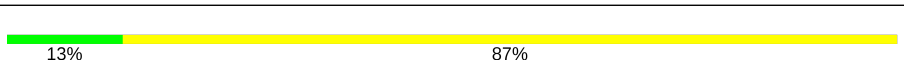
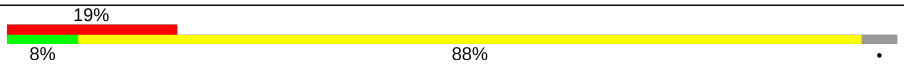
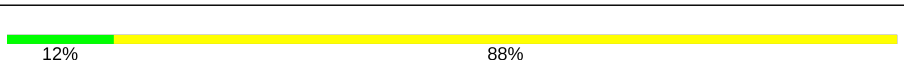
Mol	Chain	Length	Quality of chain
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	O	30	
6	R	30	
7	P	26	
7	S	26	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56477 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	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			
6	R	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			

- Molecule 7 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	25	Total	C	N	O	P	0	0	0
			510	245	91	149	25			
7	S	26	Total	C	N	O	P	0	0	0
			527	255	93	154	25			

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

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

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

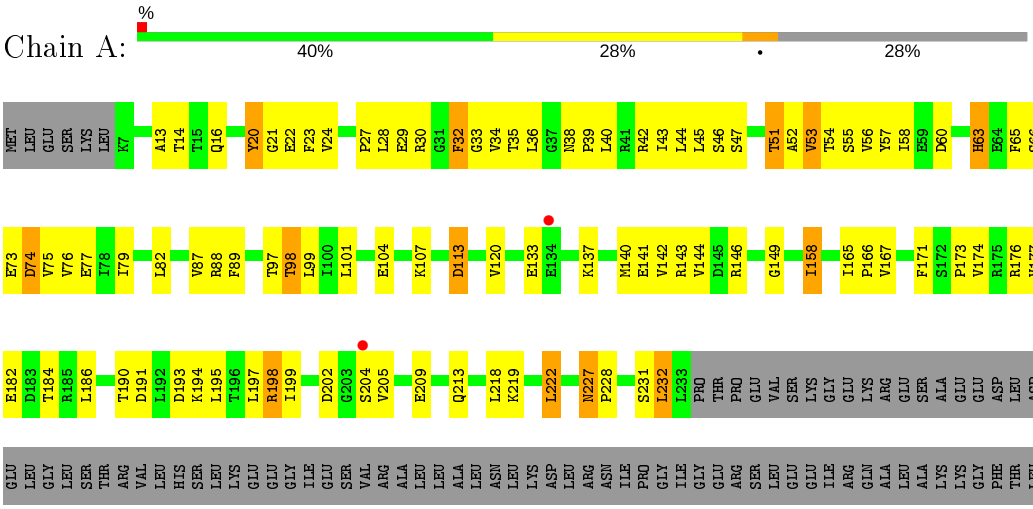
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

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 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.

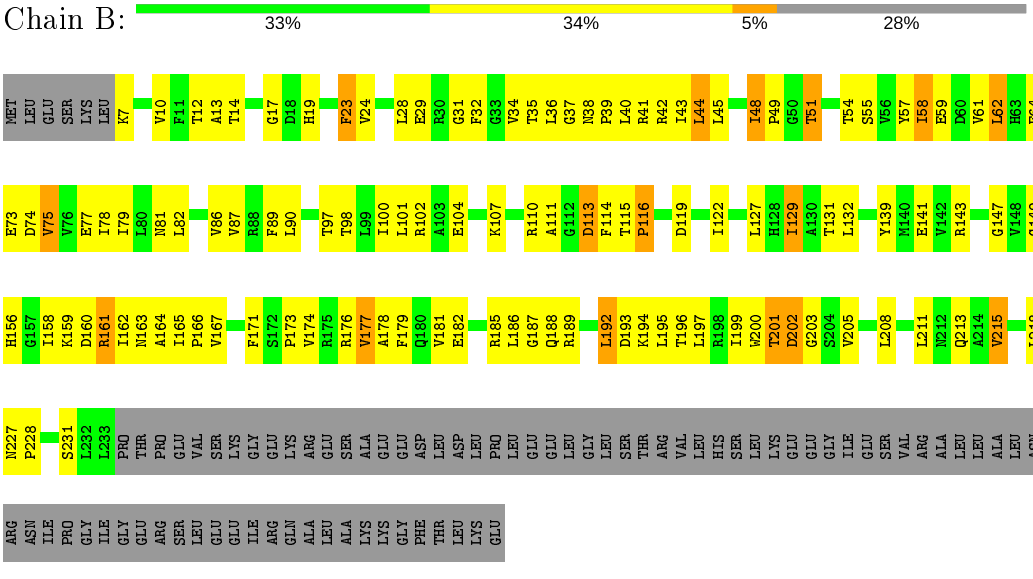
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



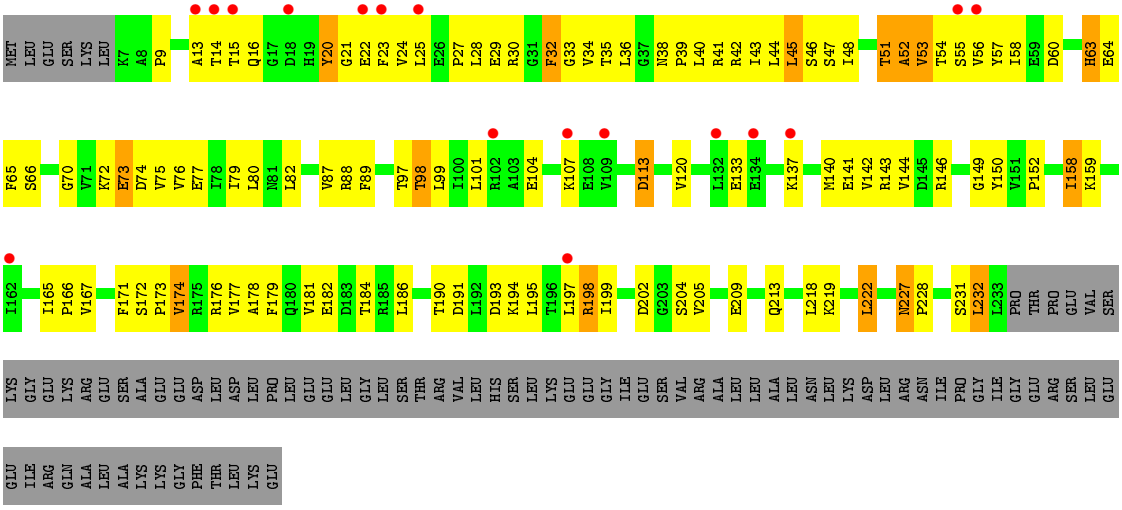
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



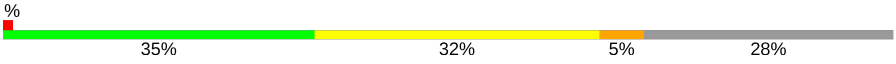
• Molecule 1: DNA-directed RNA polymerase subunit alpha

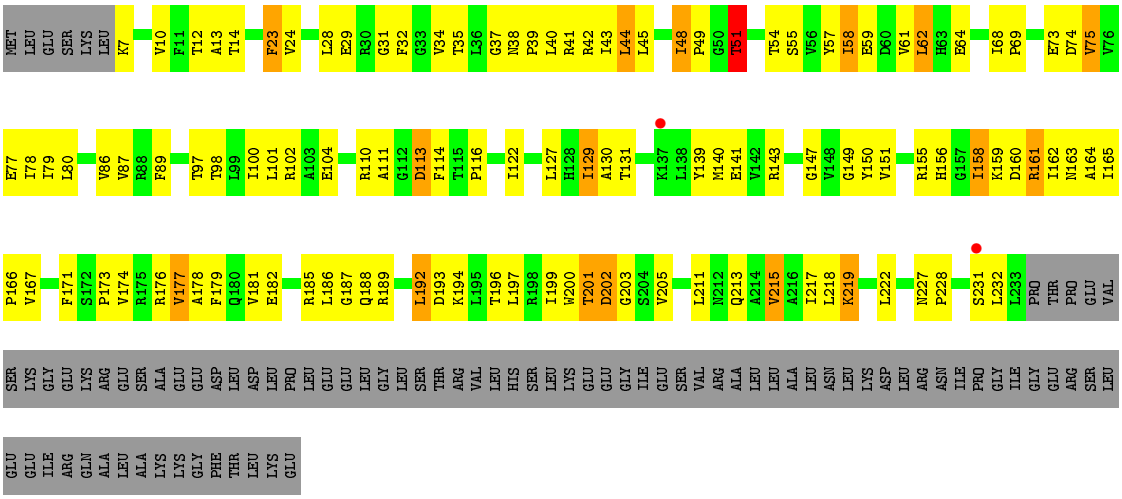
Chain G:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

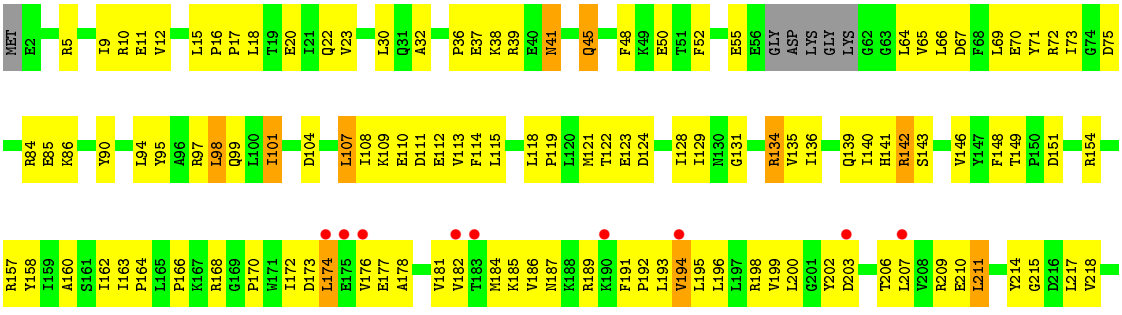
Chain H:

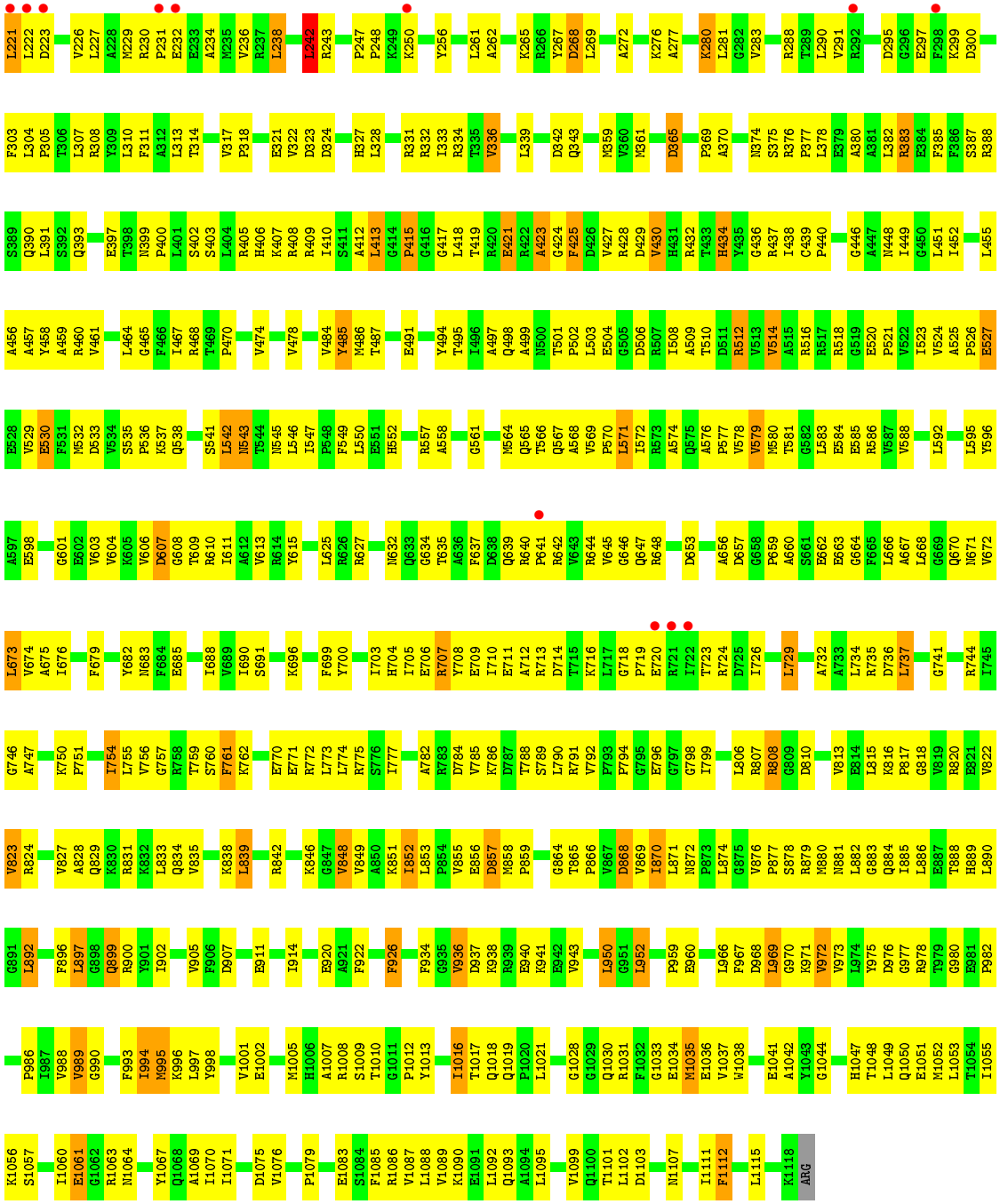




• Molecule 2: DNA-directed RNA polymerase subunit beta

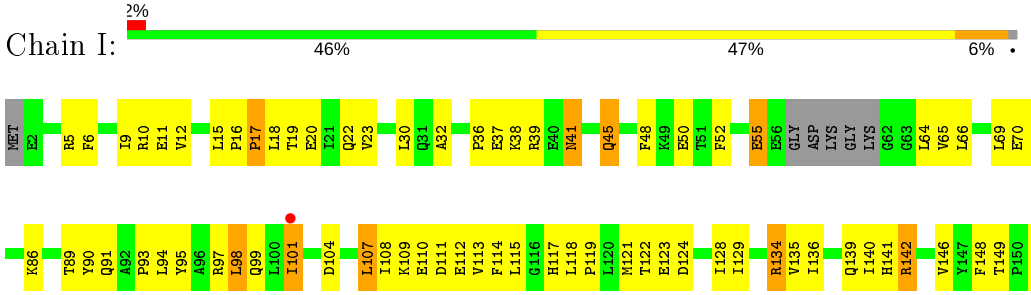
Chain C:

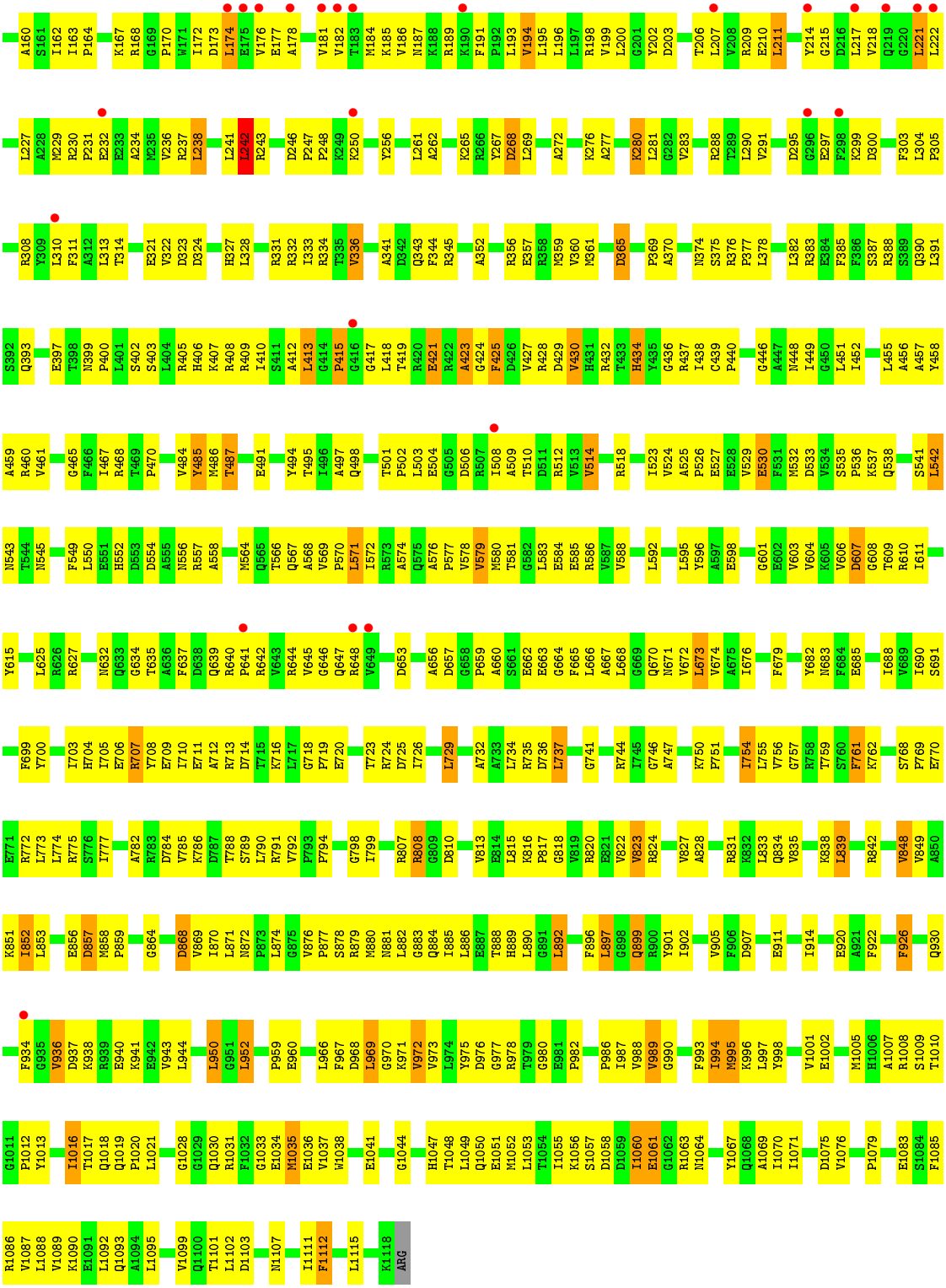




• Molecule 2: DNA-directed RNA polymerase subunit beta

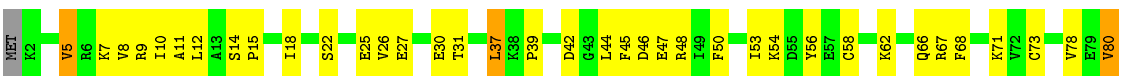
Chain I:

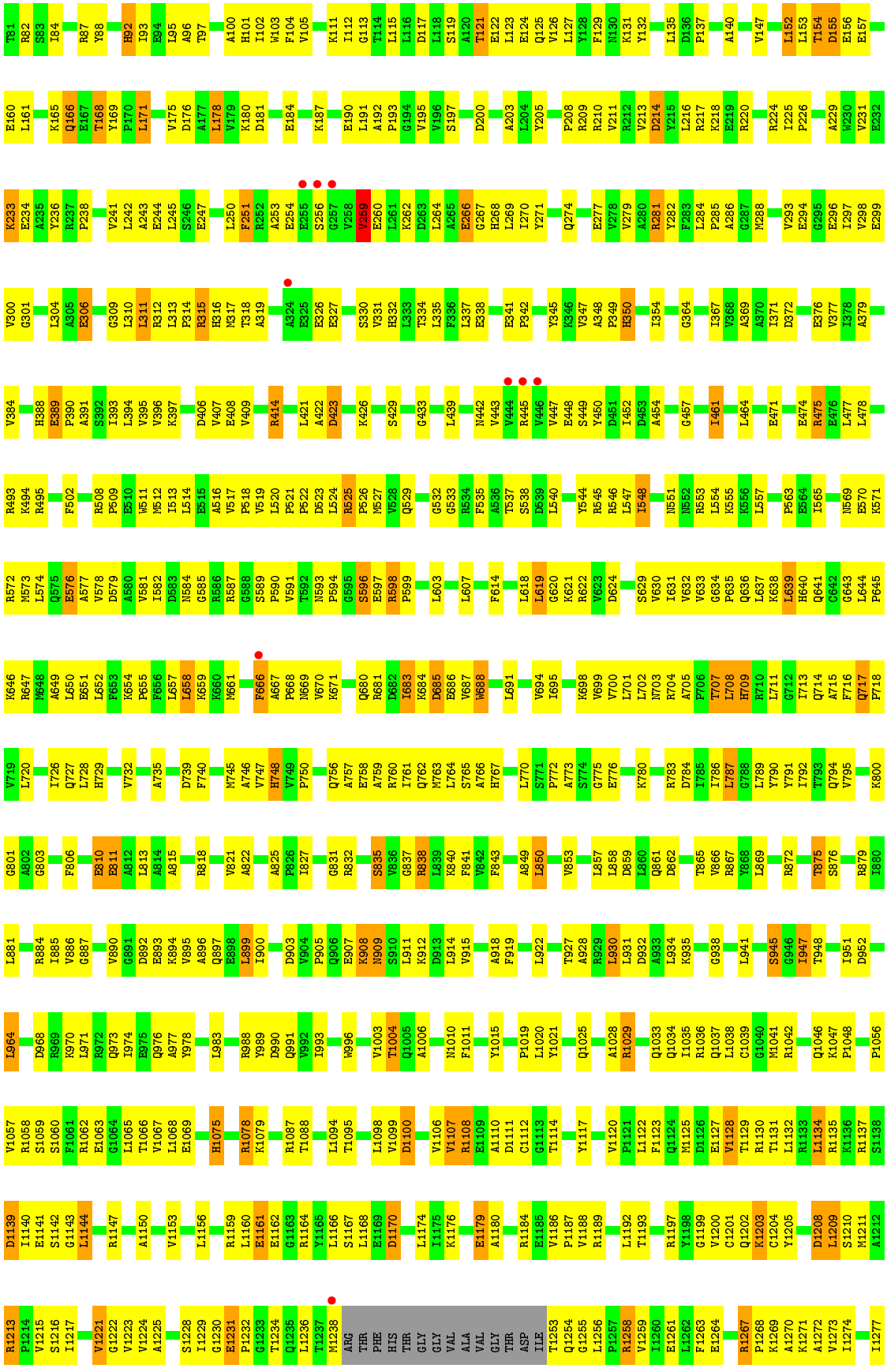


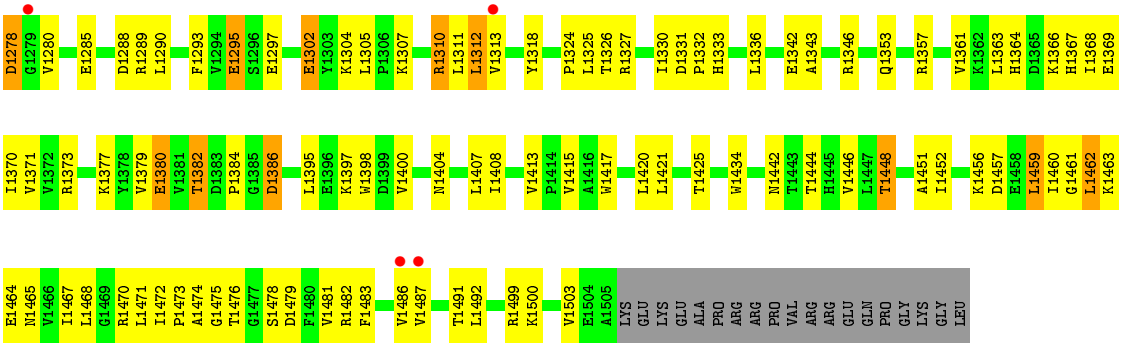


• Molecule 3: DNA-directed RNA polymerase subunit beta'

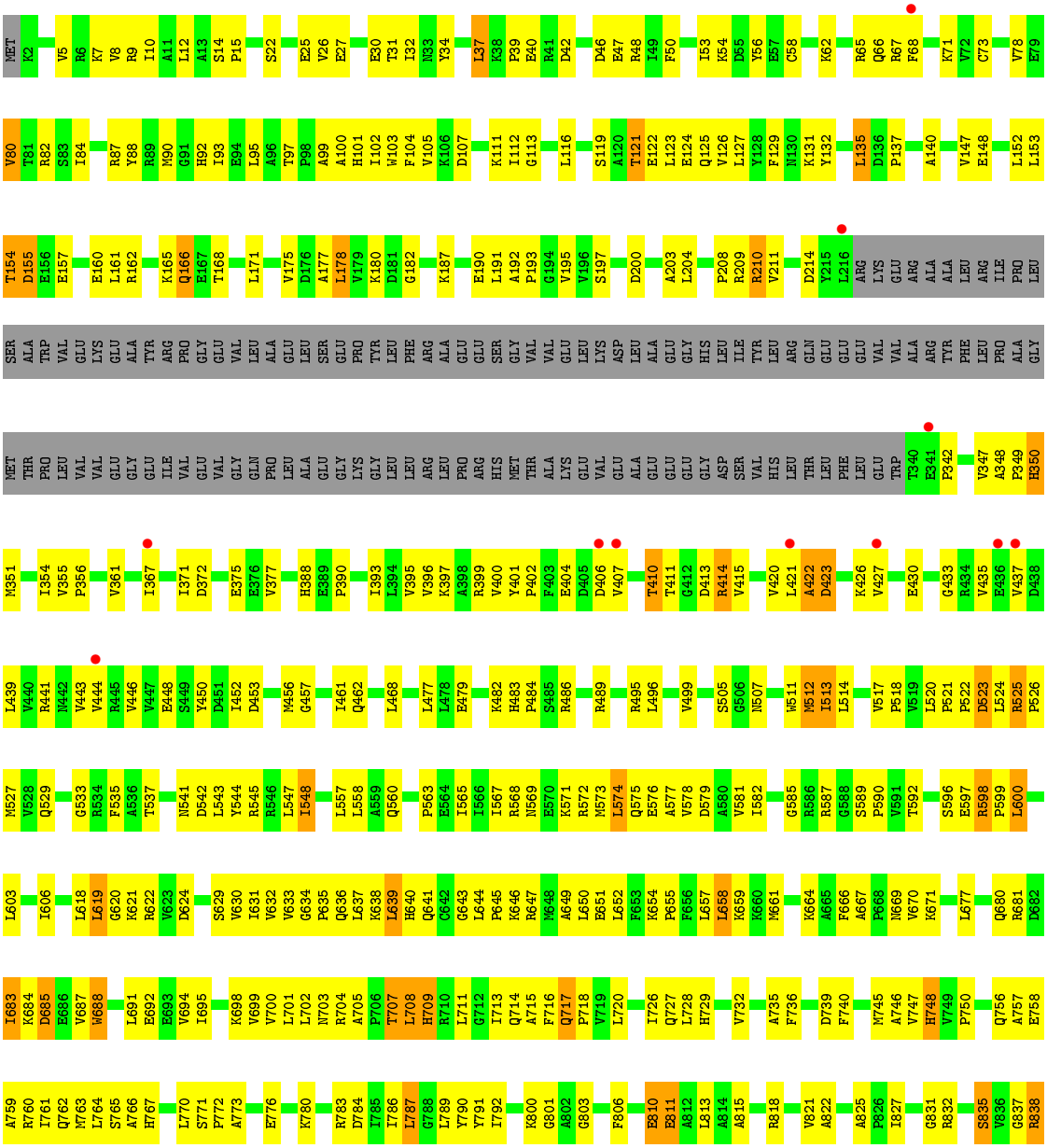
Chain D:

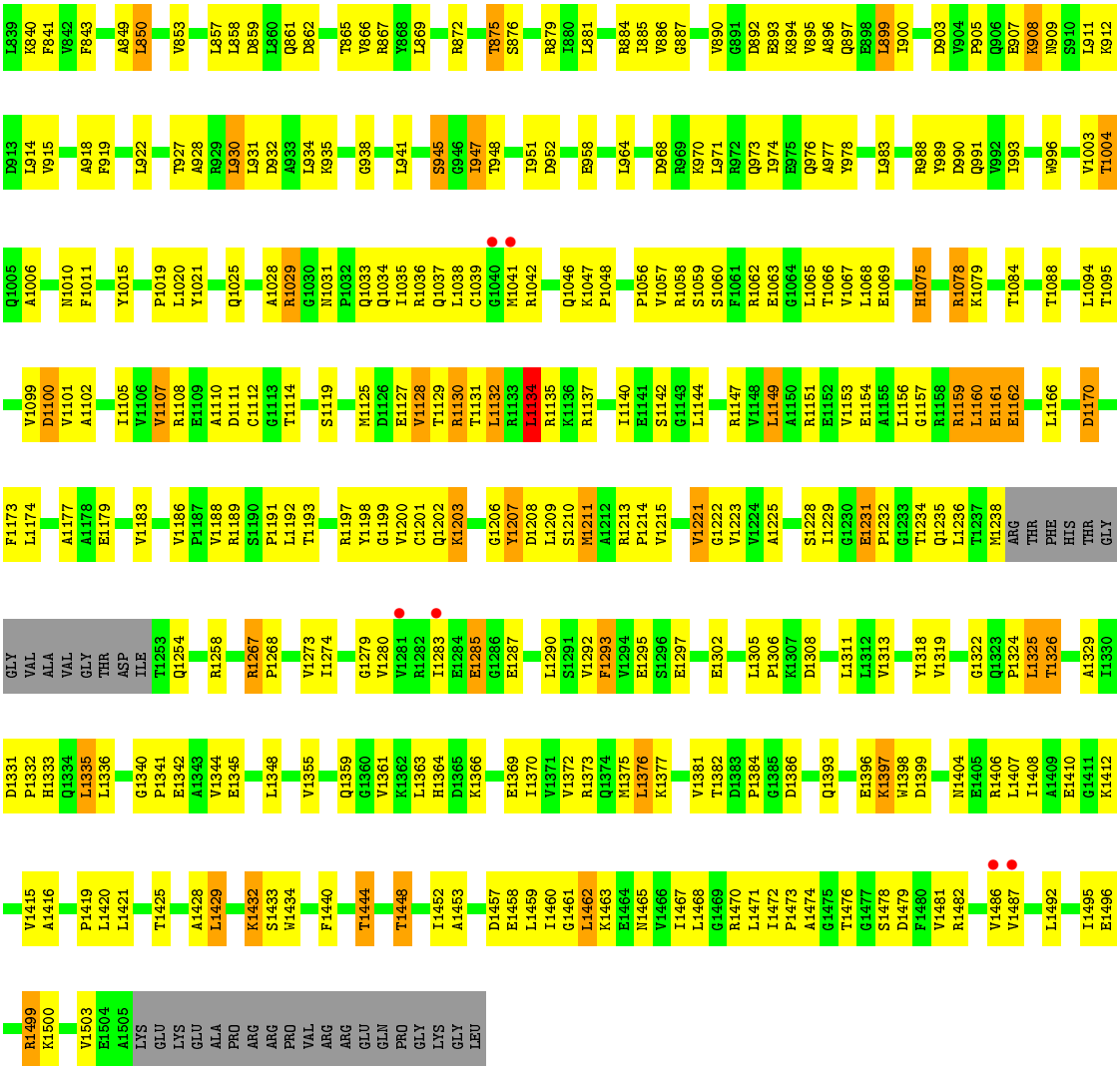



T81 R82 S83 I84 R87 Y88 H92 I93 E94 L95 A96 T97 A100 H101 I102 W103 F104 V105 K111 I112 G113 T114 L115 L116 D117 L118 S119 A120 T121 E122 L123 E124 Q125 V126 L127 Y128 F129 N130 K131 Y132 L135 D136 P137 A140 V147 L152 L153 T154 D155 E156 E157
E160 L161 K165 Q166 E167 T168 Y169 P170 L171 V175 D176 A177 L178 V179 K180 D181 E184 K187 E190 L191 A192 P193 G194 V195 Y196 S197 D200 A203 L204 Y205 P208 R209 R210 V211 R212 V213 D214 Y215 L216 R217 K218 E219 R220 R224 I225 P226 A229 W230 V231 E232
K233 E234 A235 Y236 R237 P238 V241 L242 A243 E244 L245 S246 E247 L250 F251 R252 A253 E254 E255 S256 G257 V258 V259 E260 L261 K262 D263 L264 A265 E266 G267 H268 L269 I270 Y271 Q274 E277 V278 V279 A280 R281 Y282 F283 L284 P285 A286 G287 M288 V293 E294 G295 E296 I297 V298 E299
V300 G301 L304 A305 E306 G309 L310 I311 R312 L313 P314 R315 H316 M317 T318 A319 A324 E325 E326 E327 S330 V331 H332 L333 T334 L335 F336 L337 E338 E341 P342 Y345 K346 V347 A348 P349 H350 I354 G364 I367 V368 A369 A370 I371 D372 E376 V377 I378 A379
V384 H388 E389 P390 A391 S392 I393 L394 V395 V396 K397 D406 V407 E408 V409 R414 L421 A422 D423 K426 S429 G433 L439 N442 V443 V444 R445 V446 V447 E448 S449 Y450 D451 I452 D453 A454 G457 I461 L464 E471 E474 R475 E476 L477 L478
R493 K494 R495 F502 R508 P509 E510 W511 M512 I513 L514 E515 A516 V517 P518 V519 L520 P521 P522 D523 L524 R525 P526 M527 V528 Q529 G532 G533 R534 F535 A536 T537 S538 D539 L540 Y544 R545 R546 L547 I548 N551 N552 R553 L554 K555 K556 L557 P563 E564 I565 N569 E570 K571
R572 M573 L574 Q575 E576 A577 V578 D579 A580 V581 I582 D583 N584 G585 R586 R587 G588 S589 P590 V591 T592 N593 P594 G595 S596 E597 R598 P599 L603 L607 F614 L618 L619 G620 K621 R622 V623 D624 S629 V630 I631 V632 V633 G634 P635 Q636 L637 K638 L639 H640 Q641 G642 G643 L644 P645
K646 R647 W648 A649 L650 E651 L652 F653 K654 P655 F656 L657 L658 K659 K660 M661 F666 A667 P668 N669 V670 K671 Q680 R681 D682 I683 K684 D685 E686 V687 W688 L691 V694 I695 K698 V699 V700 L701 L702 N703 R704 A705 P706 T707 L708 H709 R710 L711 G712 I713 Q714 A715 F716 Q717 P718
V719 L720 I726 Q727 L728 H729 V732 A735 D739 F740 M745 A746 V747 H748 V749 P750 Q756 A757 E758 A759 R760 I761 Q762 M763 L764 S765 A766 H767 L770 S771 P772 A773 S774 G775 E776 K780 R783 D784 T785 T786 L787 G788 L789 Y790 Y791 T792 T793 Q794 V795 K800
G801 A802 G803 F806 E810 E811 A812 L813 A814 A815 R818 V821 A822 A825 P826 I827 G831 R832 S835 Y836 G837 R838 L839 K840 F841 V842 F843 A849 L850 V853 L857 L858 D859 L860 Q861 D862 T865 V866 R867 Y868 L869 R872 T875 S876 R879 I880
L881 R884 I885 V886 G887 V890 G891 D892 E893 K894 V895 A896 Q897 E898 L899 I900 D903 V904 P905 Q906 E907 K908 N909 S910 L911 K912 D913 L914 V915 A918 F919 L922 T927 A928 R929 L930 L931 D932 A933 L934 K935 G938 L941 S945 G946 I947 T948 I951 D952
L964 D968 R969 K970 L971 R972 Q973 I974 E975 Q976 A977 Y978 L983 R988 Y989 D990 Q991 V992 I993 W996 V1003 T1004 Q1005 A1006 N1010 F1011 Y1015 P1019 L1020 Y1021 Q1025 A1028 R1029 Q1033 Q1034 I1035 R1036 Q1037 L1038 C1039 G1040 M1041 R1042 Q1046 K1047 P1048 P1056
V1057 R1058 S1059 S1060 F1061 R1062 E1063 G1064 L1065 T1066 V1067 L1068 E1069 H1075 R1078 K1079 R1087 T1088 L1094 T1095 L1098 V1099 D1100 V1106 V1107 R1108 E1109 A1110 D1111 C1112 G1113 T1114 Y1117 V1120 P1121 L1122 F1123 Q1124 M1125 D1126 E1127 V1128 T1129 R1130 T1131 L1132 R1133 L1134 R1135 K1136 R1137 S1138
D1139 I1140 E1141 S1142 G1143 L1144 R1147 A1150 V1153 L1156 R1159 L1160 E1161 E1162 G1163 R1164 Y1165 L1166 S1167 L1168 E1169 D1170 L1174 I1175 K1176 E1179 A1180 R1184 E1185 V1186 P1187 V1188 R1189 L1192 T1193 R1197 Y1198 G1199 V1200 C1201 Q1202 K1203 C1204 Y1205 D1208 L1209 S1210 M1211 A1212
R1213 P1214 V1215 S1216 I1217 V1221 G1222 V1223 V1224 A1225 S1228 I1229 G1230 E1231 P1232 G1233 T1234 Q1235 L1236 T1237 M1238 ARG THR PHE HIS THR GLY GLY VAL ALA VAL GLY THR ASP ILE T1253 Q1254 G1255 L1256 P1257 R1258 V1259 I1260 E1261 L1262 F1263 E1264 R1267 P1268 K1269 A1270 K1271 A1272 V1273 I1274 I1277

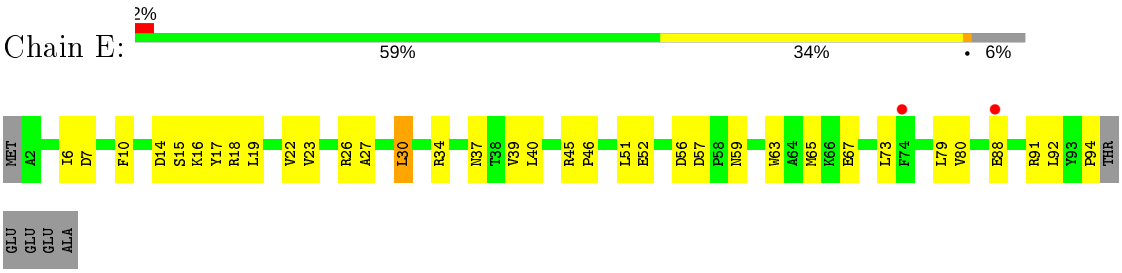


• Molecule 3: DNA-directed RNA polymerase subunit beta'

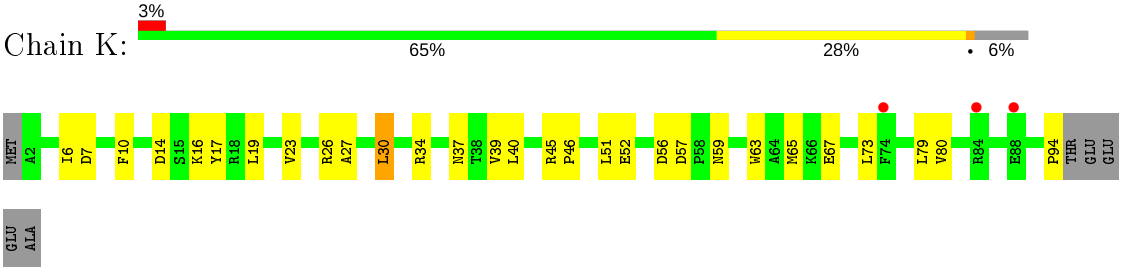




• Molecule 4: DNA-directed RNA polymerase subunit omega

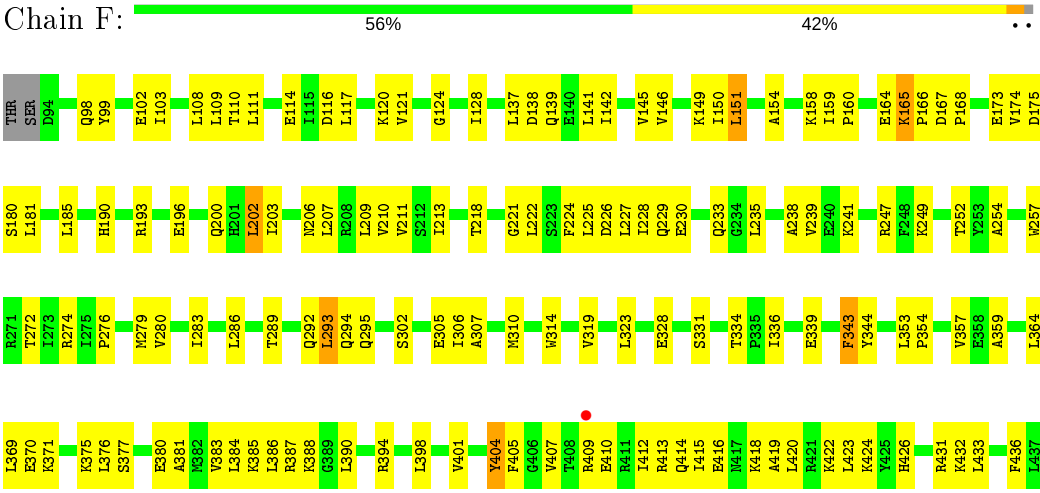


• Molecule 4: DNA-directed RNA polymerase subunit omega



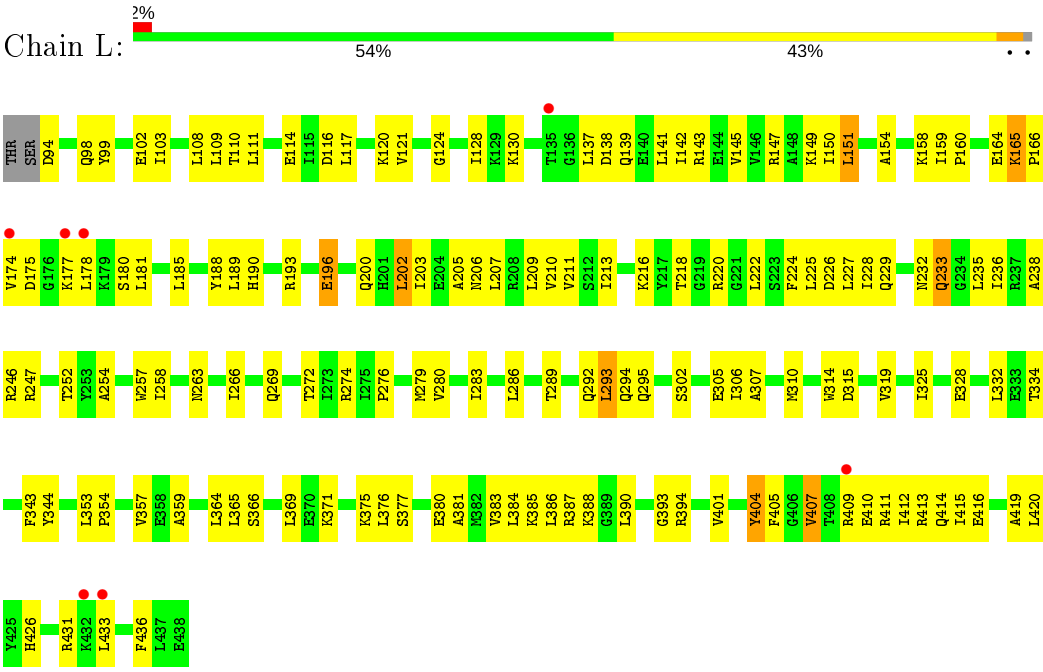
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



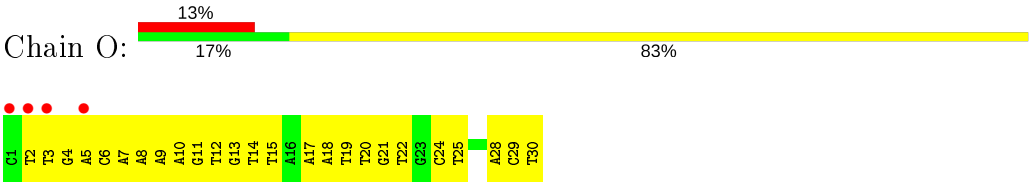
• Molecule 5: RNA polymerase sigma factor SigA

Chain L:



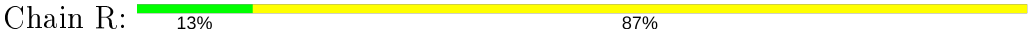
• Molecule 6: DNA (30-MER)

Chain O:



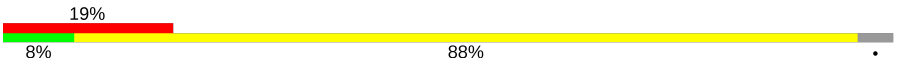
• Molecule 6: DNA (30-MER)

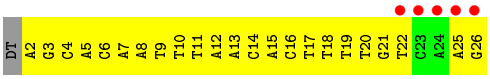
Chain R:



- Molecule 7: DNA (26-MER)

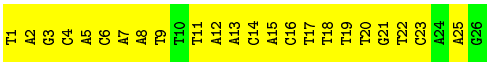
Chain P:





- Molecule 7: DNA (26-MER)

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	288.23Å 288.23Å 535.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 4.60 49.81 – 4.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.81-4.60) 98.6 (49.81-4.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 4.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.245 , 0.281 0.245 , 0.281	Depositor DCC
R_{free} test set	6224 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	154.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 174.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	56477	wwPDB-VP
Average B, all atoms (Å^2)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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	0.31	0/1804	0.64	1/2455 (0.0%)
1	B	0.30	0/1804	0.61	0/2455
1	G	0.31	0/1804	0.64	1/2455 (0.0%)
1	H	0.30	0/1804	0.61	0/2455
2	C	0.27	0/8905	0.55	2/12040 (0.0%)
2	I	0.27	0/8905	0.55	2/12040 (0.0%)
3	D	0.28	0/11963	0.55	3/16165 (0.0%)
3	J	0.28	0/10959	0.57	1/14802 (0.0%)
4	E	0.25	0/783	0.54	0/1054
4	K	0.25	0/783	0.53	0/1054
5	F	0.27	0/2829	0.55	1/3804 (0.0%)
5	L	0.27	0/2829	0.55	1/3804 (0.0%)
6	O	0.50	0/687	0.92	0/1059
6	R	0.50	0/687	0.91	0/1059
7	P	0.54	0/571	0.93	0/878
7	S	0.54	0/590	0.93	0/908
All	All	0.29	0/57707	0.59	12/78487 (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	3
2	I	0	3
3	D	0	1
3	J	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	311	LEU	CA-CB-CG	7.45	132.43	115.30
3	D	1134	LEU	CA-CB-CG	6.98	131.36	115.30
2	I	417	GLY	N-CA-C	6.42	129.14	113.10
2	C	417	GLY	N-CA-C	6.40	129.09	113.10
3	J	1134	LEU	CA-CB-CG	5.63	128.26	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	415	PRO	Peptide
2	C	423	ALA	Peptide
2	C	737	LEU	Peptide
3	D	1208	ASP	Peptide
2	I	415	PRO	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	1770	0	1799	89	0
1	B	1770	0	1799	101	0
1	G	1770	0	1799	103	0
1	H	1770	0	1799	95	0
2	C	8739	0	8841	499	0
2	I	8739	0	8841	485	0
3	D	11761	0	11976	585	0
3	J	10779	0	10993	503	0
4	E	768	0	784	37	0
4	K	768	0	784	29	0
5	F	2787	0	2866	120	0
5	L	2787	0	2866	133	0
6	O	613	0	343	28	0
6	R	613	0	343	26	0
7	P	510	0	284	27	0
7	S	527	0	297	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	J	2	0	0	0	0
9	D	1	0	0	0	0
9	J	1	0	0	0	0
All	All	56477	0	56414	2598	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 23.

The worst 5 of 2598 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:C:707:ARG:HE	2:C:824:ARG:HE	1.17	0.90
6:R:24:DC:H42	7:S:3:DG:H1	1.18	0.90
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.88
4:E:30:LEU:HD12	4:E:37:ASN:HD21	1.39	0.88
4:K:30:LEU:HD12	4:K:37:ASN:HD21	1.39	0.87

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	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	17 56
1	B	225/314 (72%)	200 (89%)	20 (9%)	5 (2%)	6 37
1	G	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	17 56
1	H	225/314 (72%)	201 (89%)	18 (8%)	6 (3%)	5 34
2	C	1108/1119 (99%)	958 (86%)	139 (12%)	11 (1%)	15 54
2	I	1108/1119 (99%)	956 (86%)	140 (13%)	12 (1%)	14 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D	1486/1524 (98%)	1315 (88%)	162 (11%)	9 (1%)	25 65
3	J	1361/1524 (89%)	1201 (88%)	150 (11%)	10 (1%)	22 62
4	E	91/99 (92%)	75 (82%)	16 (18%)	0	100 100
4	K	91/99 (92%)	75 (82%)	16 (18%)	0	100 100
5	F	343/347 (99%)	299 (87%)	42 (12%)	2 (1%)	25 65
5	L	343/347 (99%)	302 (88%)	40 (12%)	1 (0%)	41 76
All	All	6831/7434 (92%)	5982 (88%)	789 (12%)	60 (1%)	17 56

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	1128	VAL
3	D	1209	LEU
1	G	53	VAL
3	J	1128	VAL

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	194/270 (72%)	179 (92%)	15 (8%)	13 39
1	B	194/270 (72%)	172 (89%)	22 (11%)	6 24
1	G	194/270 (72%)	178 (92%)	16 (8%)	11 36
1	H	194/270 (72%)	171 (88%)	23 (12%)	5 22
2	C	931/936 (100%)	840 (90%)	91 (10%)	8 28
2	I	931/936 (100%)	840 (90%)	91 (10%)	8 28
3	D	1252/1281 (98%)	1114 (89%)	138 (11%)	6 25
3	J	1150/1281 (90%)	1028 (89%)	122 (11%)	6 26
4	E	83/88 (94%)	79 (95%)	4 (5%)	25 52
4	K	83/88 (94%)	79 (95%)	4 (5%)	25 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	296/299 (99%)	276 (93%)	20 (7%)	16 42
5	L	296/299 (99%)	276 (93%)	20 (7%)	16 42
All	All	5798/6288 (92%)	5232 (90%)	566 (10%)	8 28

5 of 566 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1382	THR
1	H	113	ASP
3	J	1293	PHE
3	D	1459	LEU
5	F	409	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1235	GLN
1	G	63	HIS
4	K	37	ASN
3	D	1359	GLN
5	F	294	GLN

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 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

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	227/314 (72%)	0.08	2 (0%) 84 77	107, 189, 236, 264	0
1	B	227/314 (72%)	-0.23	0 100 100	94, 161, 214, 264	0
1	G	227/314 (72%)	0.39	17 (7%) 14 12	116, 199, 240, 276	0
1	H	227/314 (72%)	-0.13	2 (0%) 84 77	116, 173, 216, 267	0
2	C	1112/1119 (99%)	-0.03	21 (1%) 66 58	90, 179, 243, 314	0
2	I	1112/1119 (99%)	0.01	26 (2%) 60 51	94, 185, 244, 315	0
3	D	1490/1524 (97%)	-0.13	13 (0%) 84 77	64, 149, 204, 259	0
3	J	1367/1524 (89%)	-0.08	17 (1%) 79 70	79, 159, 217, 264	0
4	E	93/99 (93%)	0.06	2 (2%) 62 53	100, 159, 205, 238	0
4	K	93/99 (93%)	0.03	3 (3%) 47 38	112, 168, 216, 253	0
5	F	345/347 (99%)	-0.10	1 (0%) 94 90	115, 185, 255, 300	0
5	L	345/347 (99%)	-0.10	7 (2%) 65 56	121, 188, 252, 300	0
6	O	30/30 (100%)	0.70	4 (13%) 3 4	154, 221, 293, 311	0
6	R	30/30 (100%)	0.21	0 100 100	164, 221, 257, 267	0
7	P	25/26 (96%)	0.83	5 (20%) 1 1	172, 235, 306, 326	0
7	S	26/26 (100%)	0.06	0 100 100	184, 224, 263, 283	0
All	All	6976/7546 (92%)	-0.04	120 (1%) 70 61	64, 171, 235, 326	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	176	VAL	5.1
2	I	175	GLU	4.5
2	C	221	LEU	4.4
1	G	13	ALA	4.0
2	C	175	GLU	3.7

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

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

6.3 Carbohydrates (i)

There are no 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. 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
9	MG	D	2003	1/1	0.82	0.45	286,286,286,286	0
9	MG	J	2003	1/1	0.84	0.41	331,331,331,331	0
8	ZN	J	2002	1/1	0.93	0.07	147,147,147,147	0
8	ZN	D	2002	1/1	0.96	0.16	182,182,182,182	0
8	ZN	J	2001	1/1	0.97	0.12	166,166,166,166	0
8	ZN	D	2001	1/1	0.99	0.13	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.