wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2024 – 10:17 AM EDT

PDB ID	:	4XLR
Title	:	Crystal structure of T.aquaticus transcription initiation complex with CarD containing bubble promoter and RNA
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2015-01-13
Resolution	:	4.30 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:

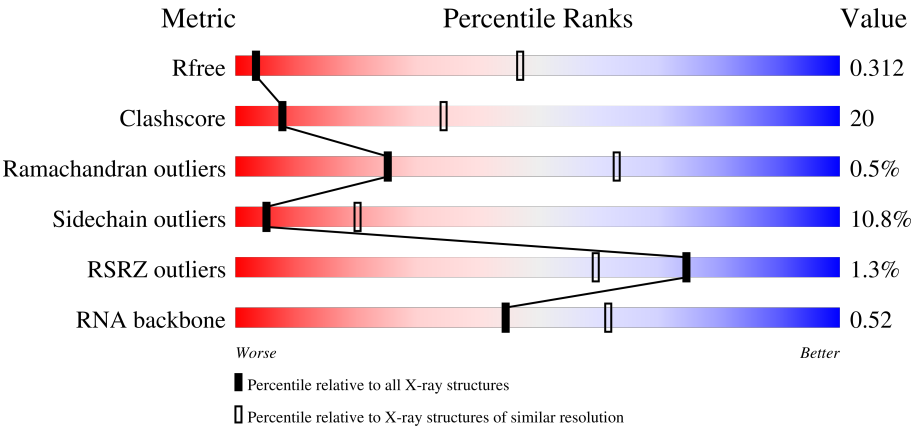
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.30 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}	164625	1028 (4.72-3.86)
Clashscore	180529	1030 (4.70-3.90)
Ramachandran outliers	177936	1014 (4.76-3.84)
Sidechain outliers	177891	1022 (4.76-3.82)
RSRZ outliers	164620	1026 (4.72-3.86)
RNA backbone	3690	1156 (5.60-3.00)

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	314	% 37% 31% . 28%
1	B	314	% 42% 26% . 28%
1	G	314	% 37% 31% . 28%
1	H	314	42% 26% . 28%

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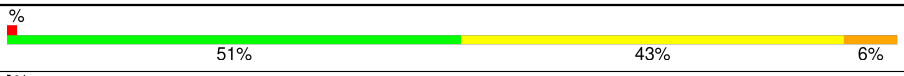
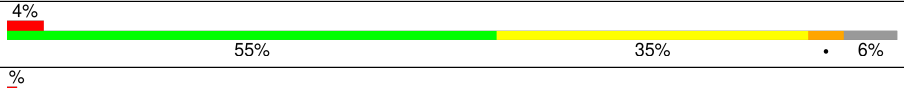
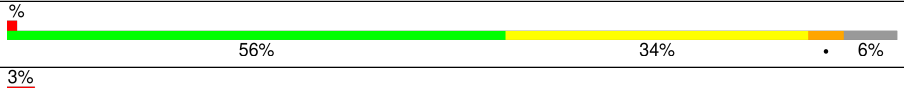
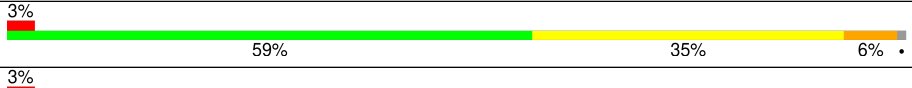
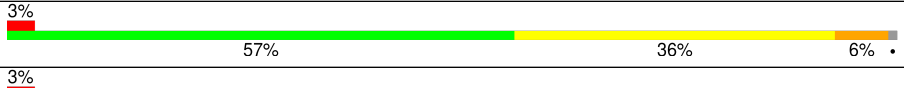
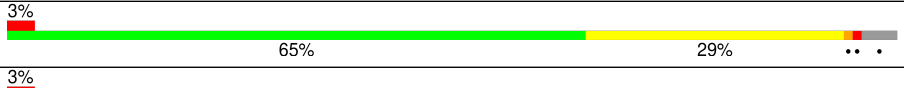
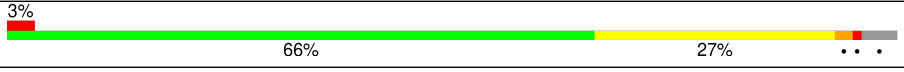
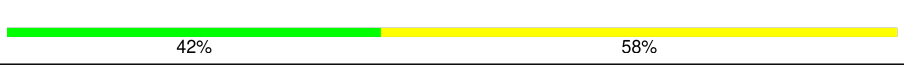
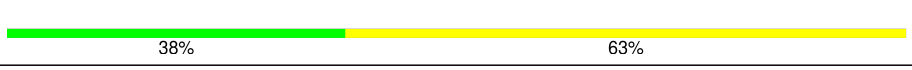
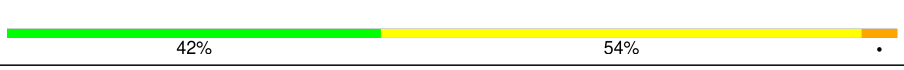
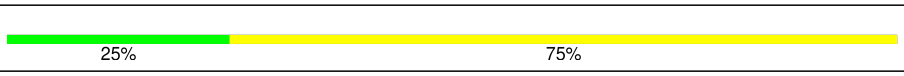
Mol	Chain	Length	Quality of chain
2	C	1119	
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	M	164	
6	N	164	
7	O	48	
7	R	48	
8	P	48	
8	S	48	
9	Q	4	
9	T	4	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 60854 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	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			
2	I	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	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 protein called CarD-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			
6	N	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			
7	R	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			

- Molecule 8 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			
8	S	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			

- Molecule 9 is a RNA chain called RNA (5'-R(P*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Q	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			
9	T	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

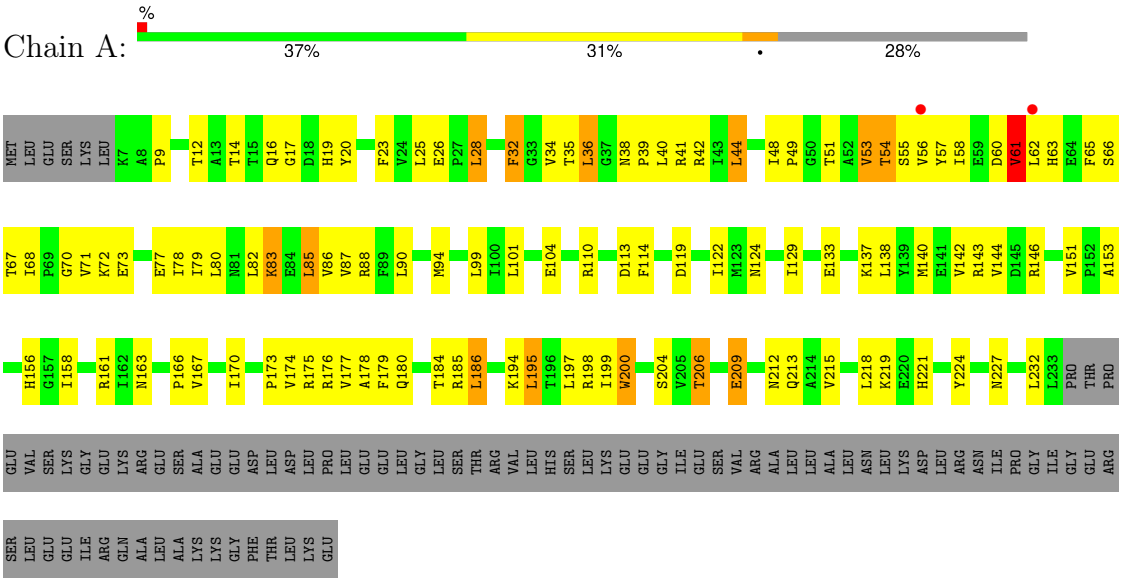
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total Mg 1 1	0	0
11	J	1	Total Mg 1 1	0	0

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.

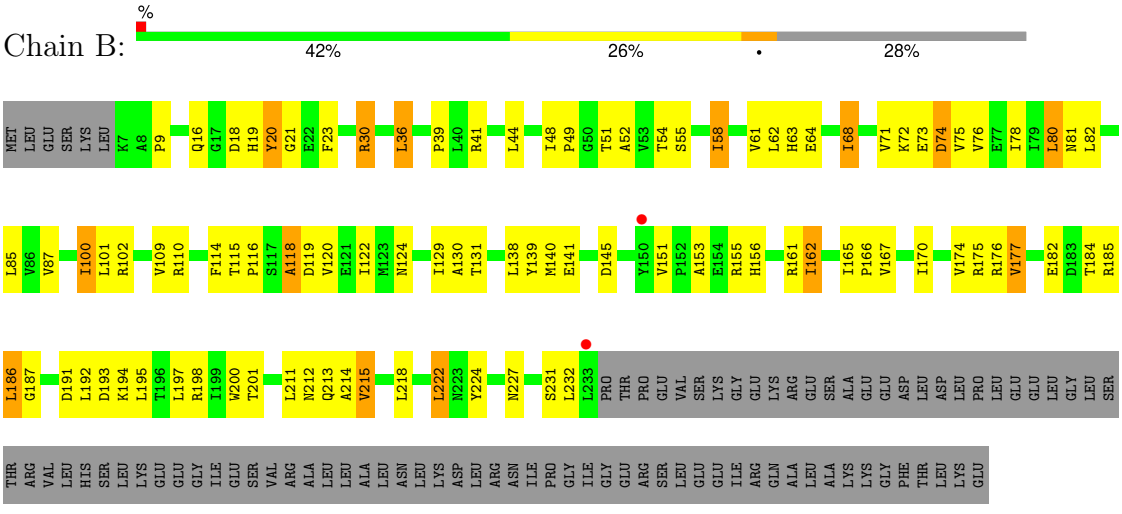
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



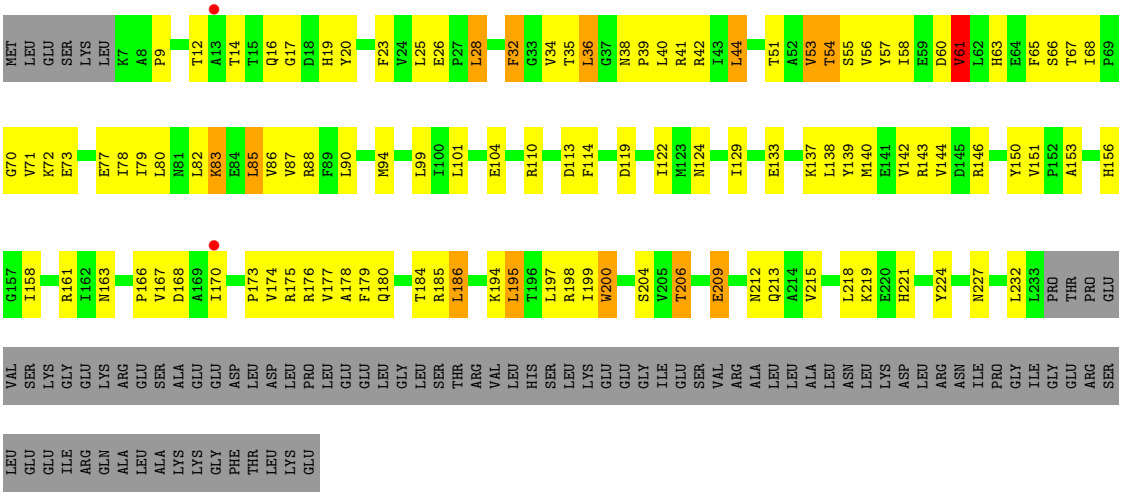
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



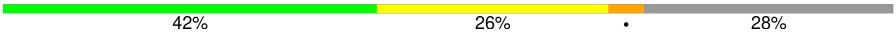
• Molecule 1: DNA-directed RNA polymerase subunit alpha

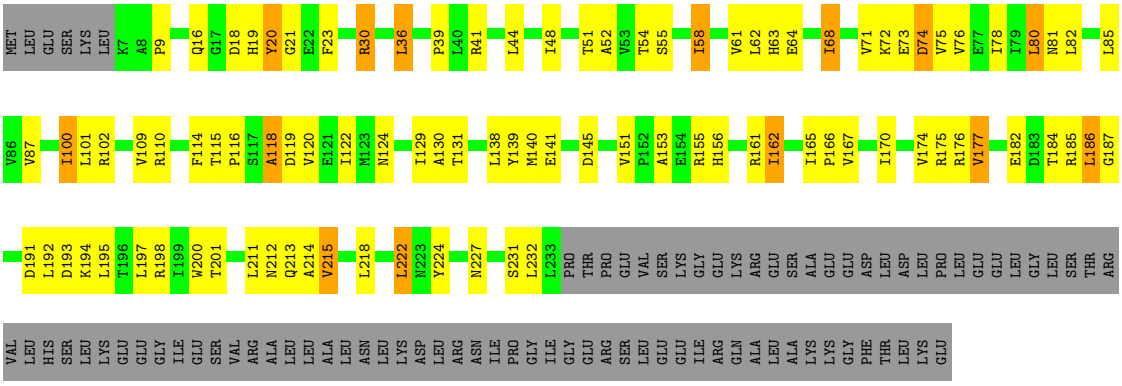
Chain G:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

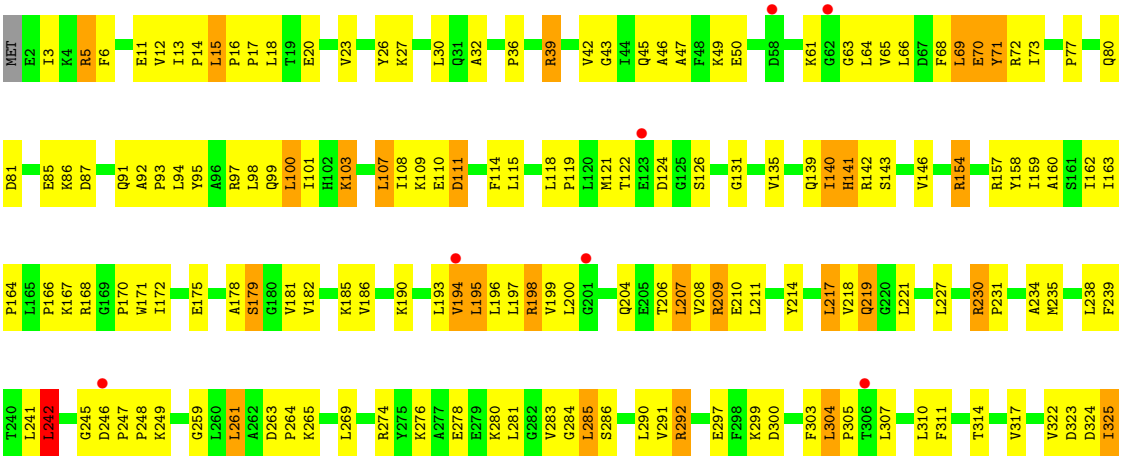
Chain H:

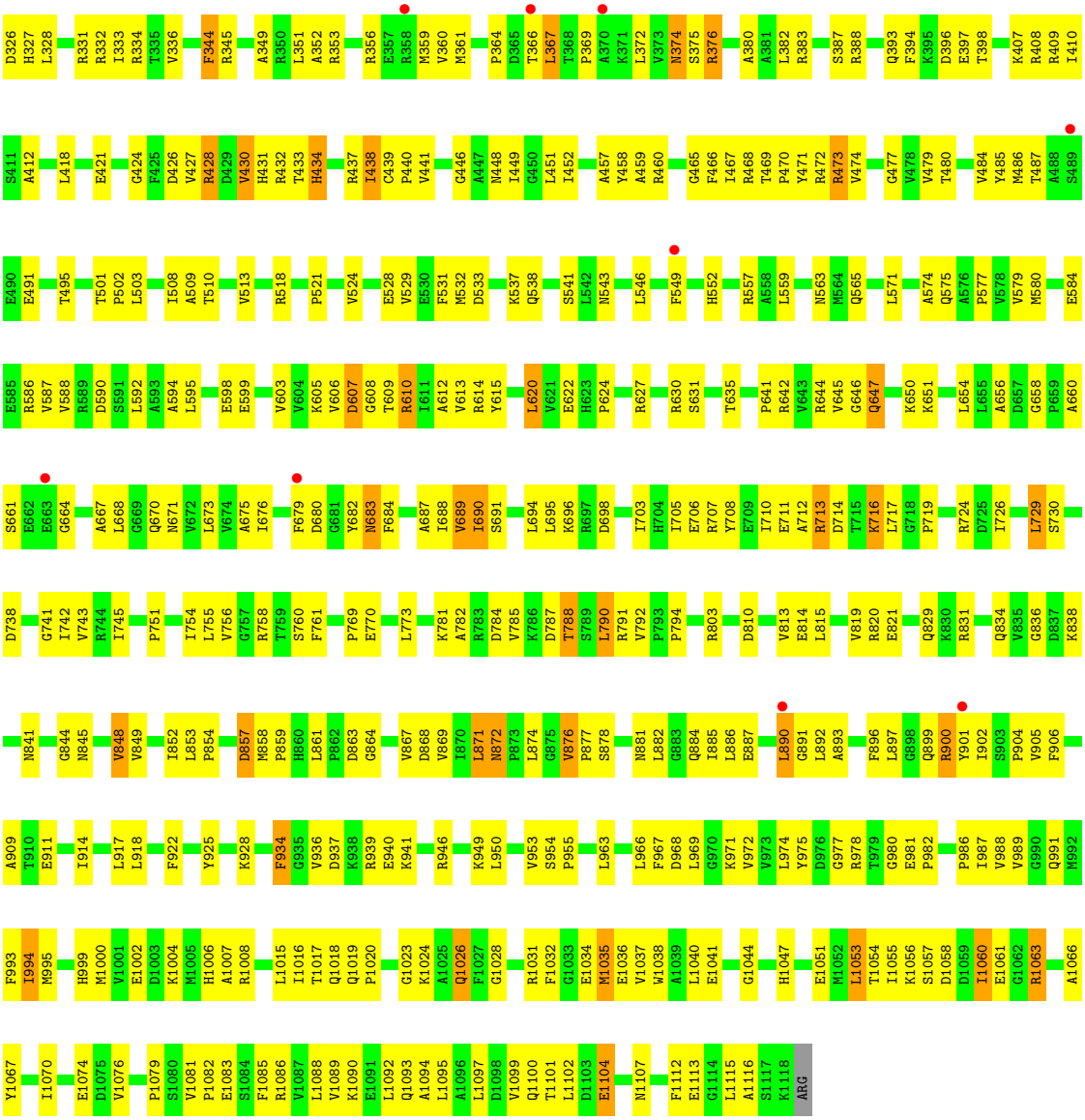




• Molecule 2: DNA-directed RNA polymerase subunit beta

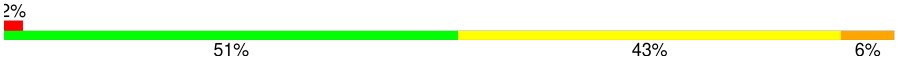
Chain C:

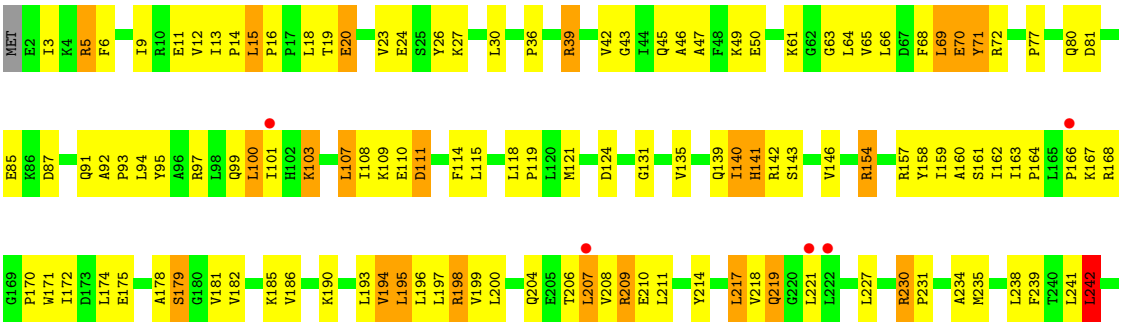


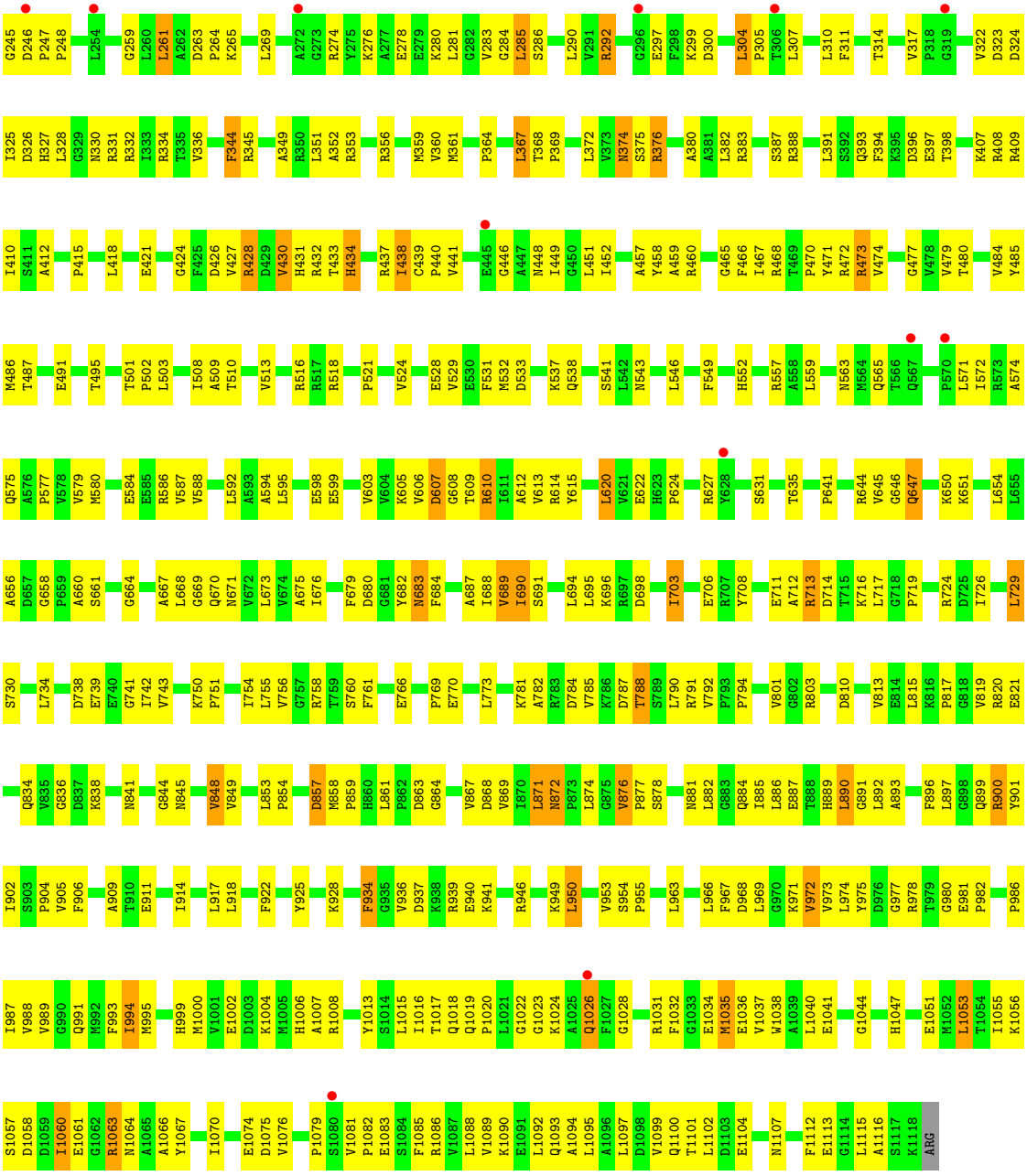


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I:

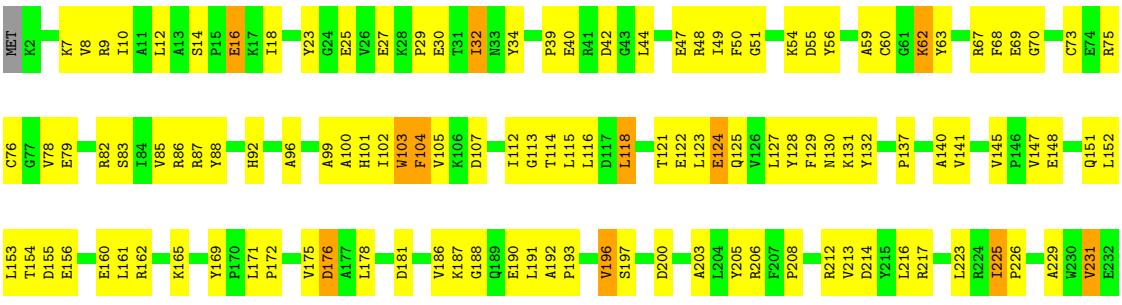


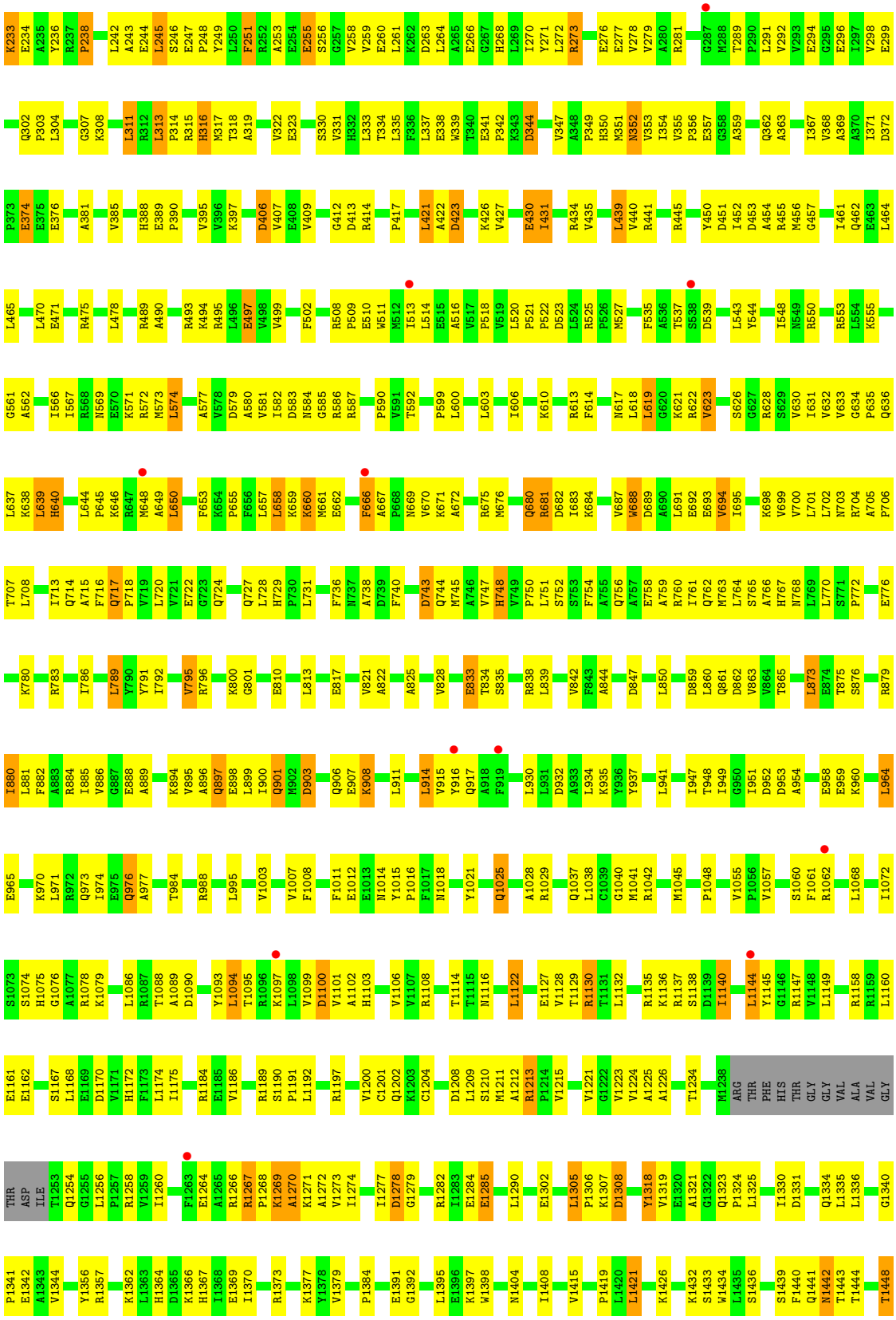


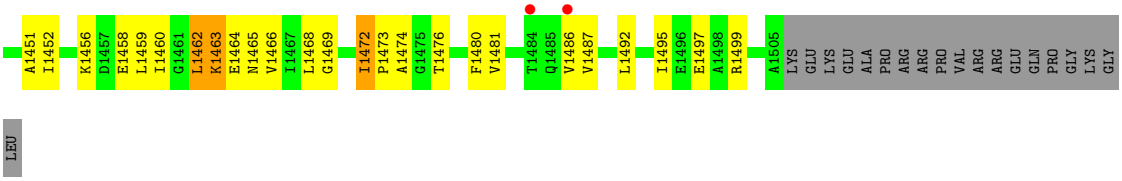


• Molecule 3: DNA-directed RNA polymerase subunit beta'

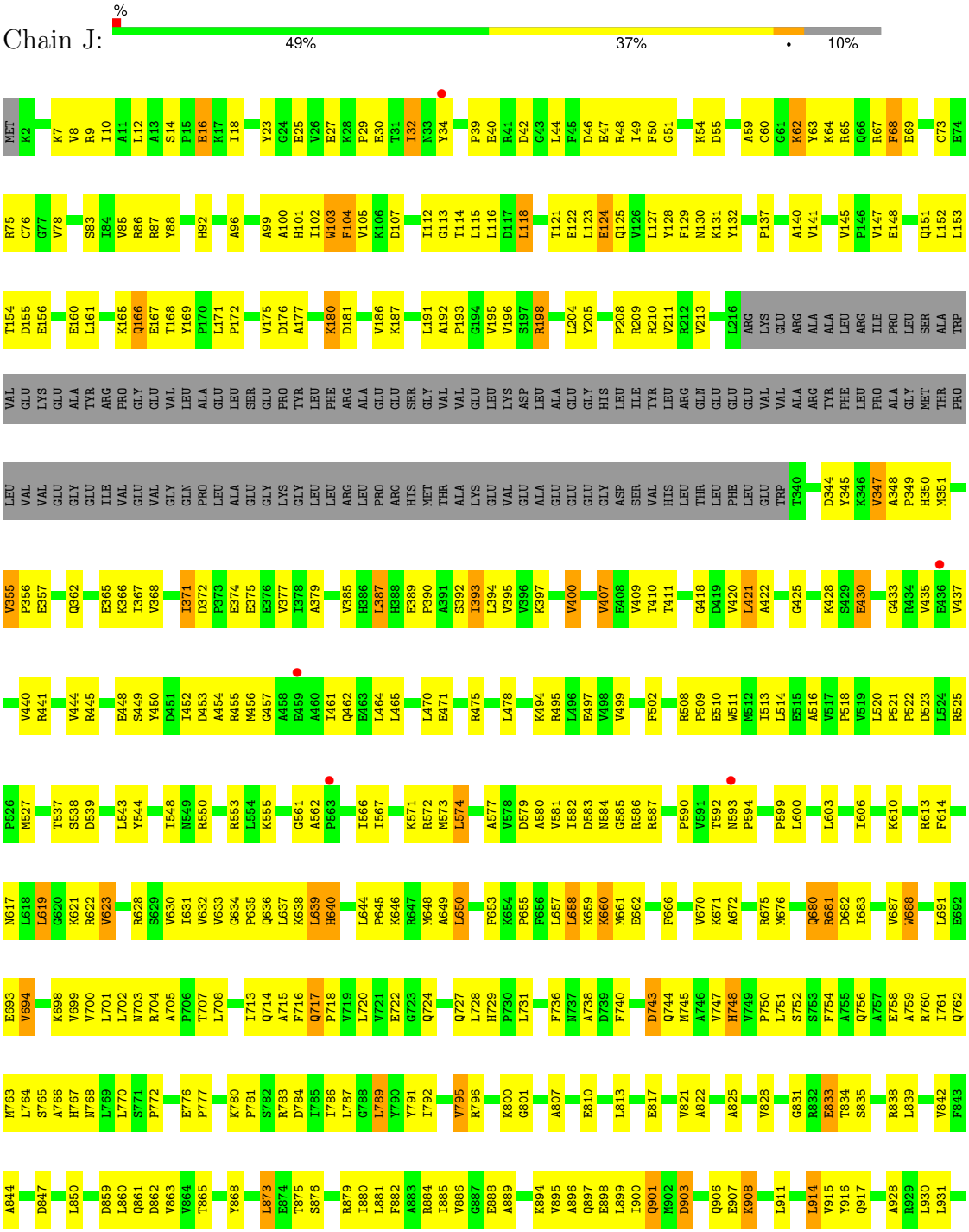
Chain D:

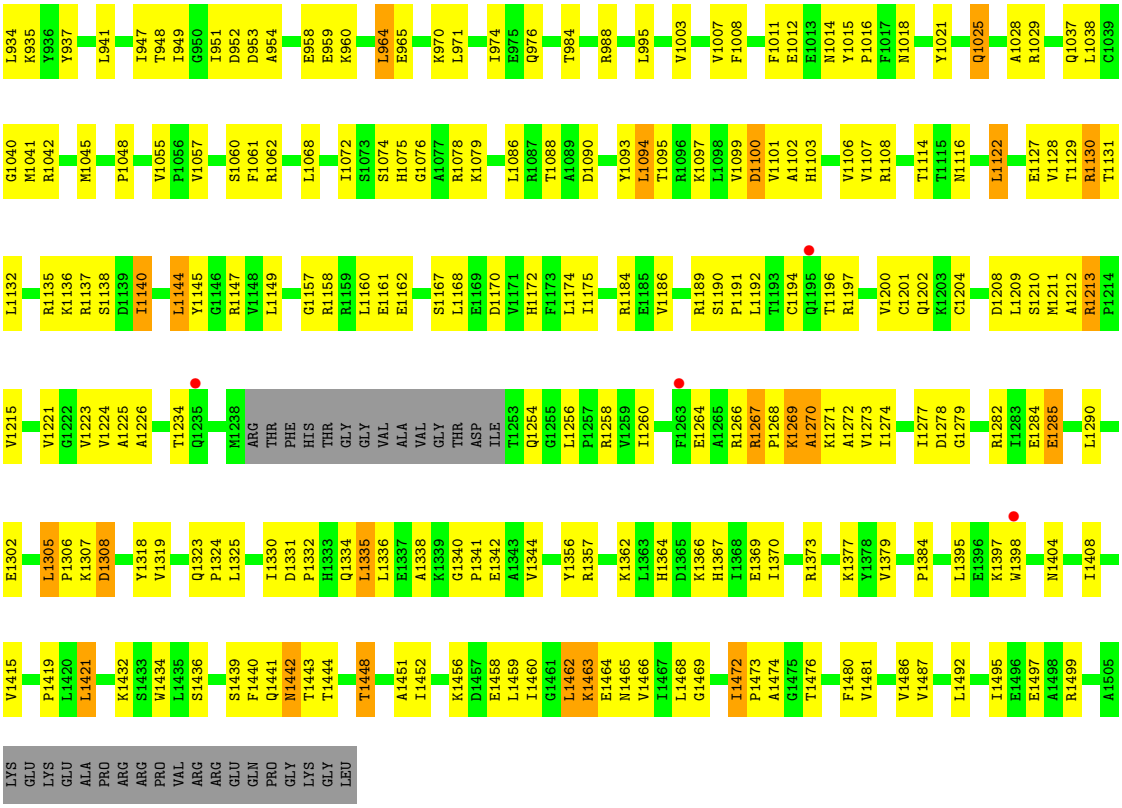



K233 E234 A235 Y236 R237 P238 L242 A243 E244 L245 S246 E247 P248 Y249 L250 F251 R252 A253 E254 E255 S256 G257 V258 V259 E260 L261 K262 D263 L264 A265 E266 G267 H268 L269 I270 Y271 L272 R273 E276 E277 V278 V279 A280 R281 G287 M288 T289 P290 L291 V292 V293 E294 G295 E296 I297 V298 E299
Q302 P303 L304 G307 K308 L311 R312 L313 P314 R315 H316 M317 T318 A319 V322 E323 S330 V331 H332 L333 T334 L335 F336 L337 E338 W339 T340 E341 P342 K343 D344 V347 A348 P349 H350 M351 N352 V353 I354 V355 P356 E357 G358 A359 Q362 A363 I367 V368 A369 A370 I371 D372
P373 E374 E375 E376 A381 V385 H388 E389 P390 V395 V396 K397 D406 V407 E408 V409 G412 D413 R414 P417 L421 A422 D423 K426 V427 E430 I431 R434 V435 L439 V440 R441 R445 Y450 D451 I452 D453 A454 R455 M456 G457 I461 Q462 E463 L464
L465 L470 E471 R475 L478 R489 A490 R493 K494 R495 L496 E497 V498 V499 F502 R508 P509 E510 W511 M512 I513 L514 E515 A516 V517 P518 V519 L520 P521 P522 D523 L524 R525 P526 M527 F535 A536 T537 S538 D539 L543 Y544 I548 N549 R550 R553 L554 K555
G561 A562 I566 I567 R568 N569 E570 K571 R572 M573 L574 A577 V578 D579 A580 V581 I582 D583 N584 G585 R586 R587 P590 V591 T592 P599 L600 L603 I606 K610 R613 F614 N617 L618 L619 G620 K621 R622 V623 S626 G627 R628 S629 V630 I631 V632 V633 G634 P635 Q636
L637 K638 L639 H640 L644 P645 K646 R647 M648 A649 L650 F653 K654 P655 F656 L657 L658 K659 K660 M661 E662 F666 A667 P668 N669 V670 K671 A672 R675 M676 Q680 R681 D682 I683 K684 V687 W688 D689 A690 L691 E692 E693 V694 I695 K698 V699 V700 L701 L702 N703 R704 A705 P706
T707 L708 I713 Q714 A715 F716 Q717 P718 V719 L720 V721 E722 G723 Q724 Q727 L728 H729 P730 L731 F736 N737 A738 D739 F740 D743 Q744 M745 A746 V747 H748 V749 P750 L751 S752 S753 F754 A755 Q756 A757 E758 A759 R760 I761 Q762 M763 L764 S765 A766 H767 N768 L769 L770 S771 P772 E776
K780 R783 I786 L789 Y790 Y791 I792 V795 R796 K800 G801 E810 L813 E817 V821 A822 A825 V828 E833 T834 S835 R838 L839 V842 F843 A844 D847 L850 D859 L860 Q861 D862 V863 V864 T865 L873 E874 T875 S876 R879
I880 L881 F882 A883 R884 I885 V886 G887 E888 A889 K894 V895 A896 Q897 E898 L899 I900 Q901 M902 D903 Q906 E907 K908 L911 L914 V915 Y916 Q917 A918 F919 L930 L931 D932 A933 L934 K935 Y936 Y937 L941 I947 T948 I949 G950 I951 D952 D953 A954 E958 E959 K960 L964
E965 K970 L971 R972 Q973 I974 E975 Q976 A977 T984 R988 L995 V1003 V1007 F1008 F1011 E1012 E1013 N1014 Y1015 P1016 F1017 N1018 Y1021 Q1025 A1028 R1029 Q1037 L1038 C1039 G1040 M1041 R1042 M1045 P1048 V1055 P1056 V1057 S1060 F1061 R1062 L1068 I1072
S1073 S1074 H1075 G1076 A1077 R1078 K1079 L1086 R1087 T1088 A1089 D1090 Y1093 L1094 T1095 R1096 K1097 L1098 V1099 D1100 V1101 A1102 H1103 V1106 V1107 R1108 T1114 T1115 N1116 L1122 E1127 V1128 T1129 R1130 T1131 L1132 R1135 K1136 R1137 S1138 D1139 T1140 L1144 Y1145 G1146 R1147 V1148 L1149 R1158 R1159 L1160
E1161 E1162 S1167 L1168 E1169 D1170 V1171 H1172 F1173 L1174 I1175 R1184 E1185 V1186 R1189 S1190 P1191 L1192 R1197 V1200 C1201 Q1202 K1203 C1204 D1208 L1209 S1210 M1211 A1212 R1213 P1214 V1215 V1221 G1222 V1223 V1224 A1225 A1226 T1234 M1238 ARG THR PHE HIS THR GLY GLY VAL ALA VAL GLY
THR ASP ILE T1253 Q1254 G1255 L1256 P1257 R1258 V1259 I1260 F1263 E1264 A1265 R1266 R1267 P1268 K1269 A1270 K1271 A1272 V1273 I1274 I1277 D1278 G1279 R1282 I1283 E1284 E1285 L1290 E1302 L1305 P1306 K1307 D1308 Y1318 V1319 E1320 A1321 G1322 Q1323 P1324 L1325 I1330 D1331 Q1334 L1335 L1336 G1340
P1341 E1342 A1343 V1344 Y1356 R1357 K1362 L1363 H1364 D1365 K1366 H1367 I1368 E1369 I1370 R1373 K1377 Y1378 V1379 P1384 E1391 G1392 L1395 E1396 K1397 W1398 N1404 I1408 V1415 P1419 L1420 L1421 K1426 K1432 S1433 W1434 L1435 S1436 S1439 F1440 Q1441 N1442 T1443 T1444 T1448

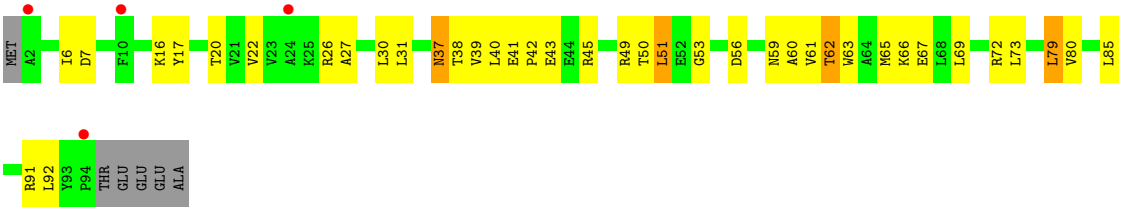


• Molecule 3: DNA-directed RNA polymerase subunit beta'

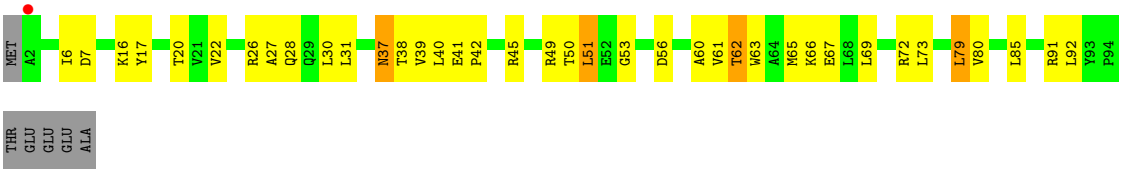




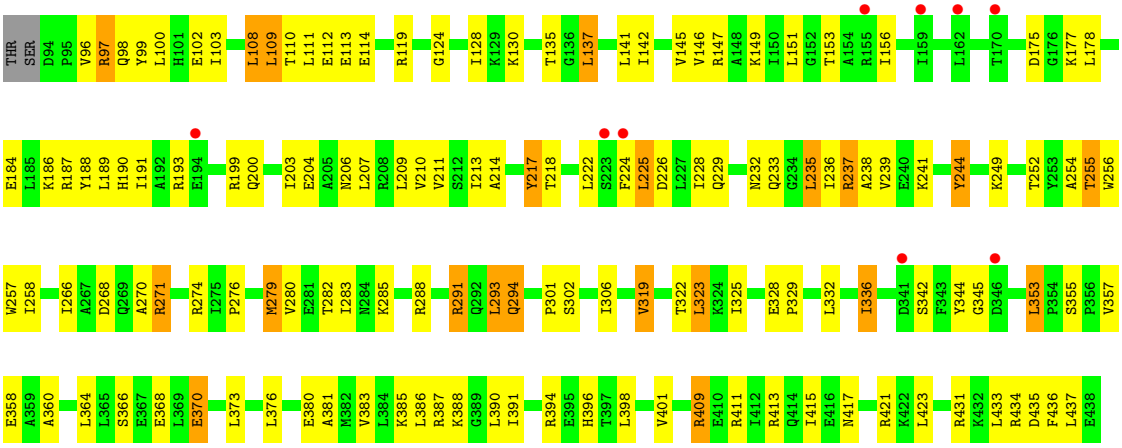
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega

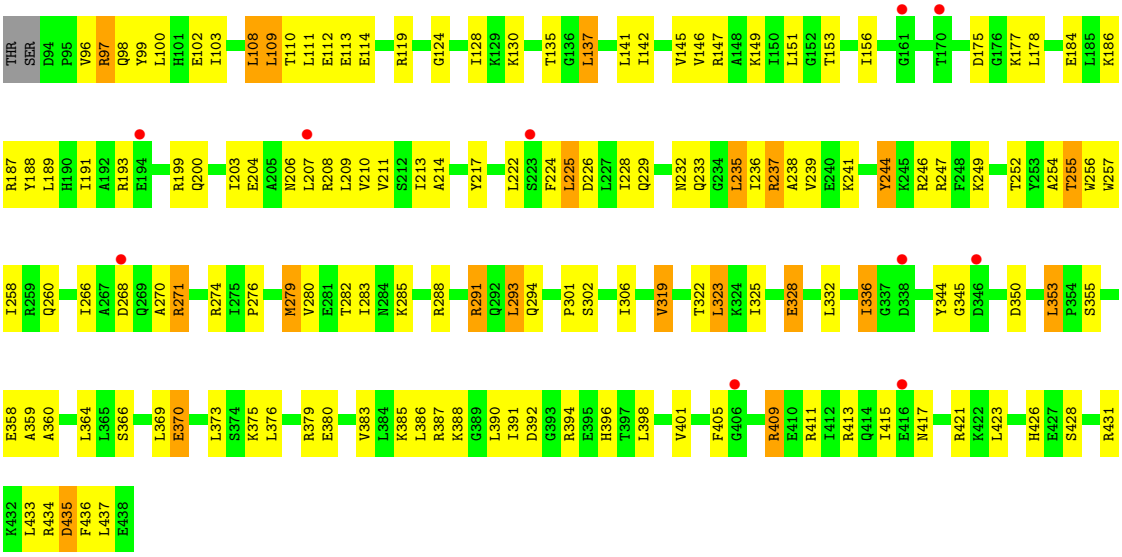


• Molecule 5: RNA polymerase sigma factor SigA



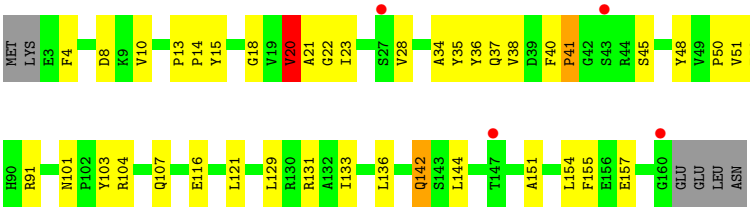
• Molecule 5: RNA polymerase sigma factor SigA

Chain L:



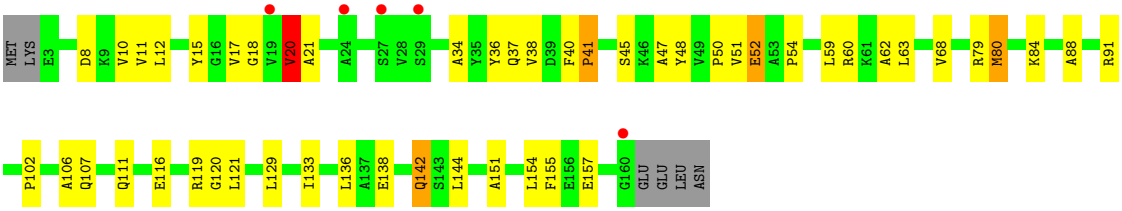
• Molecule 6: CarD-like transcriptional regulator

Chain M:



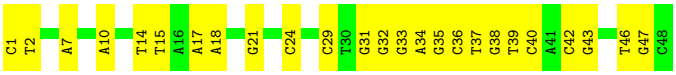
• Molecule 6: CarD-like transcriptional regulator

Chain N:



• Molecule 7: DNA (48-MER)

Chain O:

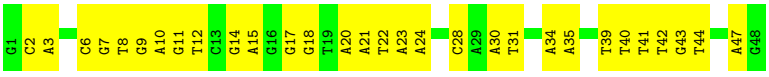


• Molecule 7: DNA (48-MER)

Chain R:

• Molecule 8: DNA (48-MER)

Chain P:

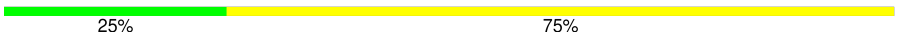


• Molecule 8: DNA (48-MER)

Chain S:

• Molecule 9: RNA (5'-R(P*UP*CP*GP*A)-3')

Chain Q:



• Molecule 9: RNA (5'-R(P*UP*CP*GP*A)-3')

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	289.84Å 289.84Å 536.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 4.30 39.56 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.56-4.30) 94.6 (39.56-4.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.275 , 0.310 0.277 , 0.312	Depositor DCC
R_{free} test set	7337 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	165.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 165.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	60854	wwPDB-VP
Average B, all atoms (Å^2)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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	0.29	0/1804	0.52	0/2455
1	B	0.27	0/1804	0.49	0/2455
1	G	0.30	0/1804	0.52	0/2455
1	H	0.27	0/1804	0.49	0/2455
2	C	0.29	0/8929	0.51	1/12074 (0.0%)
2	I	0.29	0/8929	0.51	1/12074 (0.0%)
3	D	0.29	0/11963	0.50	0/16165
3	J	0.28	0/10959	0.49	0/14802
4	E	0.27	0/783	0.53	0/1054
4	K	0.27	0/783	0.53	0/1054
5	F	0.34	0/2829	0.54	0/3804
5	L	0.33	0/2829	0.54	0/3804
6	M	0.35	0/1267	0.55	0/1719
6	N	0.35	0/1267	0.55	0/1719
7	O	0.59	0/1109	0.92	0/1712
7	R	0.56	0/1109	0.92	0/1712
8	P	0.64	0/1106	0.88	0/1706
8	S	0.61	0/1106	0.90	2/1706 (0.1%)
9	Q	0.24	0/94	0.71	0/144
9	T	0.24	0/94	0.76	0/144
All	All	0.33	0/62372	0.55	4/85213 (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	I	0	2
3	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
6	M	0	2
6	N	0	2
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	23	DA	O5'-P-OP1	-6.61	99.75	105.70
2	C	242	LEU	CA-CB-CG	5.68	128.36	115.30
2	I	242	LEU	CA-CB-CG	5.57	128.10	115.30
8	S	22	DT	OP1-P-O3'	5.13	116.48	105.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	360	VAL	Peptide
2	C	71	TYR	Mainchain
3	D	1270	ALA	Peptide
2	I	360	VAL	Peptide
2	I	71	TYR	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	1770	0	1799	87	0
1	B	1770	0	1799	66	0
1	G	1770	0	1799	88	0
1	H	1770	0	1799	65	0
2	C	8762	0	8854	435	0
2	I	8762	0	8854	436	0
3	D	11761	0	11976	537	0
3	J	10779	0	10993	490	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	768	0	784	38	0
4	K	768	0	784	36	0
5	F	2787	0	2866	122	0
5	L	2787	0	2866	127	0
6	M	1239	0	1259	38	0
6	N	1239	0	1259	39	0
7	O	988	0	544	30	0
7	R	988	0	544	38	0
8	P	985	0	543	36	0
8	S	985	0	543	30	0
9	Q	85	0	43	1	0
9	T	85	0	43	2	0
10	D	2	0	0	0	0
10	J	2	0	0	0	0
11	D	1	0	0	0	0
11	J	1	0	0	0	0
All	All	60854	0	59951	2363	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 20.

The worst 5 of 2363 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:73:CYS:HB3	3:D:76:CYS:SG	1.97	1.04
3:J:73:CYS:HB3	3:J:76:CYS:SG	1.97	1.04
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.89
3:D:412:GLY:HA2	3:D:434:ARG:HD3	1.55	0.89
3:J:105:VAL:HA	3:J:112:ILE:HD11	1.55	0.88

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%)	191 (85%)	32 (14%)	2 (1%)	14	50
1	B	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	14	50
1	G	225/314 (72%)	190 (84%)	33 (15%)	2 (1%)	14	50
1	H	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	14	50
2	C	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	30	67
2	I	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	30	67
3	D	1486/1524 (98%)	1306 (88%)	171 (12%)	9 (1%)	22	59
3	J	1361/1524 (89%)	1200 (88%)	156 (12%)	5 (0%)	30	67
4	E	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
5	F	343/347 (99%)	301 (88%)	41 (12%)	1 (0%)	37	72
5	L	343/347 (99%)	300 (88%)	42 (12%)	1 (0%)	37	72
6	M	156/164 (95%)	143 (92%)	11 (7%)	2 (1%)	10	42
6	N	156/164 (95%)	142 (91%)	12 (8%)	2 (1%)	10	42
All	All	7157/7762 (92%)	6277 (88%)	844 (12%)	36 (0%)	25	63

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	681	ARG
3	D	683	ILE
3	D	1128	VAL
1	G	53	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%)	171 (88%)	23 (12%)	4 18
1	B	194/270 (72%)	167 (86%)	27 (14%)	3 15
1	G	194/270 (72%)	171 (88%)	23 (12%)	4 18
1	H	194/270 (72%)	167 (86%)	27 (14%)	3 15
2	C	931/936 (100%)	820 (88%)	111 (12%)	4 18
2	I	931/936 (100%)	820 (88%)	111 (12%)	4 18
3	D	1252/1281 (98%)	1115 (89%)	137 (11%)	5 20
3	J	1150/1281 (90%)	1033 (90%)	117 (10%)	6 21
4	E	83/88 (94%)	77 (93%)	6 (7%)	12 32
4	K	83/88 (94%)	77 (93%)	6 (7%)	12 32
5	F	296/299 (99%)	267 (90%)	29 (10%)	6 22
5	L	296/299 (99%)	267 (90%)	29 (10%)	6 22
6	M	127/133 (96%)	122 (96%)	5 (4%)	27 50
6	N	127/133 (96%)	122 (96%)	5 (4%)	27 50
All	All	6052/6554 (92%)	5396 (89%)	656 (11%)	5 20

5 of 656 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	848	VAL
3	J	1078	ARG
2	I	934	PHE
2	I	834	GLN
3	J	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	80	GLN
2	I	1050	GLN
5	L	263	ASN
2	I	187	ASN
2	I	683	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	Q	3/4 (75%)	2 (66%)	0
9	T	3/4 (75%)	0	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	Q	2	C
9	Q	3	G

There are no RNA pucker outliers to report.

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 oligosaccharides 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	227/314 (72%)	0.10	2 (0%) 81 66	144, 176, 208, 241	0
1	B	227/314 (72%)	0.03	2 (0%) 81 66	143, 164, 196, 228	0
1	G	227/314 (72%)	0.16	2 (0%) 81 66	148, 188, 218, 252	0
1	H	227/314 (72%)	0.04	0 100 100	145, 175, 207, 241	0
2	C	1117/1119 (99%)	0.17	16 (1%) 73 58	144, 172, 211, 253	0
2	I	1117/1119 (99%)	0.17	17 (1%) 71 56	144, 182, 221, 270	0
3	D	1490/1524 (97%)	0.13	13 (0%) 81 66	117, 162, 195, 251	0
3	J	1367/1524 (89%)	0.13	9 (0%) 84 70	120, 171, 204, 250	0
4	E	93/99 (93%)	0.37	4 (4%) 40 32	144, 165, 194, 217	0
4	K	93/99 (93%)	0.28	1 (1%) 77 62	144, 179, 206, 228	0
5	F	345/347 (99%)	0.17	9 (2%) 57 42	144, 179, 222, 245	0
5	L	345/347 (99%)	0.30	10 (2%) 54 40	145, 186, 225, 258	0
6	M	158/164 (96%)	0.35	5 (3%) 50 38	159, 207, 235, 243	0
6	N	158/164 (96%)	0.46	5 (3%) 50 38	171, 215, 240, 267	0
7	O	48/48 (100%)	0.27	0 100 100	157, 217, 256, 270	0
7	R	48/48 (100%)	0.19	0 100 100	163, 207, 251, 276	0
8	P	48/48 (100%)	0.33	0 100 100	161, 219, 260, 270	0
8	S	48/48 (100%)	0.36	0 100 100	161, 212, 250, 261	0
9	Q	4/4 (100%)	-0.18	0 100 100	175, 177, 186, 189	0
9	T	4/4 (100%)	-0.53	0 100 100	165, 183, 184, 196	0
All	All	7391/7962 (92%)	0.17	95 (1%) 74 59	117, 174, 219, 276	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	159	ILE	3.6
2	I	445	GLU	3.6
6	M	43	SER	3.5
6	N	160	GLY	3.4
2	I	207	LEU	3.4

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 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
11	MG	D	2003	1/1	0.83	0.08	283,283,283,283	0
11	MG	J	2003	1/1	0.92	0.06	270,270,270,270	0
10	ZN	J	2001	1/1	0.98	0.09	277,277,277,277	0
10	ZN	D	2002	1/1	0.99	0.07	237,237,237,237	0
10	ZN	J	2002	1/1	0.99	0.03	157,157,157,157	0
10	ZN	D	2001	1/1	1.00	0.06	116,116,116,116	0

6.5 Other polymers (i)

There are no such residues in this entry.