wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 09:43 AM EDT

PDB ID	:	1SMY
Title	:	Structural basis for transcription regulation by alarmone ppGpp
Authors	:	Artsimovitch, I.; Patlan, V.; Sekine, S.; Vassylyeva, M.N.; Hosaka, T.; Ochi, K.; Yokoyama, S.; Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-03-10
Resolution	:	2.70 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 (i)) were used in the production of this report:

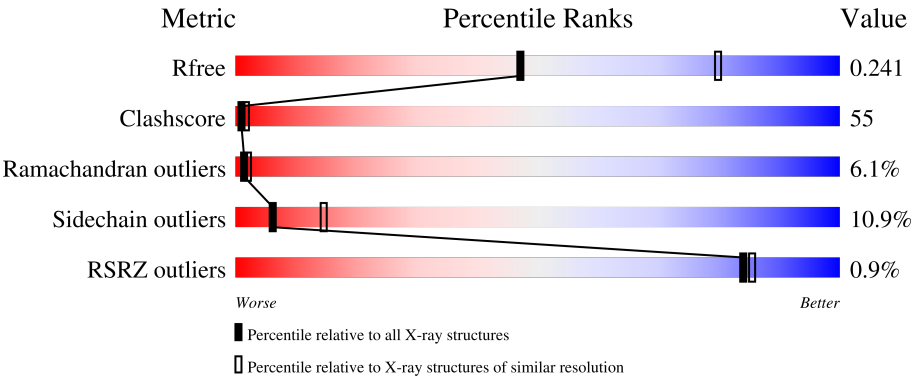
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	315	21% 44% 8% 27%
1	B	315	21% 46% 5% 27%
1	K	315	21% 46% 5% 27%
1	L	315	23% 46% . 27%

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Mol	Chain	Length	Quality of chain
2	C	1119	28% 59% 12%
2	M	1119	27% 62% 10%
3	D	1524	27% 53% 10% 9%
3	N	1524	29% 52% 9% 9%
4	E	99	25% 58% 9%
4	O	99	33% 51% 8%
5	F	423	22% 50% 8% 18%
5	P	423	21% 52% 7% 18%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 63021 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8828	5581	1577	1646	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8828	5581	1577	1646	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA POLYMERASE OMEGA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

- Molecule 5 is a protein called principal sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total 2770	C 1744	N 504	O 518	S 4	0	0	0
5	P	345	Total 2770	C 1744	N 504	O 518	S 4	0	0	0

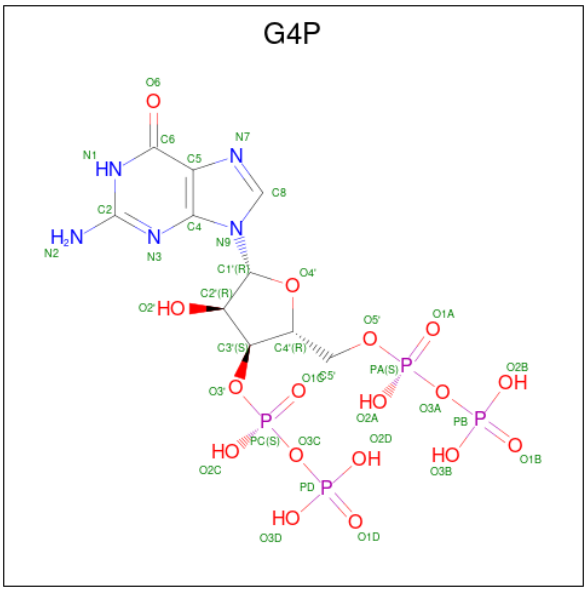
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total 29	Mg 29	0	0
6	B	22	Total 22	Mg 22	0	0
6	C	92	Total 92	Mg 92	0	0
6	D	150	Total 150	Mg 150	0	0
6	E	17	Total 17	Mg 17	0	0
6	F	49	Total 49	Mg 49	0	0
6	M	1	Total 1	Mg 1	0	0
6	N	2	Total 2	Mg 2	0	0

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

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

- Molecule 8 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	N	1	Total C N O P 36 10 5 17 4	0	0
8	N	1	Total C N O P 36 10 5 17 4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	296	Total O 296 296	0	0
9	B	307	Total O 307 307	0	0
9	C	1308	Total O 1308 1308	0	0
9	D	1745	Total O 1745 1745	0	0
9	E	160	Total O 160 160	0	0
9	F	619	Total O 619 619	0	0
9	K	316	Total O 316 316	0	0
9	L	341	Total O 341 341	0	0
9	M	1401	Total O 1401 1401	0	0
9	N	1794	Total O 1794 1794	0	0

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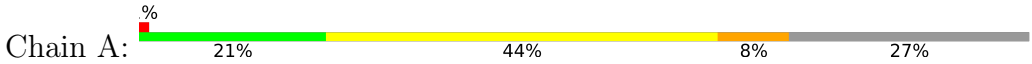
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	O	203	Total O 203 203	0	0
9	P	541	Total O 541 541	0	0

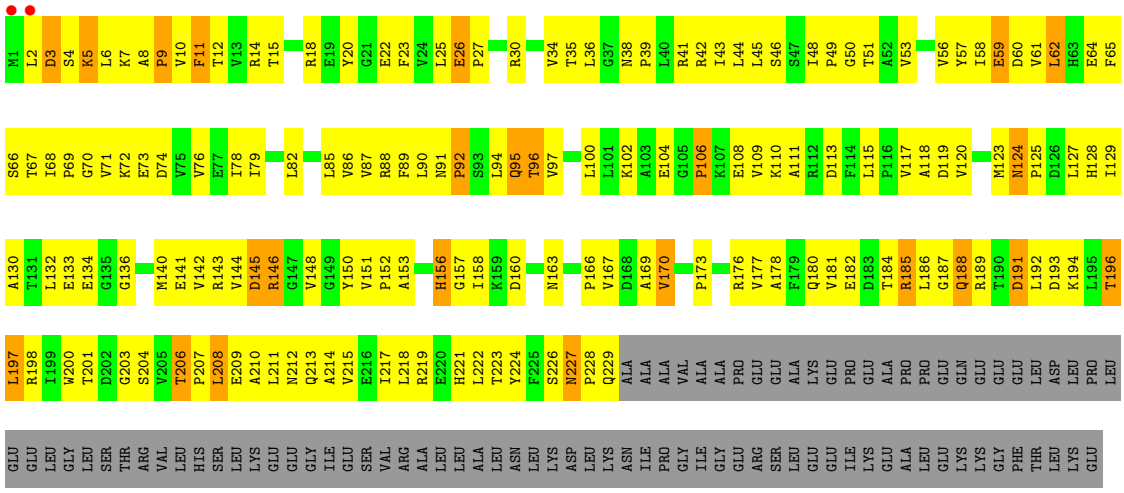
3 Residue-property plots (i)

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 alpha chain

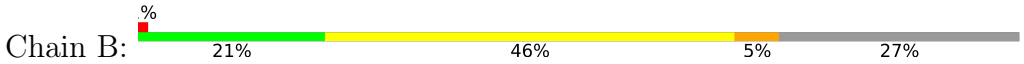
Chain A:

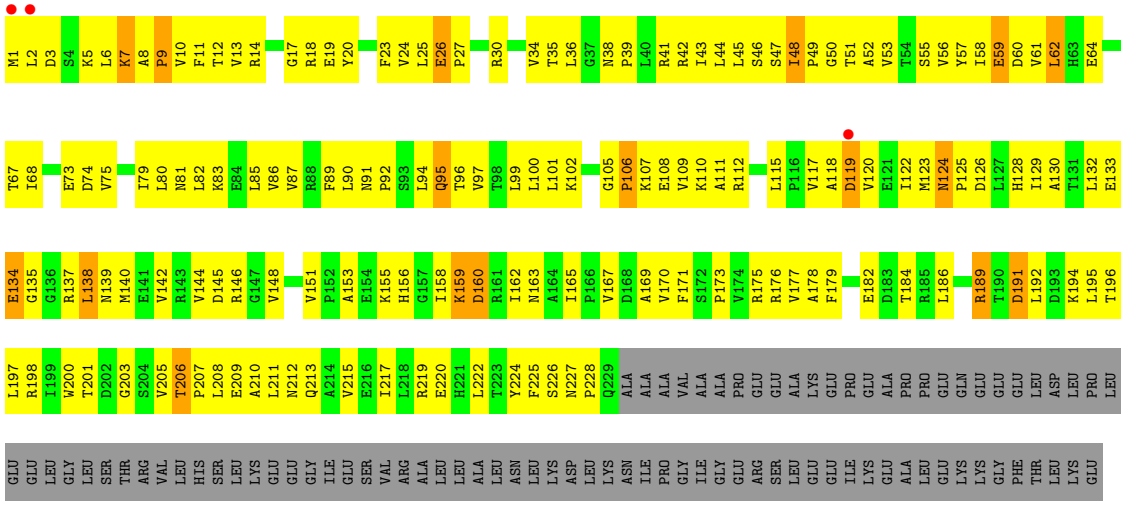




• Molecule 1: DNA-directed RNA polymerase alpha chain

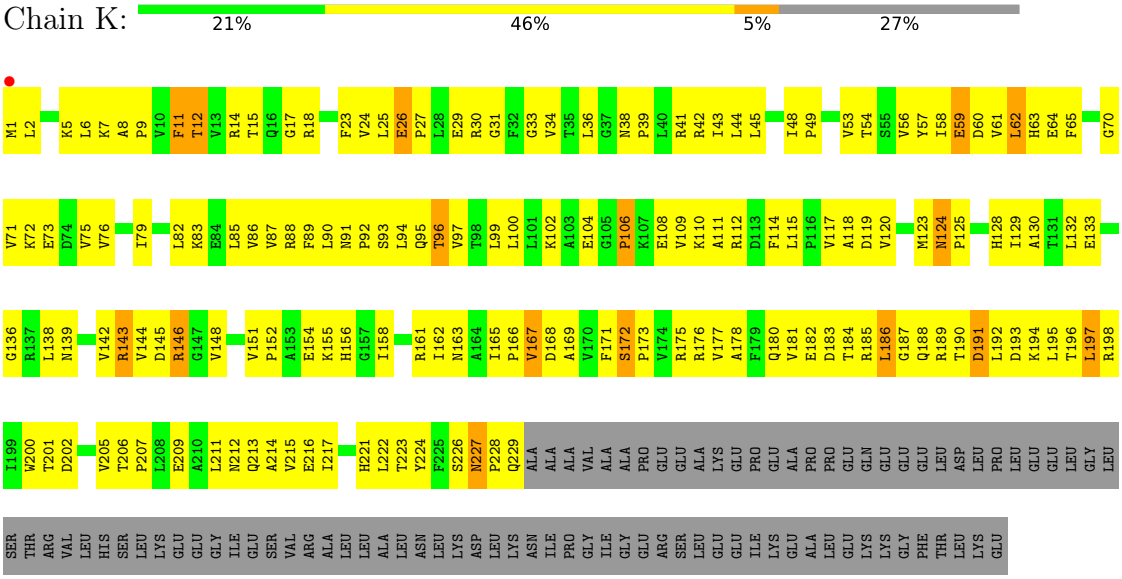
Chain B:





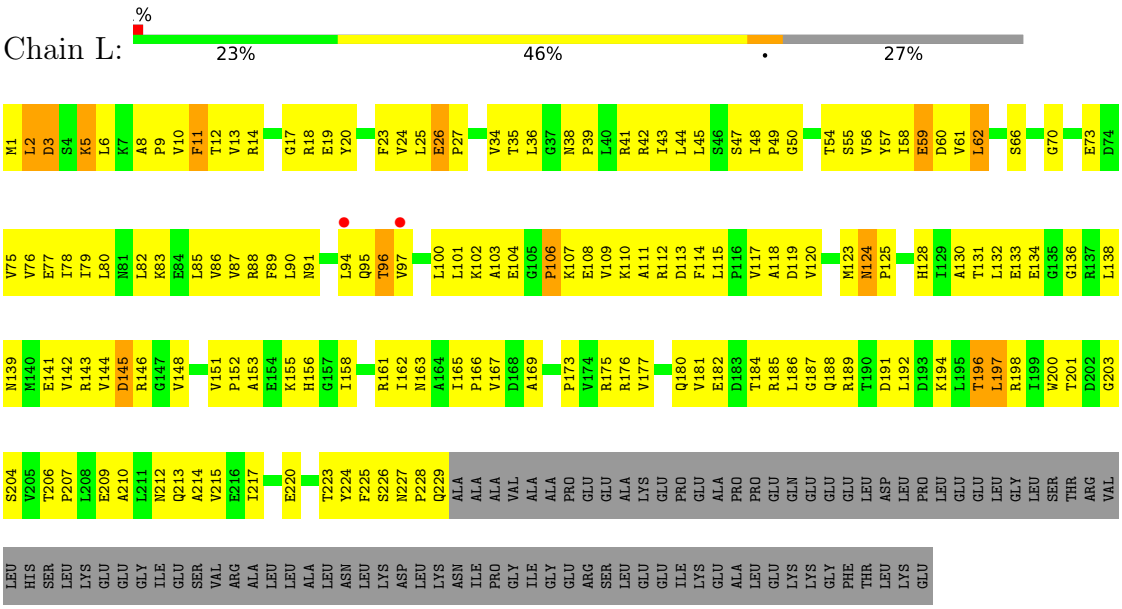
• Molecule 1: DNA-directed RNA polymerase alpha chain

Chain K:



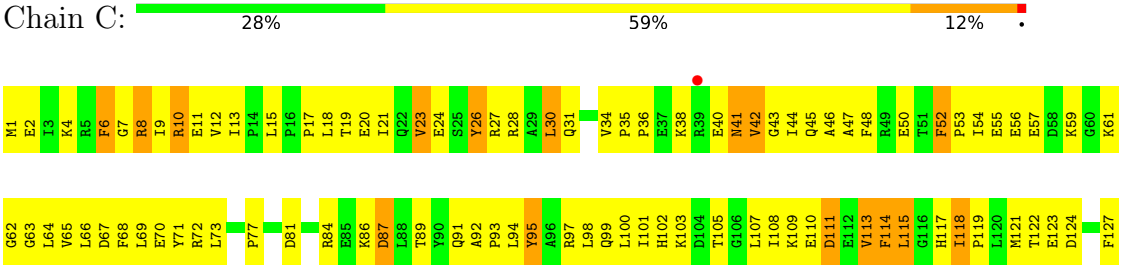
• Molecule 1: DNA-directed RNA polymerase alpha chain

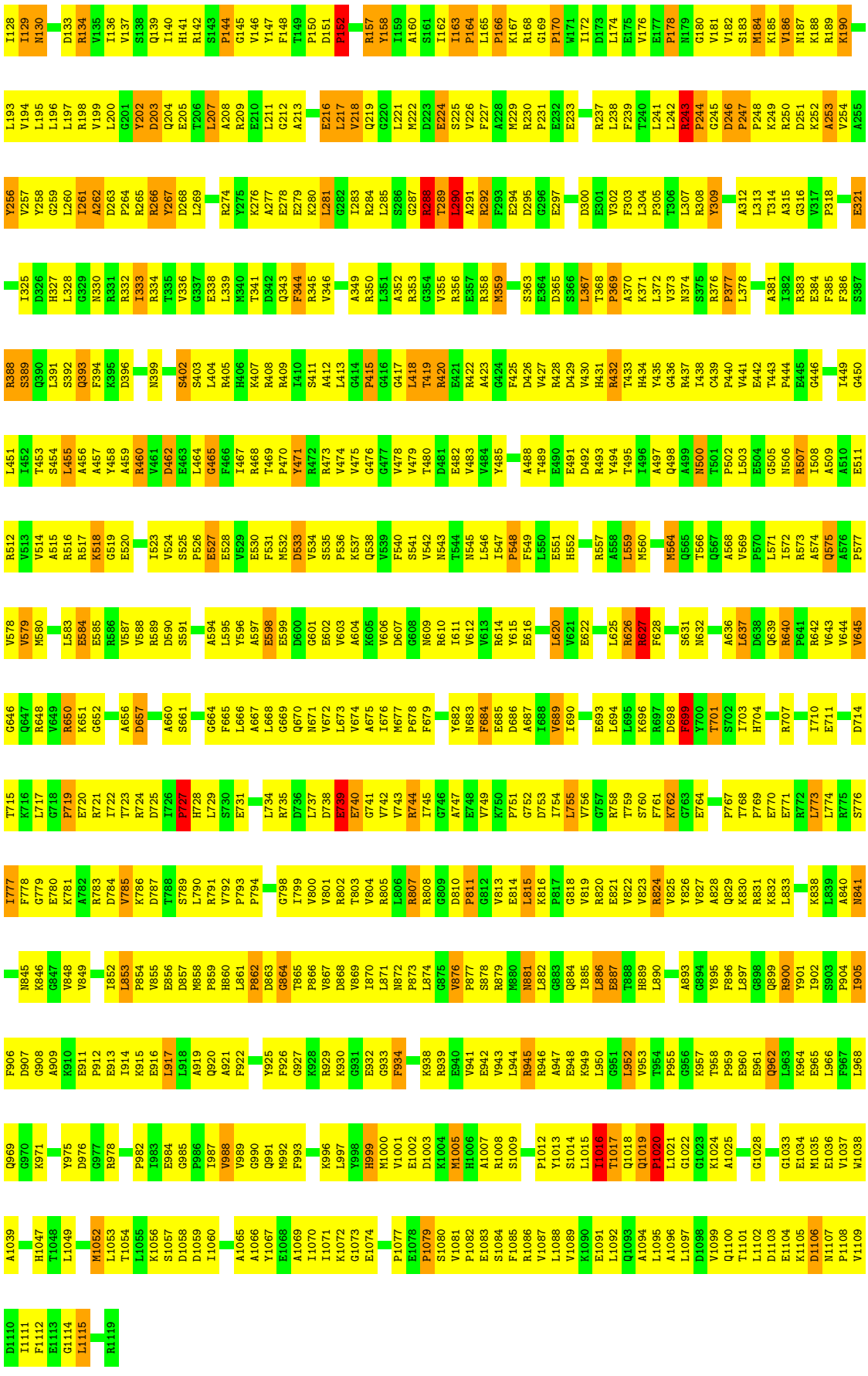
Chain L:



• Molecule 2: DNA-directed RNA polymerase beta chain

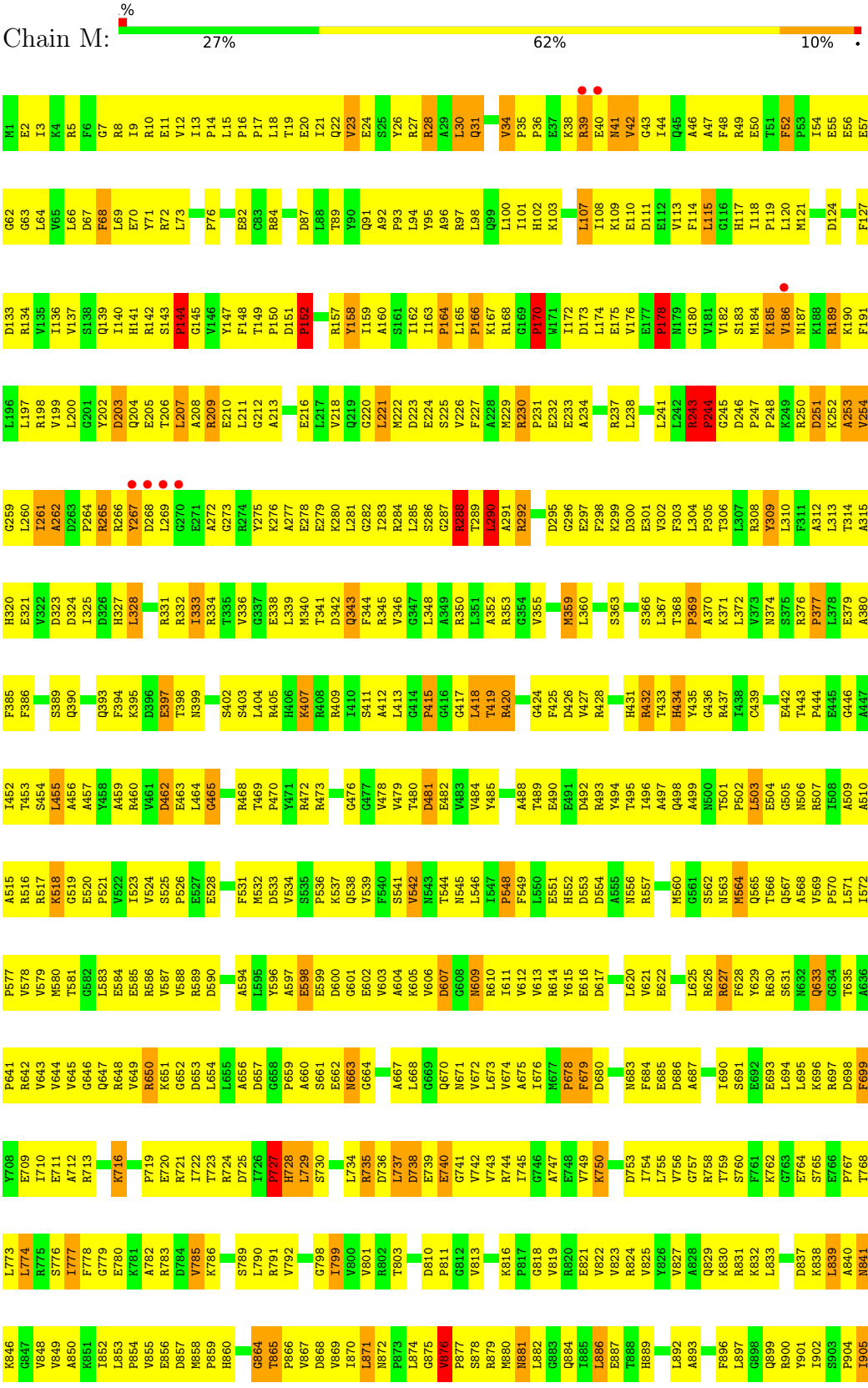
Chain C:

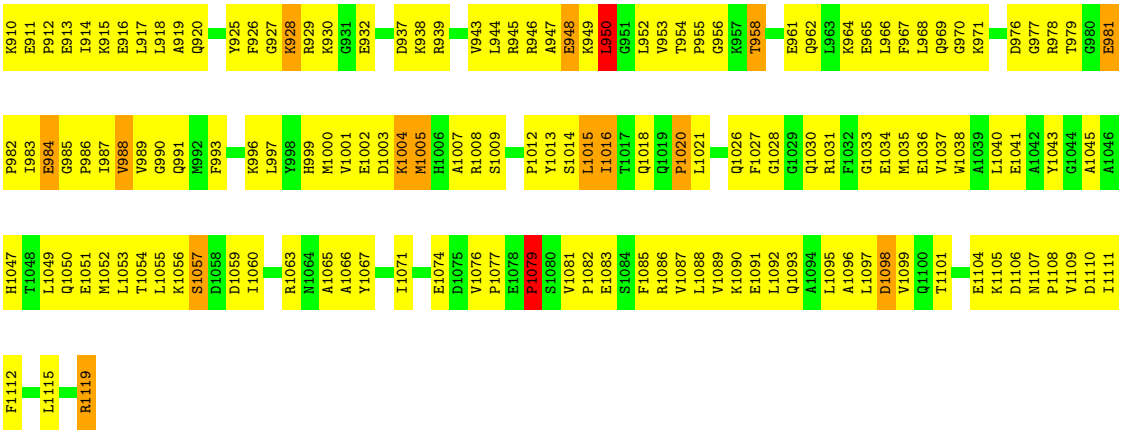



I128 I129 N130 D133 R134 V135 I136 V137 S138 Q139 I140 H141 R142 S143 P144 G145 V146 Y147 F148 T149 P150 D151 P152 R157 Y158 I159 A160 S161 I162 I163 P164 L165 P166 K167 R168 G169 P170 W171 I172 D173 L174 E175 V176 E177 P178 N179 G180 V181 V182 S183 M184 K185 V186 N187 K188 R189 K190
L193 V194 L195 L196 L197 R198 V199 L200 G201 Y202 D203 Q204 E205 T206 L207 A208 R209 E210 L211 G212 A213 E216 L217 V218 Q219 G220 L221 M222 D223 E224 S225 V226 F227 A228 M229 R230 P231 E232 E233 R237 L238 F239 T240 L241 L242 R243 P244 G245 D246 P247 P248 K249 R250 D251 K252 A253 V254 A255
Y256 V257 Y258 G259 L260 I261 A262 D263 P264 R265 R266 Y267 D268 L269 R274 Y275 K276 A277 E278 E279 K280 L281 G282 I283 R284 L285 S286 G287 R288 T289 L290 A291 R292 F293 E294 D295 G296 E297 D300 E301 V302 F303 L304 P305 T306 L307 R308 Y309 A312 L313 T314 A315 G316 V317 P318 E321
I325 D326 H327 L328 G329 N330 R331 R332 I333 R334 T335 V336 G337 E338 L339 M340 T341 D342 Q343 F344 R345 V346 A349 R350 L351 A352 R353 G354 V355 R356 E357 R358 M359 S363 E364 D365 S366 L367 T368 P369 A370 K371 L372 V373 N374 S375 R376 P377 L378 A381 I382 R383 E384 F385 F386 S387
R388 S389 Q390 L391 S392 Q393 F394 K395 D396 N399 S402 S403 L404 R405 H406 K407 R408 R409 I410 S411 A412 L413 G414 P415 G416 G417 G417 L418 T419 R420 E421 R422 A423 G424 F425 D426 V427 R428 D429 V430 H431 R432 T433 H434 Y435 G436 R437 I438 C439 P440 V441 E442 T443 P444 E445 G446 I449 G450
L451 I452 T453 S454 L455 A456 A457 Y458 A459 R460 V461 D462 E463 L464 G465 F466 I467 R468 T469 P470 Y471 R472 R473 V474 V475 G476 G477 V478 V479 T480 D481 E482 V483 V484 Y485 A488 T489 E490 E491 D492 R493 Y494 T495 I496 A497 Q498 A499 N500 T501 P502 L503 E504 G505 N506 R507 I508 A509 A510 E511
R512 V513 V514 A515 R516 R517 K518 G519 E520 I523 V524 S525 P526 E527 E528 V529 E530 F531 M532 D533 V534 S535 P536 K537 Q538 V539 F540 S541 V542 N543 T544 N545 L546 I547 P548 F549 L550 E551 H552 R557 A558 L559 M560 M564 Q565 T566 Q567 A568 V569 P570 L571 I572 R573 A574 Q575 A576 P577
V578 V579 M580 L583 E584 E585 R586 V587 V588 R589 D590 S591 A594 L595 Y596 A597 E598 E599 D600 G601 E602 V603 A604 K605 V606 D607 G608 N609 R610 I611 V612 V613 R614 Y615 E616 L620 V621 E622 L625 R626 E627 F628 S631 N632 A636 L637 D638 Q639 R640 P641 R642 V643 V644 V645
G646 Q647 R648 V649 R650 K651 G652 A656 D657 A660 S661 G664 F665 L666 A667 L668 G669 Q670 N671 E602 V672 L673 V674 A675 I676 M677 P678 F679 Y682 N683 F684 E685 D686 A687 I688 V689 I690 E693 L694 L695 K696 R697 D698 F699 Y700 T701 S702 I703 H704 R707 I710 E711 D714
T715 K716 L717 G718 P719 E720 R721 I722 T723 R724 D725 T726 P727 H728 L729 S730 E731 L734 R735 D736 L737 D738 E739 E740 G741 V742 V743 R744 I745 G746 A747 E748 V749 K750 P751 G752 D753 I754 L755 V756 G757 R758 T759 S760 F761 R762 G763 E764 P767 T768 P769 E770 E771 R772 L773 L774 R775 S776
I777 F778 G779 E780 K781 A782 R783 D784 V785 K786 D787 T788 S789 L790 R791 V792 P793 P794 G798 I799 V800 V801 R802 T803 V804 R805 L806 R807 R808 G809 D810 P811 G812 V813 E814 L815 K816 P817 G818 V819 R820 E821 V822 V823 R824 V825 Y826 V827 A828 Q829 K830 R831 K832 L833 K838 L839 A840 N841
Q969 G970 K971 Y975 D976 G977 R978 P982 I983 E984 G985 P986 I987 V988 V989 G990 Q991 M992 F993 K996 L997 Y998 H999 M1000 V1001 E1002 D1003 K1004 M1005 H1006 A1007 R1008 S1009 P1012 Y1013 S1014 L1015 I1016 T1017 Q1018 Q1019 P1020 L1021 G1022 G1023 K1024 A1025 G1028 G1033 E1034 M1035 E1036 V1037 W1038
A1039 H1047 T1048 L1049 M1052 L1053 T1054 L1055 K1056 S1057 D1058 D1059 I1060 A1065 A1066 Y1067 E1068 A1069 I1070 I1071 K1072 G1073 E1074 P1077 E1078 P1079 S1080 V1081 P1082 E1083 S1084 F1085 R1086 V1087 L1088 V1089 K1090 E1091 L1092 Q1093 A1094 L1095 A1096 L1097 D1098 V1099 Q1100 T1101 L1102 D1103 E1104 K1105 D1106 N1107 P1108 V1109
D1110 I1111 F1112 E1113 G1114 L1115 R1119

• Molecule 2: DNA-directed RNA polymerase beta chain

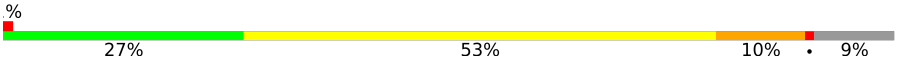
Chain M:

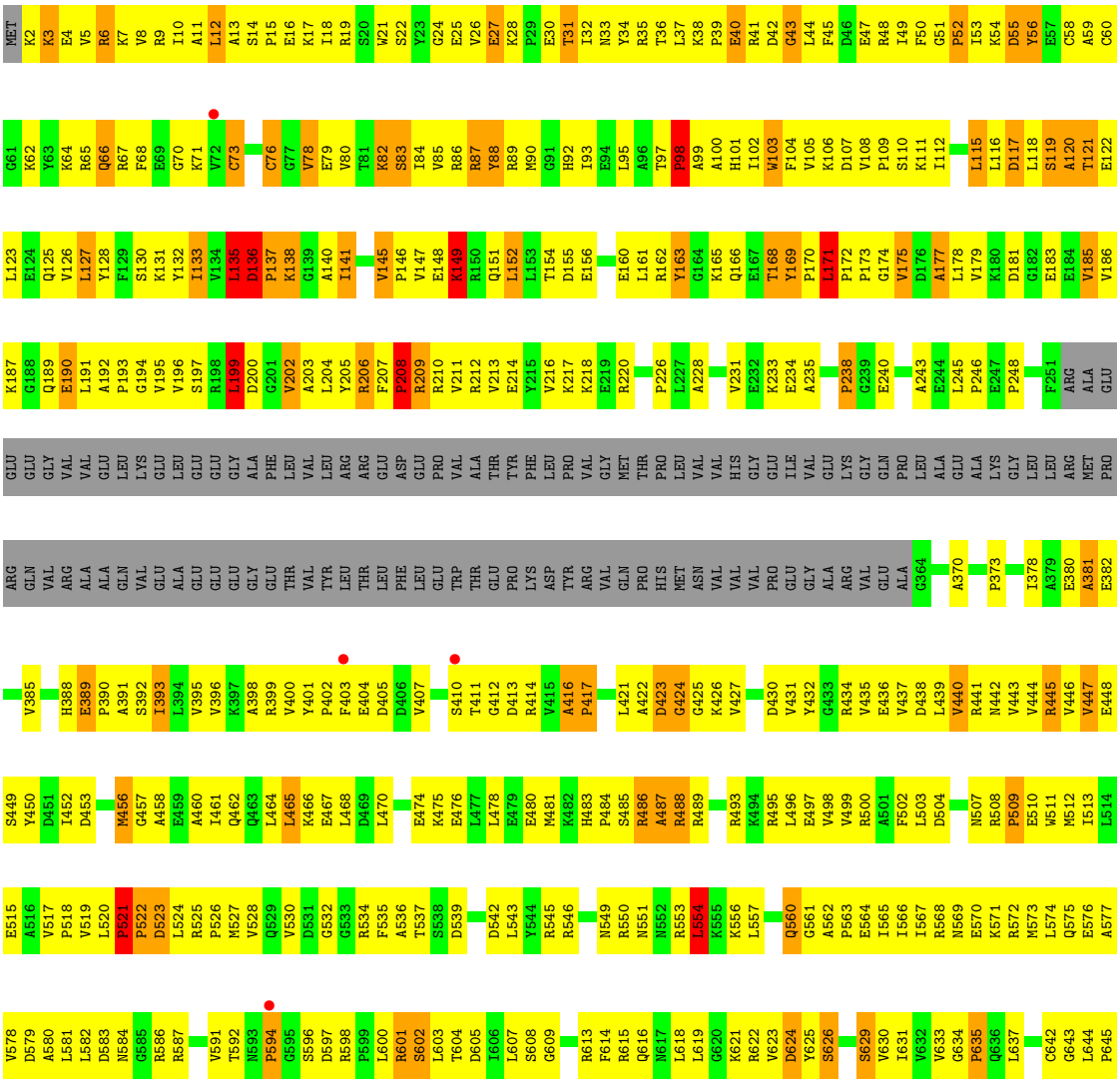


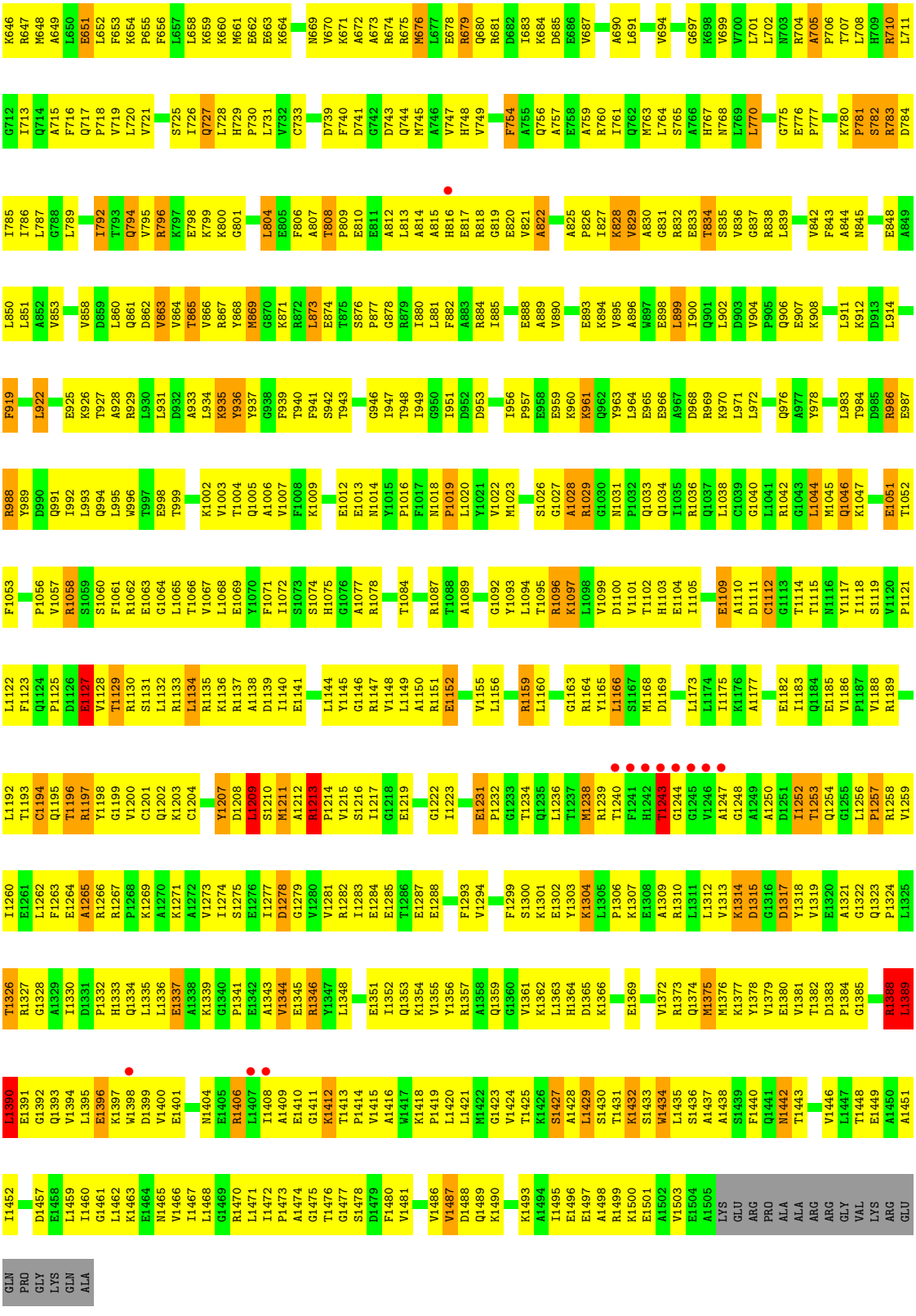


• Molecule 3: DNA-directed RNA polymerase beta' chain

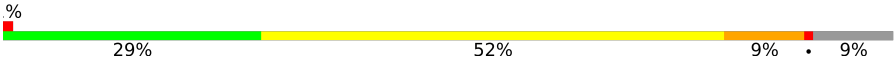
Chain D:

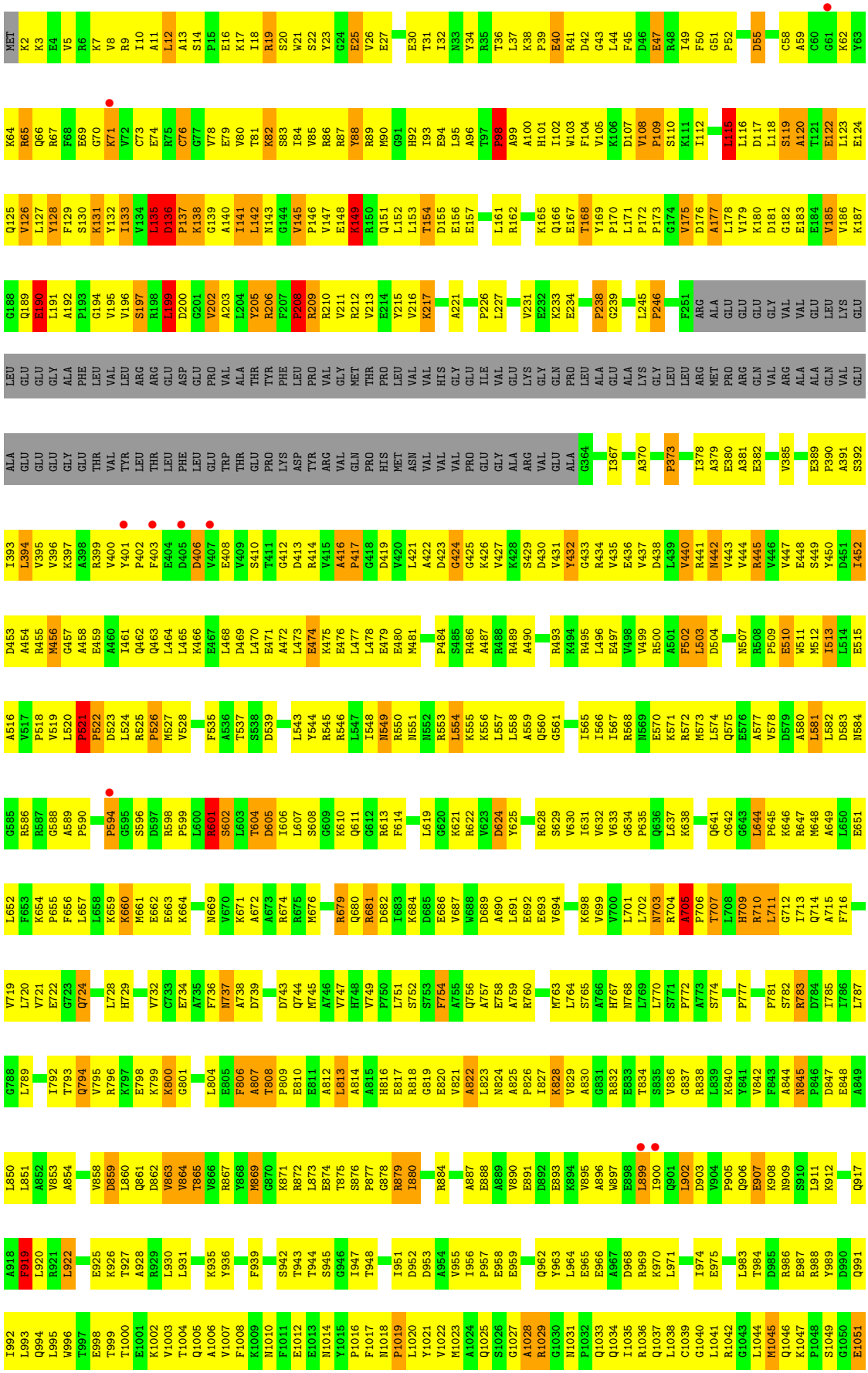


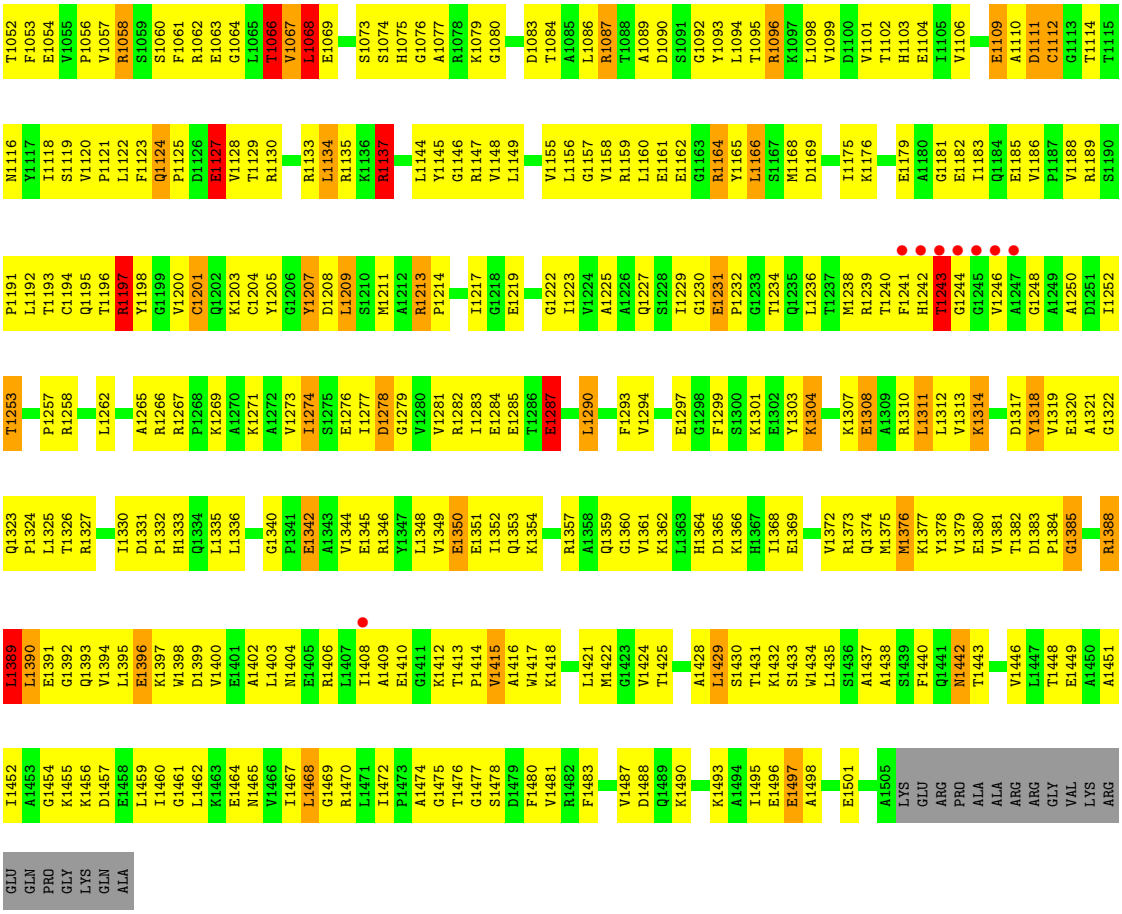




• Molecule 3: DNA-directed RNA polymerase beta' chain

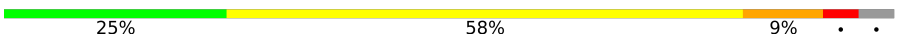


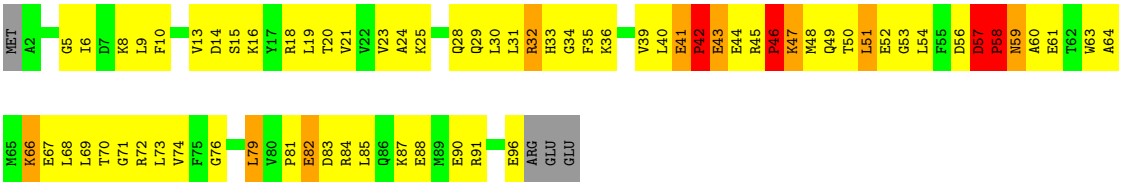




• Molecule 4: RNA POLYMERASE OMEGA SUBUNIT

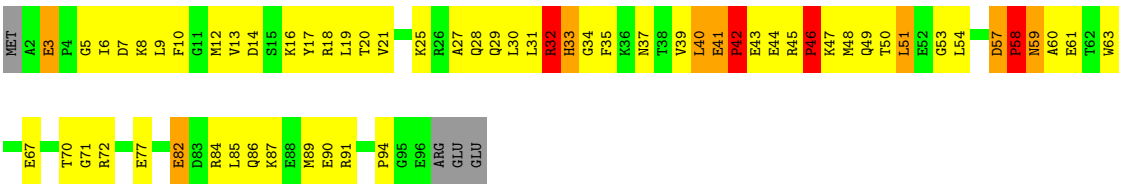
Chain E:





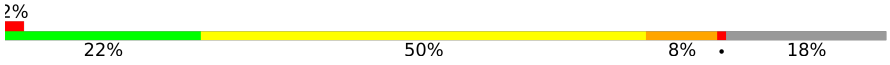
• Molecule 4: RNA POLYMERASE OMEGA SUBUNIT

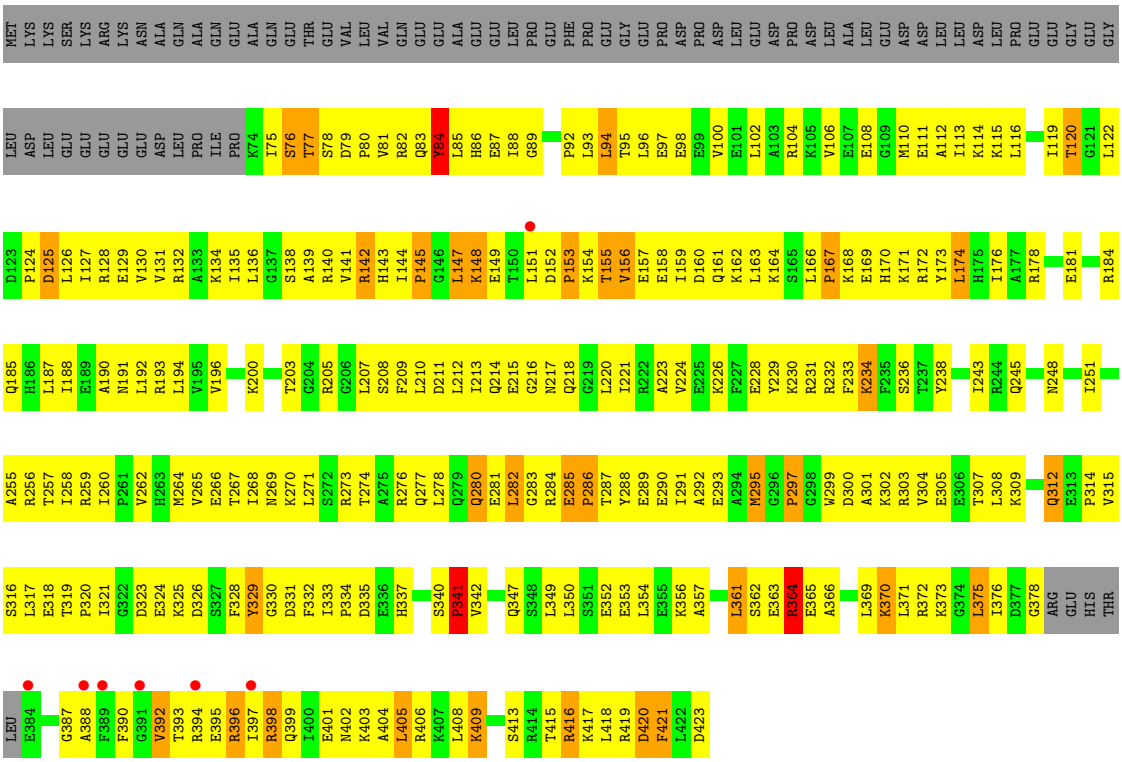
Chain O:



• Molecule 5: principal sigma factor

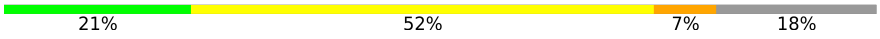
Chain F:

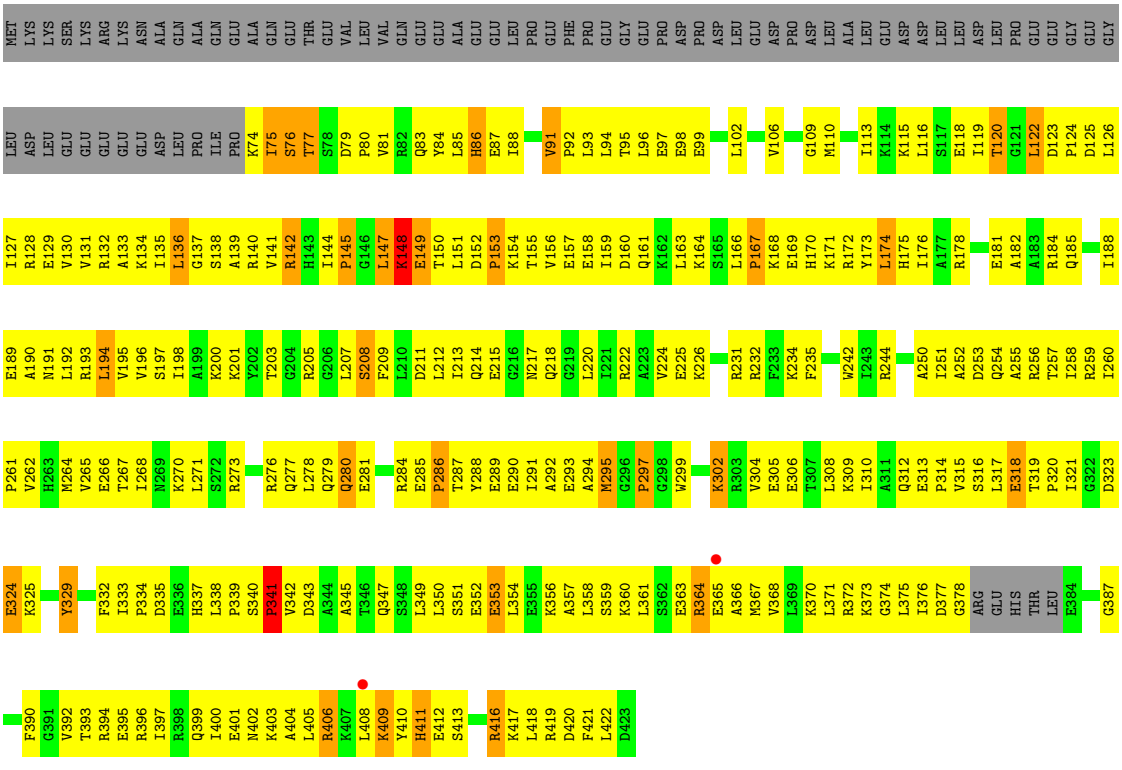




• Molecule 5: principal sigma factor

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 50.12 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 97.1 (50.12-2.71)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.266 0.186 , 0.241	Depositor DCC
R_{free} test set	14873 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.086 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	63021	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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, G4P, 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	0.68	0/1838	0.70	0/2498
1	B	0.68	0/1838	0.68	0/2498
1	K	0.68	0/1838	0.72	1/2498 (0.0%)
1	L	0.68	0/1838	0.67	1/2498 (0.0%)
2	C	0.75	0/8996	0.79	4/12164 (0.0%)
2	M	0.74	0/8996	0.78	4/12164 (0.0%)
3	D	0.74	0/10975	0.81	10/14836 (0.1%)
3	N	0.73	0/10975	0.81	14/14836 (0.1%)
4	E	0.74	0/783	0.81	0/1054
4	O	0.75	0/783	0.81	0/1054
5	F	0.65	0/2811	0.75	1/3781 (0.0%)
5	P	0.64	0/2811	0.74	1/3781 (0.0%)
All	All	0.72	0/54482	0.78	36/73662 (0.0%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	243	ARG	C-N-CD	-9.21	100.34	120.60
3	D	199	LEU	CA-CB-CG	-8.95	94.72	115.30
3	N	199	LEU	CA-CB-CG	-8.85	94.94	115.30
1	K	197	LEU	CA-CB-CG	8.22	134.21	115.30
2	C	243	ARG	C-N-CD	-7.23	104.69	120.60

There are no chirality outliers.

There are no planarity outliers.

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	1806	0	1861	211	0
1	B	1806	0	1861	191	0
1	K	1806	0	1861	196	0
1	L	1806	0	1861	183	0
2	C	8828	0	8933	1013	0
2	M	8828	0	8933	1065	0
3	D	10797	0	10873	1260	0
3	N	10797	0	10873	1227	0
4	E	769	0	775	104	0
4	O	769	0	775	96	0
5	F	2770	0	2844	327	0
5	P	2770	0	2844	363	0
6	A	29	0	0	0	0
6	B	22	0	0	0	0
6	C	92	0	0	0	0
6	D	150	0	0	0	0
6	E	17	0	0	0	0
6	F	49	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	N	72	0	22	9	0
9	A	296	0	0	67	0
9	B	307	0	0	66	0
9	C	1308	0	0	281	0
9	D	1745	0	0	322	0
9	E	160	0	0	37	0
9	F	619	0	0	99	0
9	K	316	0	0	72	0
9	L	341	0	0	64	0
9	M	1401	0	0	325	0
9	N	1794	0	0	330	0
9	O	203	0	0	33	0
9	P	541	0	0	96	0
All	All	63021	0	54316	5952	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 55.

The worst 5 of 5952 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:34:VAL:HB	2:C:38:LYS:HG3	1.28	1.11
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.33	1.10
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.34	1.10
8:N:9100:G4P:H5"	8:N:9100:G4P:H8	1.14	1.09
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.35	1.08

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	227/315 (72%)	187 (82%)	33 (14%)	7 (3%)	4	9
1	B	227/315 (72%)	183 (81%)	38 (17%)	6 (3%)	5	13
1	K	227/315 (72%)	186 (82%)	32 (14%)	9 (4%)	3	6
1	L	227/315 (72%)	185 (82%)	37 (16%)	5 (2%)	6	17
2	C	1117/1119 (100%)	856 (77%)	194 (17%)	67 (6%)	1	2
2	M	1117/1119 (100%)	863 (77%)	187 (17%)	67 (6%)	1	2
3	D	1388/1524 (91%)	1047 (75%)	248 (18%)	93 (7%)	1	1
3	N	1388/1524 (91%)	1042 (75%)	251 (18%)	95 (7%)	1	1
4	E	93/99 (94%)	72 (77%)	11 (12%)	10 (11%)	0	0
4	O	93/99 (94%)	70 (75%)	13 (14%)	10 (11%)	0	0
5	F	341/423 (81%)	264 (77%)	53 (16%)	24 (7%)	1	1
5	P	341/423 (81%)	267 (78%)	53 (16%)	21 (6%)	1	2
All	All	6786/7590 (89%)	5222 (77%)	1150 (17%)	414 (6%)	1	2

5 of 414 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	188	GLN
1	B	118	ALA
2	C	10	ARG
2	C	59	LYS

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	202/273 (74%)	181 (90%)	21 (10%)	7 16
1	B	202/273 (74%)	186 (92%)	16 (8%)	12 28
1	K	202/273 (74%)	187 (93%)	15 (7%)	13 32
1	L	202/273 (74%)	190 (94%)	12 (6%)	19 43
2	C	941/941 (100%)	827 (88%)	114 (12%)	5 11
2	M	941/941 (100%)	838 (89%)	103 (11%)	6 14
3	D	1123/1279 (88%)	992 (88%)	131 (12%)	5 12
3	N	1123/1279 (88%)	987 (88%)	136 (12%)	5 11
4	E	83/87 (95%)	73 (88%)	10 (12%)	5 11
4	O	83/87 (95%)	73 (88%)	10 (12%)	5 11
5	F	295/370 (80%)	263 (89%)	32 (11%)	6 15
5	P	295/370 (80%)	273 (92%)	22 (8%)	13 31
All	All	5692/6446 (88%)	5070 (89%)	622 (11%)	6 14

5 of 622 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	98	PRO
3	N	1285	GLU
3	N	154	THR
3	N	76	CYS

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Mol	Chain	Res	Type
3	N	724	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	1107	ASN
3	N	1184	GLN
3	N	442	ASN
3	N	737	ASN
4	O	37	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 368 ligands modelled in this entry, 366 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	G4P	N	9101	6	30,38,38	1.55	5 (16%)	42,61,61	1.52	6 (14%)
8	G4P	N	9100	6	30,38,38	1.37	4 (13%)	42,61,61	1.61	9 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	G4P	N	9101	6	-	8/23/43/43	0/3/3/3
8	G4P	N	9100	6	-	8/23/43/43	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	9101	G4P	O4'-C1'	3.85	1.46	1.41
8	N	9101	G4P	C5-C6	-3.57	1.40	1.47
8	N	9101	G4P	C6-N1	3.50	1.43	1.37
8	N	9100	G4P	O4'-C1'	3.17	1.45	1.41
8	N	9101	G4P	C8-N7	-3.09	1.29	1.35

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	9101	G4P	PC-O3C-PD	-5.30	114.65	132.83
8	N	9100	G4P	PA-O3A-PB	-4.40	117.73	132.83
8	N	9101	G4P	O3'-C3'-C4'	4.26	125.47	110.08
8	N	9100	G4P	O3B-PB-O3A	-3.07	94.35	104.64
8	N	9100	G4P	C2'-C3'-C4'	3.06	108.65	103.22

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	9100	G4P	PA-O3A-PB-O2B
8	N	9100	G4P	C5'-O5'-PA-O1A
8	N	9100	G4P	C4'-C5'-O5'-PA
8	N	9100	G4P	PC-O3C-PD-O3D
8	N	9101	G4P	PA-O3A-PB-O3B

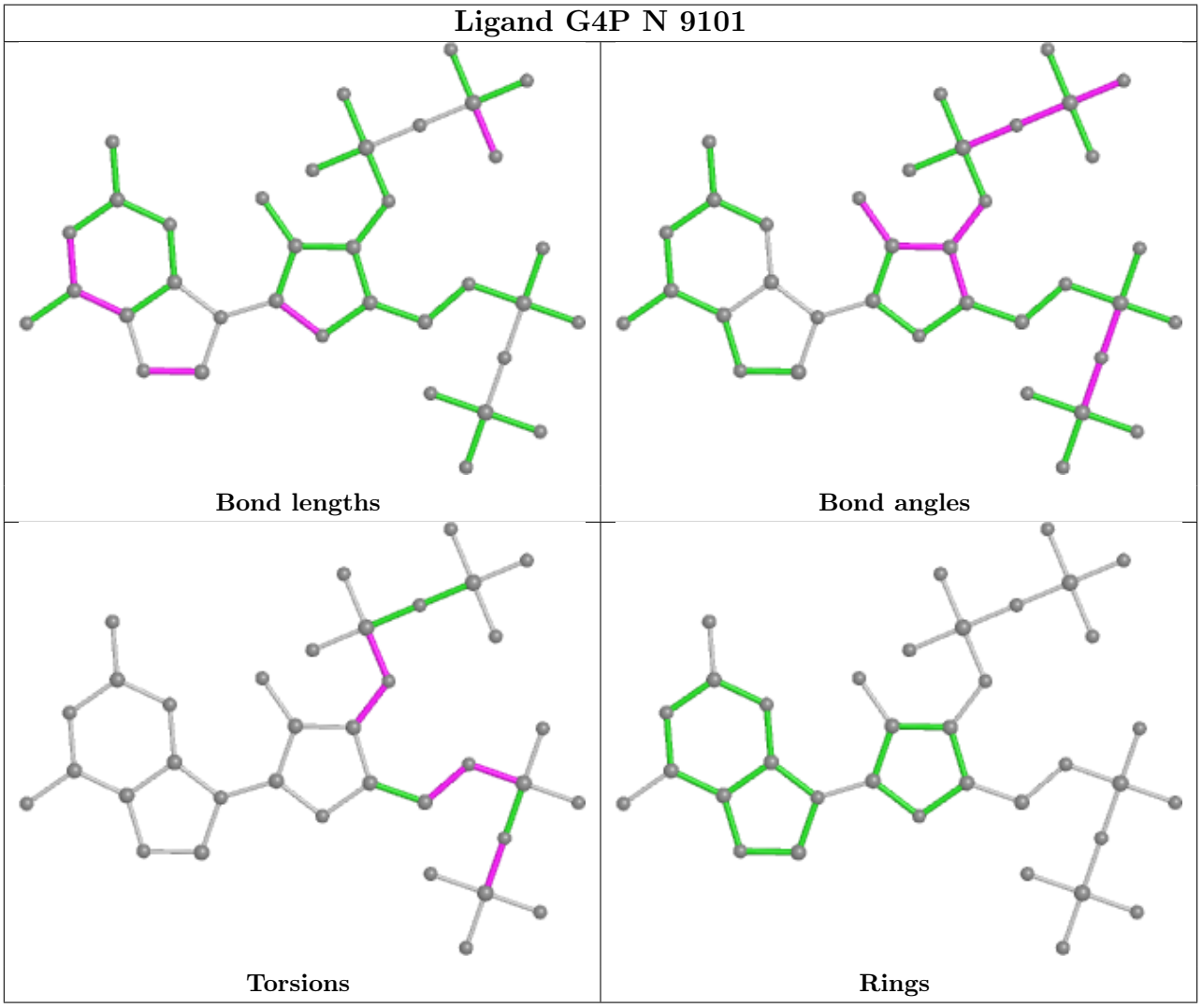
There are no ring outliers.

2 monomers are involved in 9 short contacts:

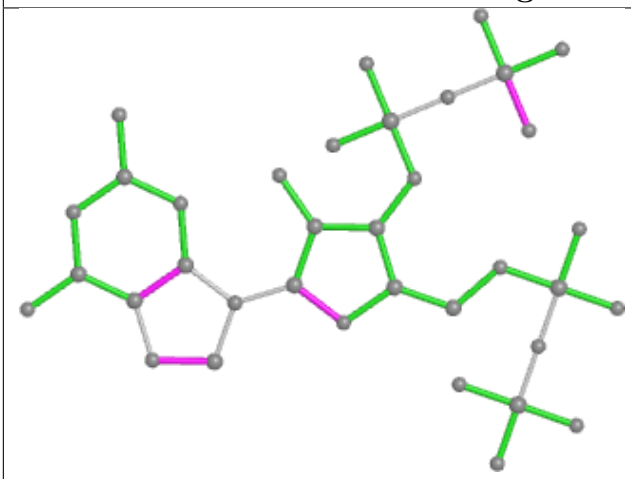
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	9101	G4P	5	0
8	N	9100	G4P	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

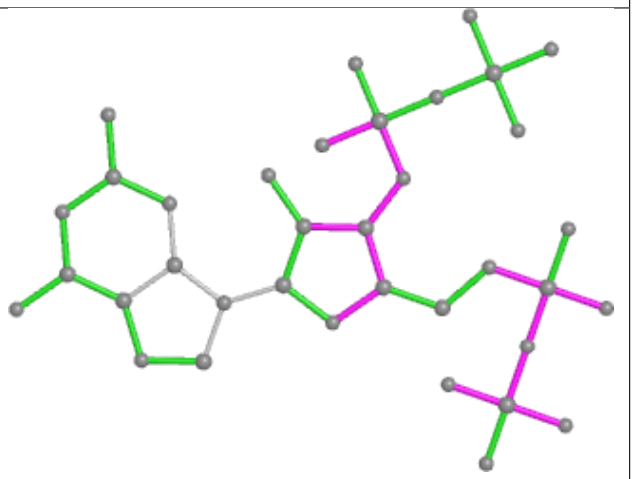
Ligand G4P N 9101



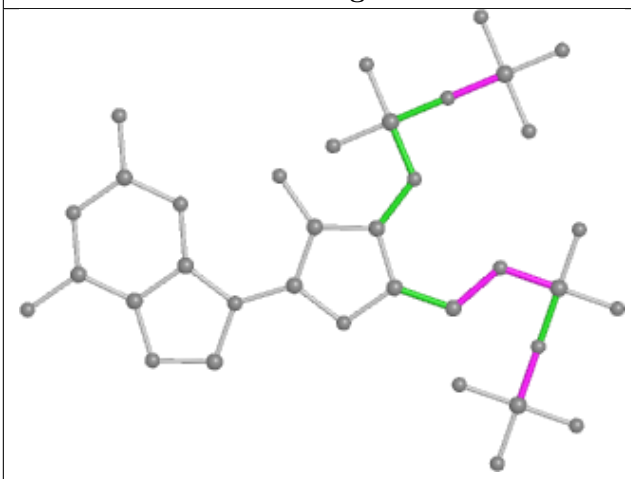
Ligand G4P N 9100



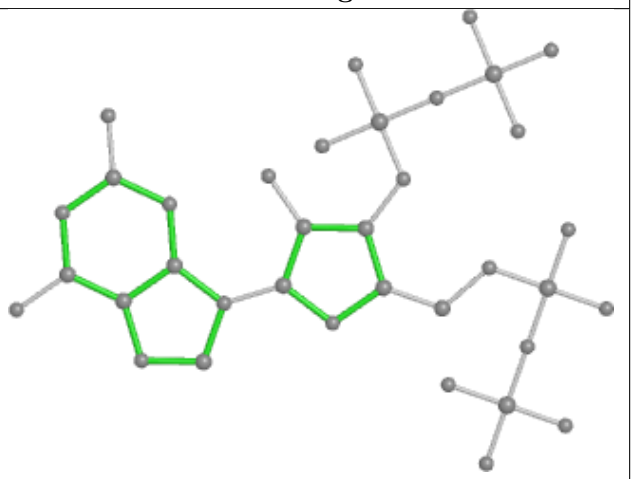
Bond lengths



Bond angles



Torsions



Rings

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	229/315 (72%)	-0.74	2 (0%) 84 85	39, 65, 90, 121	0
1	B	229/315 (72%)	-0.70	3 (1%) 77 78	58, 82, 103, 129	0
1	K	229/315 (72%)	-0.72	1 (0%) 92 93	42, 65, 87, 117	0
1	L	229/315 (72%)	-0.71	2 (0%) 84 85	54, 88, 104, 122	0
2	C	1119/1119 (100%)	-0.80	1 (0%) 95 96	31, 73, 106, 124	0
2	M	1119/1119 (100%)	-0.76	7 (0%) 89 91	30, 75, 110, 122	0
3	D	1392/1524 (91%)	-0.70	16 (1%) 80 82	33, 71, 108, 152	0
3	N	1392/1524 (91%)	-0.72	17 (1%) 79 80	35, 71, 108, 145	0
4	E	95/99 (95%)	-0.90	0 100 100	49, 79, 103, 109	0
4	O	95/99 (95%)	-0.77	0 100 100	42, 81, 111, 119	0
5	F	345/423 (81%)	-0.61	7 (2%) 65 67	53, 84, 111, 126	0
5	P	345/423 (81%)	-0.66	2 (0%) 89 91	41, 83, 110, 117	0
All	All	6818/7590 (89%)	-0.73	58 (0%) 84 85	30, 74, 108, 152	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1246	VAL	7.3
3	D	1245	GLY	7.2
3	D	1246	VAL	6.5
3	N	1247	ALA	6.2
3	D	1243	THR	5.3

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
6	MG	C	9202	1/1	0.96	0.07	43,43,43,43	0
6	MG	D	9204	1/1	0.96	0.05	38,38,38,38	0
6	MG	D	9240	1/1	0.96	0.08	20,20,20,20	0
6	MG	D	9384	1/1	0.96	0.07	20,20,20,20	0
6	MG	D	9416	1/1	0.96	0.08	20,20,20,20	0
7	ZN	D	9102	1/1	0.96	0.06	115,115,115,115	0
6	MG	A	9394	1/1	0.97	0.09	20,20,20,20	0
6	MG	C	9257	1/1	0.97	0.06	20,20,20,20	0
6	MG	C	9272	1/1	0.97	0.07	20,20,20,20	0
6	MG	C	9525	1/1	0.97	0.05	20,20,20,20	0
6	MG	D	9528	1/1	0.97	0.06	20,20,20,20	0
6	MG	F	9250	1/1	0.97	0.06	20,20,20,20	0
6	MG	M	9206	1/1	0.97	0.10	38,38,38,38	0
6	MG	D	9201	1/1	0.97	0.11	30,30,30,30	0
6	MG	C	9441	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9519	1/1	0.98	0.05	20,20,20,20	0
6	MG	B	9235	1/1	0.98	0.06	20,20,20,20	0
6	MG	C	9554	1/1	0.98	0.06	20,20,20,20	0
6	MG	C	9210	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9238	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9214	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9216	1/1	0.98	0.08	20,20,20,20	0
6	MG	D	9220	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9226	1/1	0.98	0.04	20,20,20,20	0
6	MG	D	9237	1/1	0.98	0.05	20,20,20,20	0
6	MG	B	9413	1/1	0.98	0.05	20,20,20,20	0
6	MG	D	9241	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9271	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9294	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9301	1/1	0.98	0.05	20,20,20,20	0
6	MG	D	9355	1/1	0.98	0.13	20,20,20,20	0
6	MG	B	9485	1/1	0.98	0.05	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	9386	1/1	0.98	0.04	20,20,20,20	0
6	MG	D	9390	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9406	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9299	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9460	1/1	0.98	0.04	20,20,20,20	0
6	MG	D	9480	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9518	1/1	0.98	0.06	20,20,20,20	0
6	MG	C	9320	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9532	1/1	0.98	0.04	20,20,20,20	0
6	MG	E	9249	1/1	0.98	0.09	20,20,20,20	0
6	MG	E	9341	1/1	0.98	0.06	20,20,20,20	0
6	MG	E	9431	1/1	0.98	0.07	20,20,20,20	0
6	MG	C	9354	1/1	0.98	0.07	20,20,20,20	0
6	MG	F	9290	1/1	0.98	0.06	20,20,20,20	0
6	MG	F	9305	1/1	0.98	0.07	20,20,20,20	0
6	MG	F	9398	1/1	0.98	0.07	20,20,20,20	0
6	MG	F	9496	1/1	0.98	0.05	20,20,20,20	0
6	MG	F	9500	1/1	0.98	0.08	20,20,20,20	0
6	MG	F	9545	1/1	0.98	0.08	20,20,20,20	0
6	MG	C	9356	1/1	0.98	0.07	20,20,20,20	0
6	MG	C	9364	1/1	0.98	0.06	20,20,20,20	0
7	ZN	D	9103	1/1	0.98	0.09	87,87,87,87	0
7	ZN	N	9104	1/1	0.98	0.05	116,116,116,116	0
7	ZN	N	9105	1/1	0.98	0.10	80,80,80,80	0
8	G4P	N	9100	36/36	0.98	0.11	35,45,54,55	0
6	MG	C	9316	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9423	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9321	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9328	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9330	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9339	1/1	0.99	0.11	20,20,20,20	0
6	MG	C	9345	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9348	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9442	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9464	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9358	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9359	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9473	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9367	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9371	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9378	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9381	1/1	0.99	0.05	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	C	9383	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9385	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9387	1/1	0.99	0.10	20,20,20,20	0
6	MG	C	9395	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9396	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9405	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9408	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9422	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9430	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9438	1/1	0.99	0.11	20,20,20,20	0
6	MG	A	9486	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9444	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9451	1/1	0.99	0.11	20,20,20,20	0
6	MG	C	9454	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9465	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9466	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9474	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9476	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9489	1/1	0.99	0.11	20,20,20,20	0
6	MG	C	9497	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9501	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9507	1/1	0.99	0.03	20,20,20,20	0
6	MG	C	9511	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9514	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9487	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9524	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9517	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9542	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9550	1/1	0.99	0.08	20,20,20,20	0
6	MG	A	9520	1/1	0.99	0.08	20,20,20,20	0
6	MG	C	9561	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9543	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9203	1/1	0.99	0.08	25,25,25,25	0
6	MG	B	9230	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9211	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9227	1/1	0.99	0.05	20,20,20,20	0
6	MG	B	9256	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9218	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9260	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9225	1/1	0.99	0.06	20,20,20,20	0
6	MG	B	9280	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9233	1/1	0.99	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	9236	1/1	0.99	0.08	20,20,20,20	0
6	MG	B	9306	1/1	0.99	0.10	20,20,20,20	0
6	MG	B	9311	1/1	0.99	0.11	20,20,20,20	0
6	MG	A	9273	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9246	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9247	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9252	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9253	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9258	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9261	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9262	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9265	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9269	1/1	0.99	0.05	20,20,20,20	0
6	MG	B	9427	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9274	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9277	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9283	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9285	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9286	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9291	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9446	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9296	1/1	0.99	0.06	20,20,20,20	0
6	MG	B	9458	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9304	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9307	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9308	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9315	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9317	1/1	0.99	0.12	20,20,20,20	0
6	MG	D	9325	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9331	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9332	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9333	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9336	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9337	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9342	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9344	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9353	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9295	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9357	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9361	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9362	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9363	1/1	0.99	0.05	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	9369	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9370	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9372	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9377	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9488	1/1	0.99	0.05	20,20,20,20	0
6	MG	B	9491	1/1	0.99	0.08	20,20,20,20	0
6	MG	B	9552	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9391	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9393	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9399	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9400	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9401	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9403	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9404	1/1	0.99	0.09	20,20,20,20	0
6	MG	A	9318	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9409	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9410	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9327	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9417	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9419	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9421	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9433	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9434	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9439	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9440	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9443	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9448	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9452	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9456	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9217	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9467	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9469	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9470	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9472	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9475	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9477	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9478	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9479	1/1	0.99	0.10	20,20,20,20	0
6	MG	C	9219	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9481	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9482	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9490	1/1	0.99	0.04	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	9498	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9499	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9502	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9503	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9505	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9506	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9512	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9515	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9221	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9523	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9526	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9527	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9222	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9529	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9223	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9533	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9536	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9539	1/1	0.99	0.03	20,20,20,20	0
6	MG	D	9546	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9548	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9556	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9557	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9559	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9562	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9334	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9239	1/1	0.99	0.04	20,20,20,20	0
6	MG	E	9352	1/1	0.99	0.08	20,20,20,20	0
6	MG	E	9373	1/1	0.99	0.06	20,20,20,20	0
6	MG	E	9389	1/1	0.99	0.05	20,20,20,20	0
6	MG	E	9415	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9243	1/1	0.99	0.06	20,20,20,20	0
6	MG	E	9432	1/1	0.99	0.06	20,20,20,20	0
6	MG	E	9449	1/1	0.99	0.07	20,20,20,20	0
6	MG	E	9484	1/1	0.99	0.07	20,20,20,20	0
6	MG	E	9494	1/1	0.99	0.05	20,20,20,20	0
6	MG	E	9538	1/1	0.99	0.09	20,20,20,20	0
6	MG	E	9551	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9229	1/1	0.99	0.11	20,20,20,20	0
6	MG	F	9244	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9245	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9255	1/1	0.99	0.10	20,20,20,20	0
6	MG	F	9251	1/1	0.99	0.05	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	A	9365	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9297	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9298	1/1	0.99	0.08	20,20,20,20	0
6	MG	F	9302	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9303	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9263	1/1	0.99	0.08	20,20,20,20	0
6	MG	F	9309	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9310	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9323	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9326	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9340	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9374	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9375	1/1	0.99	0.10	20,20,20,20	0
6	MG	F	9382	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9264	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9407	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9414	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9424	1/1	0.99	0.09	20,20,20,20	0
6	MG	F	9425	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9445	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9450	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9453	1/1	0.99	0.09	20,20,20,20	0
6	MG	F	9463	1/1	0.99	0.08	20,20,20,20	0
6	MG	F	9468	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9483	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9495	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9267	1/1	0.99	0.09	20,20,20,20	0
6	MG	A	9368	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9504	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9508	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9513	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9516	1/1	0.99	0.09	20,20,20,20	0
6	MG	F	9530	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9531	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9540	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9282	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9558	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9287	1/1	0.99	0.04	20,20,20,20	0
6	MG	N	9205	1/1	0.99	0.08	16,16,16,16	0
6	MG	C	9289	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9293	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9212	1/1	0.99	0.07	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	C	9300	1/1	0.99	0.03	20,20,20,20	0
6	MG	C	9313	1/1	0.99	0.10	20,20,20,20	0
8	G4P	N	9101	36/36	0.99	0.11	35,45,50,50	0
6	MG	D	9547	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9380	1/1	1.00	0.10	20,20,20,20	0
6	MG	D	9242	1/1	1.00	0.11	20,20,20,20	0
6	MG	B	9228	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9346	1/1	1.00	0.10	20,20,20,20	0
6	MG	D	9248	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9392	1/1	1.00	0.07	20,20,20,20	0
6	MG	E	9275	1/1	1.00	0.10	20,20,20,20	0
6	MG	E	9288	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9347	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9209	1/1	1.00	0.20	20,20,20,20	0
6	MG	E	9366	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9259	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9493	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9402	1/1	1.00	0.05	20,20,20,20	0
6	MG	A	9254	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9268	1/1	1.00	0.10	20,20,20,20	0
6	MG	C	9266	1/1	1.00	0.07	20,20,20,20	0
6	MG	E	9457	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9509	1/1	1.00	0.06	20,20,20,20	0
6	MG	B	9541	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9276	1/1	1.00	0.05	20,20,20,20	0
6	MG	A	9329	1/1	1.00	0.08	20,20,20,20	0
6	MG	D	9279	1/1	1.00	0.06	20,20,20,20	0
6	MG	B	9560	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9428	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9522	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9284	1/1	1.00	0.07	20,20,20,20	0
6	MG	F	9270	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9278	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9435	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9437	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9534	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9281	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9447	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9549	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9292	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9455	1/1	1.00	0.10	20,20,20,20	0
6	MG	C	9553	1/1	1.00	0.05	20,20,20,20	0

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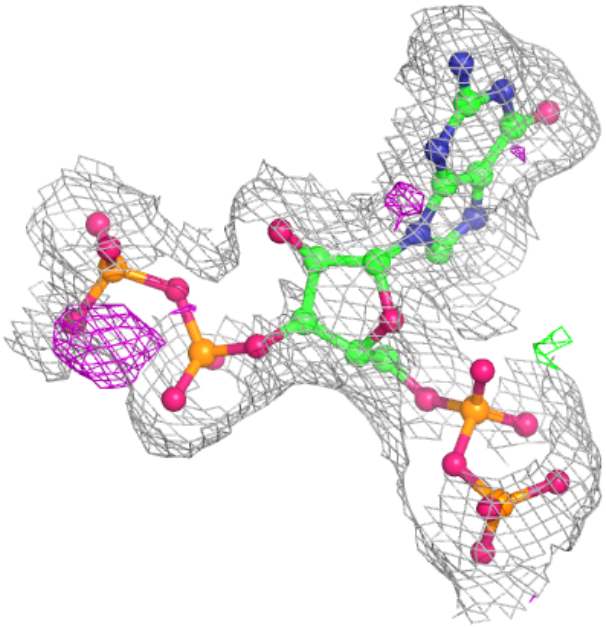
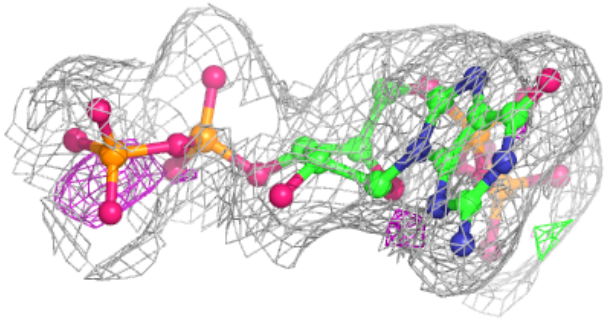
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	F	9324	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9213	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9461	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9312	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9314	1/1	1.00	0.05	20,20,20,20	0
6	MG	A	9224	1/1	1.00	0.07	20,20,20,20	0
6	MG	F	9388	1/1	1.00	0.09	20,20,20,20	0
6	MG	A	9521	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9319	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9322	1/1	1.00	0.09	20,20,20,20	0
6	MG	C	9397	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9412	1/1	1.00	0.06	20,20,20,20	0
6	MG	F	9436	1/1	1.00	0.11	20,20,20,20	0
6	MG	D	9208	1/1	1.00	0.10	20,20,20,20	0
6	MG	A	9462	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9411	1/1	1.00	0.11	20,20,20,20	0
6	MG	D	9215	1/1	1.00	0.08	20,20,20,20	0
6	MG	D	9492	1/1	1.00	0.08	20,20,20,20	0
6	MG	F	9471	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9418	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9343	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9420	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9349	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9350	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9351	1/1	1.00	0.09	20,20,20,20	0
6	MG	D	9510	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9429	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9231	1/1	1.00	0.10	20,20,20,20	0
6	MG	B	9426	1/1	1.00	0.06	20,20,20,20	0
6	MG	F	9537	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9360	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9232	1/1	1.00	0.10	20,20,20,20	0
6	MG	A	9544	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9234	1/1	1.00	0.09	20,20,20,20	0
6	MG	C	9335	1/1	1.00	0.08	20,20,20,20	0
6	MG	N	9207	1/1	1.00	0.07	37,37,37,37	0
6	MG	C	9338	1/1	1.00	0.06	20,20,20,20	0
6	MG	A	9555	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9535	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9376	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9459	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9379	1/1	1.00	0.07	20,20,20,20	0

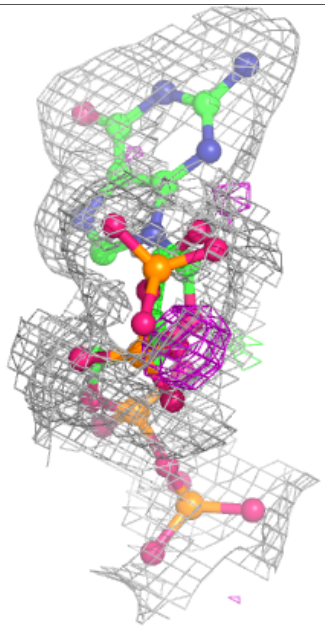
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G4P N 9100:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

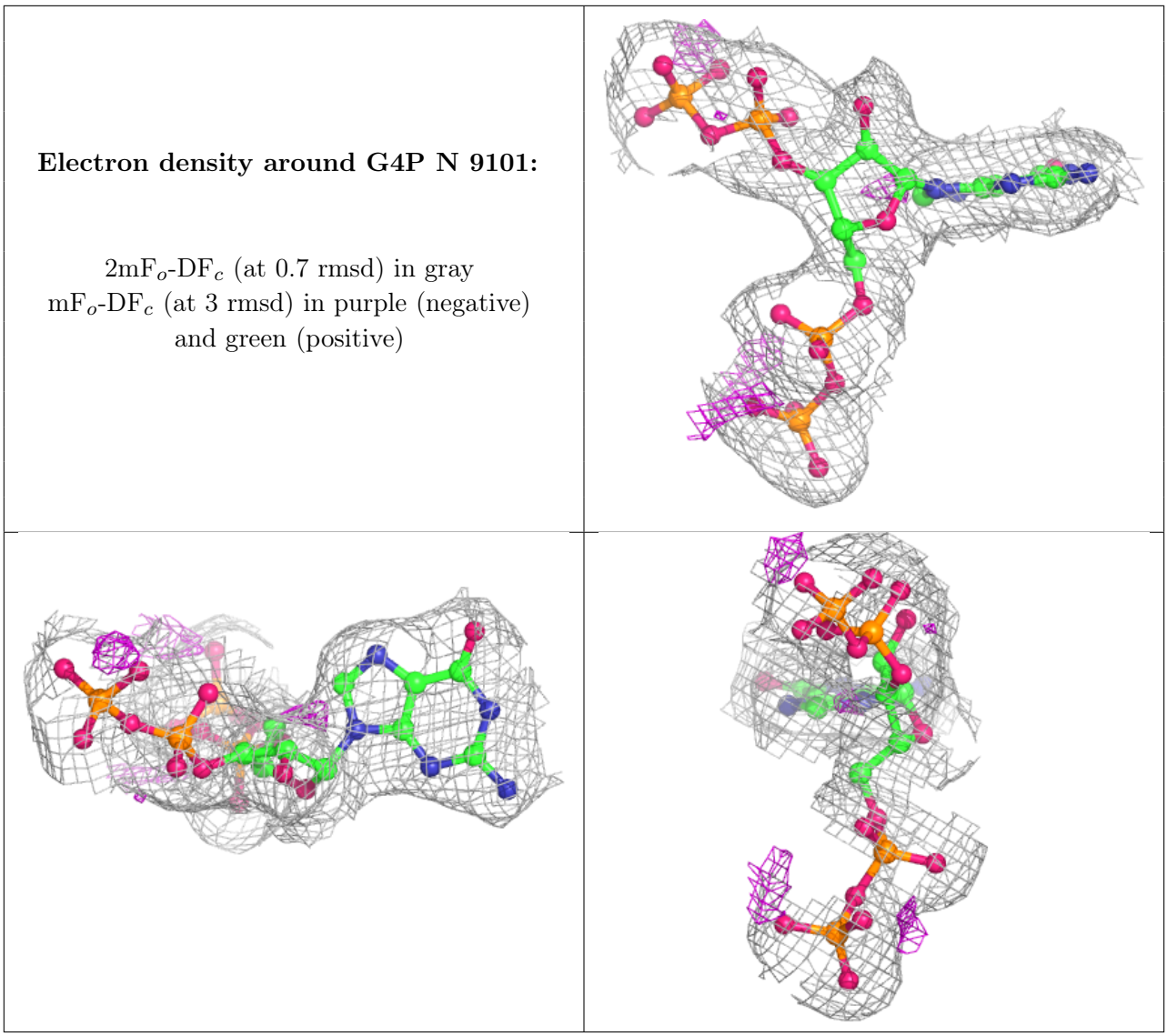






Electron density around G4P N 9101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.