wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2016 – 11:23 PM EST

PDB ID	:	5TMC
Title	:	Re-refinement of Thermus thermopiles DNA-directed RNA polymerase structure
Authors	:	Wang, J.
Deposited on	:	2016-10-12
Resolution	:	2.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

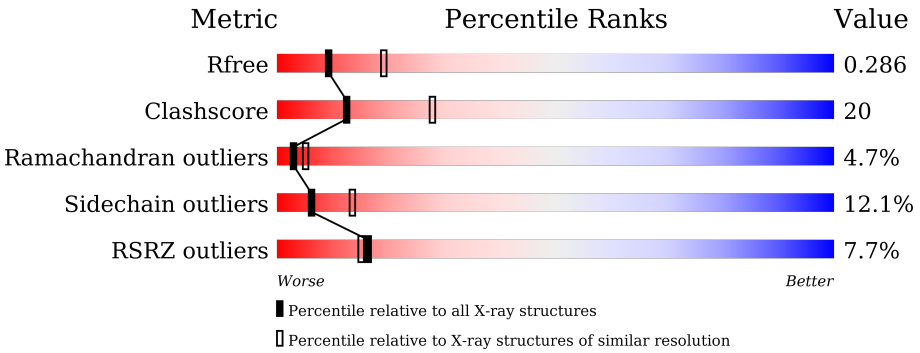
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 2.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	3% 34% 31% 8% 27%
1	B	315	10% 46% 27% · 24%
2	C	1119	6% 52% 41% 7%
3	D	1524	8% 52% 40% 7% ·
4	E	99	7% 69% 23% · · ·
5	F	423	10% 56% 23% · 17%

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Mol	Chain	Length	Quality of chain
6	Z	48	96%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	G4P	D	1605	-	-	-	X
7	PO4	A	401	-	-	-	X
8	MG	C	1201	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28419 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	231	Total	C	N	O	S	0	0	0
			1816	1159	315	339	3			
1	B	238	Total	C	N	O	S	0	0	0
			1863	1188	322	350	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1504	Total	C	N	O	S	0	0	0
			11864	7518	2091	2219	36			

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLU	VAL	conflict	UNP Q72ID6
E	92	ILE	LEU	conflict	UNP Q72ID6
E	95	GLY	VAL	conflict	UNP Q72ID6

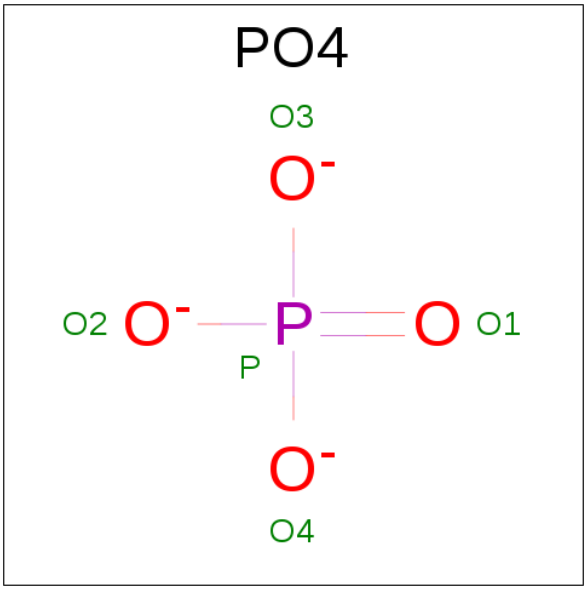
- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	351	Total	C	N	O	S	0	0	0
			2844	1794	515	531	4			

- Molecule 6 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	48	Total	C	N	O	0	0	0
			240	144	48	48			

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		

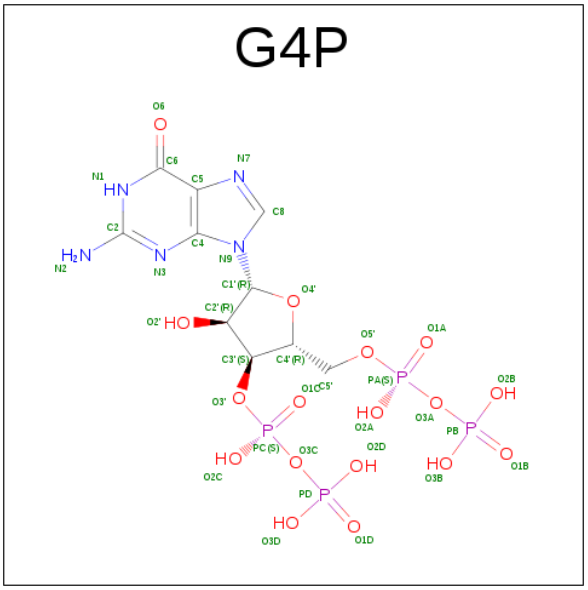
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	3	Total	Mg	0	0
			3	3		
8	C	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Zn 2 2	0	0

- Molecule 10 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
10	D	1	Total C N O P 36 10 5 17 4	0	0

- Molecule 11 is water.

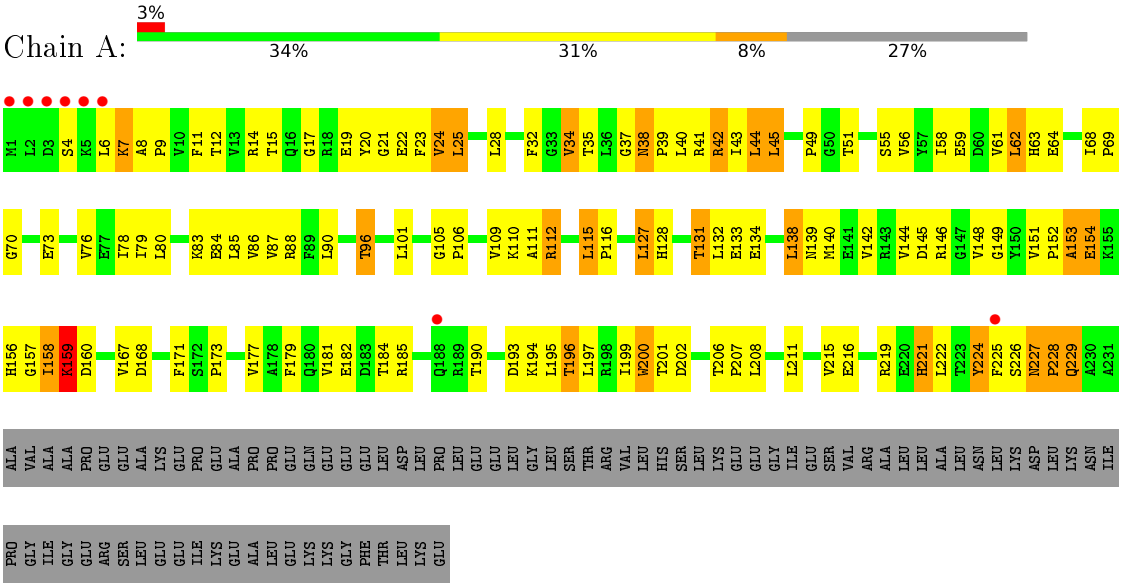
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	15	Total O 15 15	0	0
11	B	2	Total O 2 2	0	0
11	C	54	Total O 54 54	0	0
11	D	62	Total O 62 62	0	0
11	E	9	Total O 9 9	0	0
11	F	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

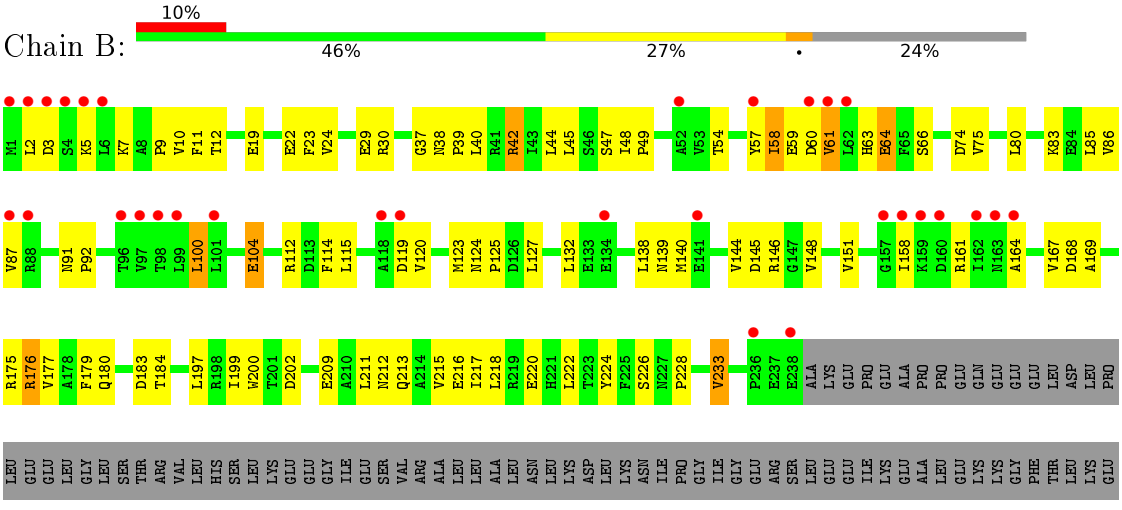
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



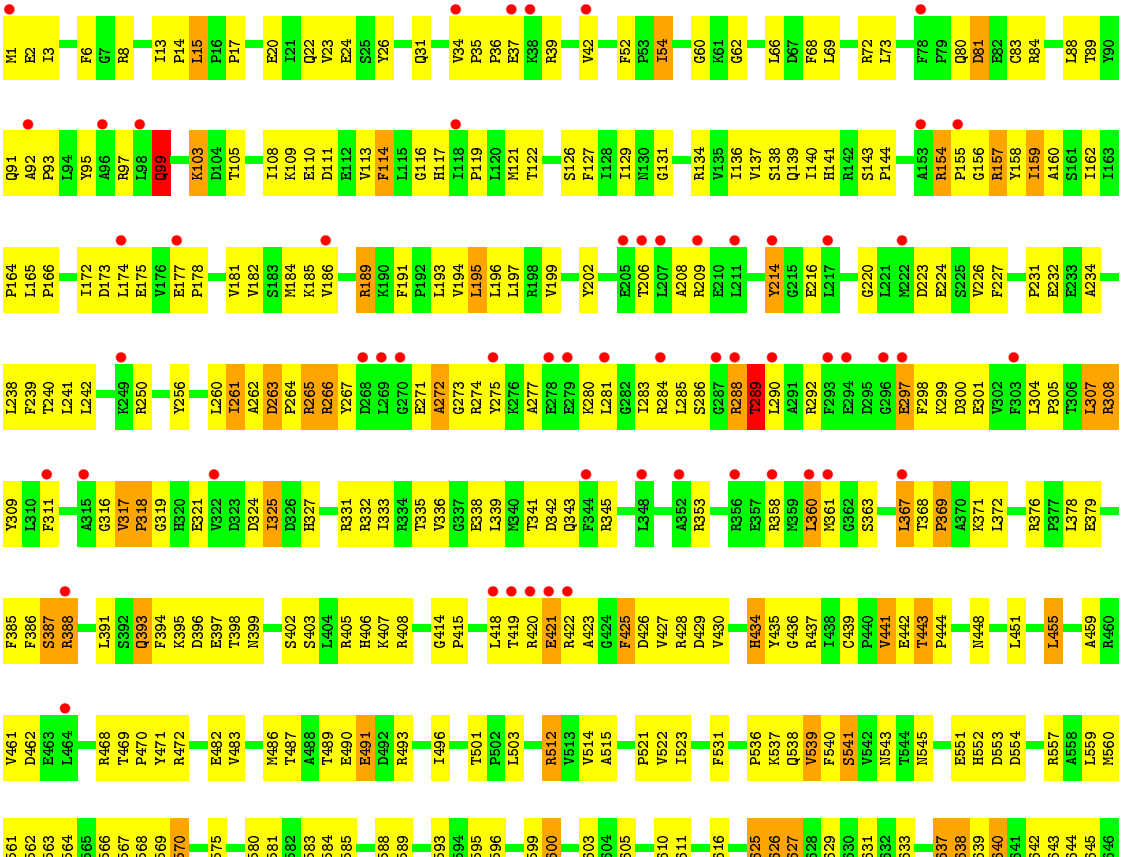
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:

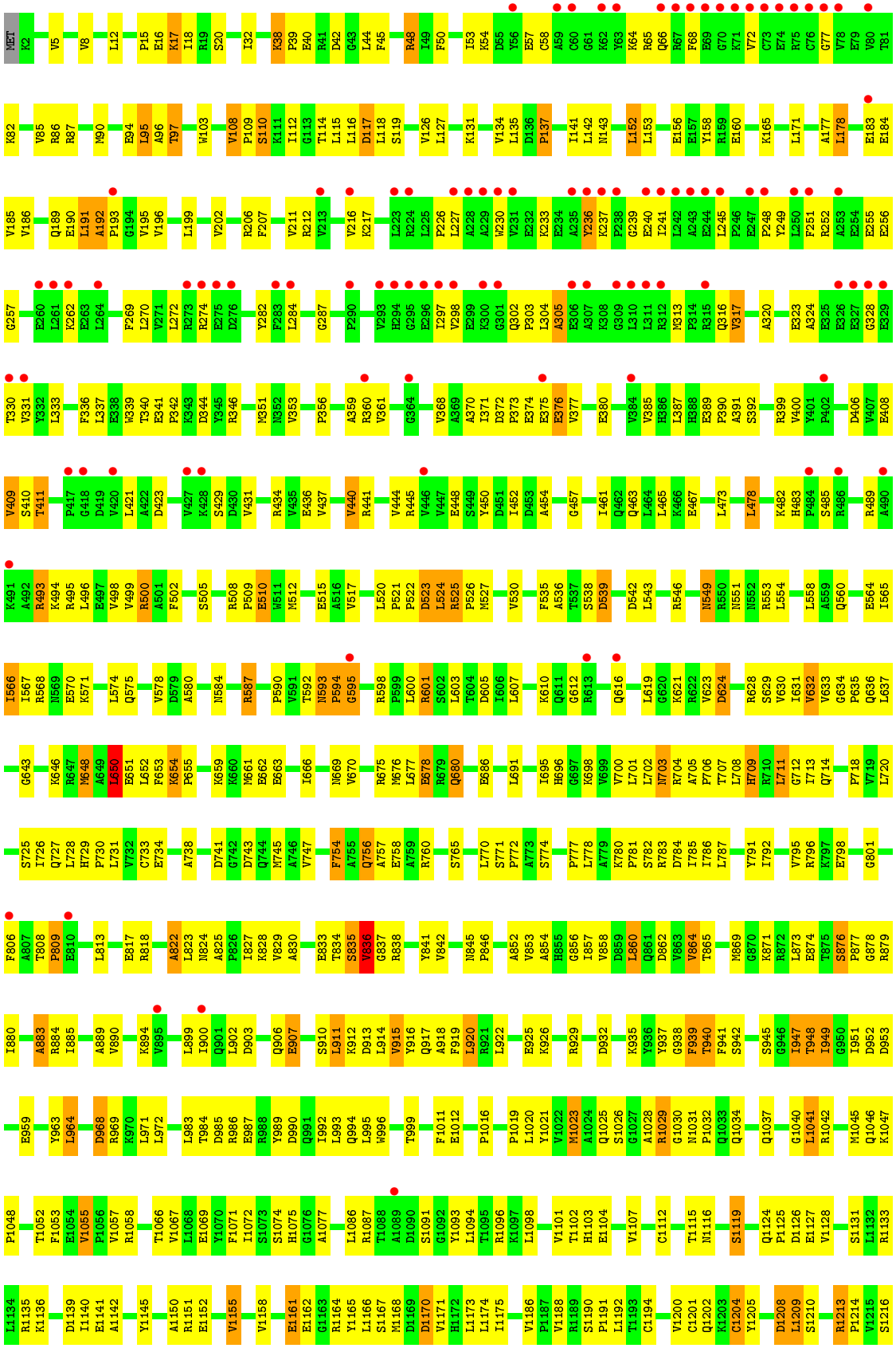


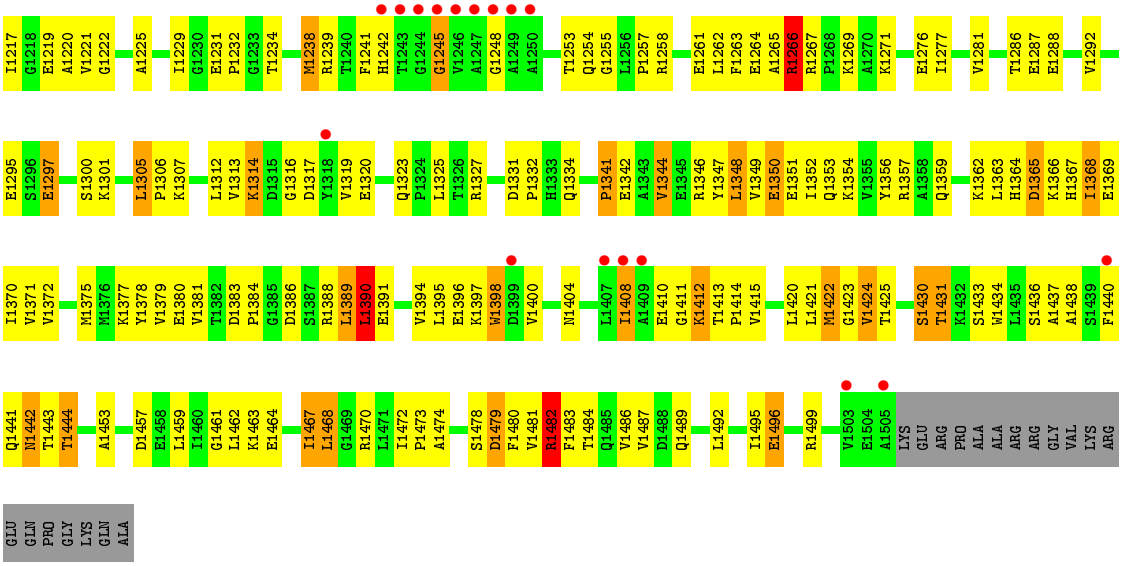
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:



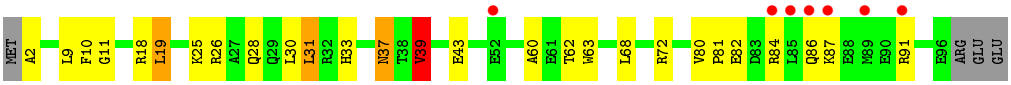
- Molecule 3: DNA-directed RNA polymerase subunit beta'


MET K2 V5 V8 L12 P15 E16 K17 I18 R19 S20 I32 K38 P39 E40 R41 D42 G43 L44 F45 R48 I49 F50 I53 K54 D55 Y56 E57 C58 A59 C60 G61 K62 Y63 K64 R65 Q66 R67 F68 E69 G70 K71 V72 C73 E74 R75 C76 G77 V78 E79 V80 T81
K82 V85 R86 R87 N90 E94 L95 A96 T97 W103 V108 P109 S110 K111 I112 G113 T114 L115 L116 D117 L118 S119 V126 L127 K131 V134 L135 D136 P137 I141 L142 N143 L152 L153 E156 E157 Y158 R159 E160 K165 L171 A177 L178 E183 E184
V185 V186 Q189 E190 L191 A192 P193 G194 V195 V196 L199 V202 R206 F207 V211 R212 V213 V216 K217 L223 R224 L225 P226 L227 A228 A229 W230 V231 E232 K233 E234 A235 Y236 K237 P238 G239 E240 I241 L242 A243 E244 L245 P246 E247 P248 Y249 L250 F251 R252 A253 E254 E255 E256
G257 E260 L261 K262 E263 L264 F269 L270 V271 L272 R273 R274 E275 D276 Y282 F283 L284 G287 P290 V293 H294 G295 E296 I297 V298 E299 K300 G301 Q302 P303 L304 A305 E306 A307 K308 G309 L310 L311 R312 M313 P314 R315 Q316 V317 A320 E323 A324 E325 E326 E327 G328 E329
T330 V331 Y332 I333 F336 I337 E338 W339 T340 E341 P342 K343 D344 Y345 R346 M351 N352 V353 P356 A359 R360 V361 G364 V368 A369 A370 I371 D372 P373 E374 E375 E376 V377 E380 V384 V385 H386 I387 H388 E389 P390 A391 S392 R399 V400 Y401 P402 D406 V407 E408
V409 S410 T411 P417 G418 D419 V420 L421 A422 D423 V427 K428 S429 D430 V431 R434 V435 E436 V437 V440 R441 V444 R445 V446 V447 E448 S449 Y450 D451 I452 D453 A454 G457 I461 Q462 Q463 L464 L465 K466 E467 L473 L478 K482 H483 P484 S485 R486 R489 A490
K491 A492 R493 K494 R495 L496 E497 V498 V499 R500 A501 F502 S505 R508 P509 E510 W511 M512 E515 A516 V517 L520 P521 P522 D523 L524 R525 P526 M527 V530 F535 A536 T537 S538 D539 D542 L543 R546 N549 R550 N551 N552 R553 L554 L558 A559 Q560 E564 I565
I566 I567 R568 N569 E570 K571 L574 Q575 V578 D579 A580 N584 R587 P590 V591 T592 N593 P594 G595 R598 P599 L600 R601 S602 L603 T604 D605 I606 L607 K610 Q611 G612 R613 Q616 L619 G620 K621 R622 V623 D624 R628 S629 V630 I631 V632 V633 G634 P635 Q636 L637
G643 K646 R647 M648 A649 L650 E651 L652 F653 K654 P655 K659 K660 M661 E662 E663 I666 M669 V670 R675 M676 L677 E678 R679 Q680 E686 L691 I695 H696 G697 K698 V699 V700 L701 L702 N703 R704 A705 P706 T707 L708 H709 R710 L711 G712 I713 Q714 P718 V719 L720
S725 I726 Q727 L728 H729 P730 L731 V732 C733 E734 A738 D741 G742 D743 Q744 M745 A746 V747 F754 A755 Q756 A757 E758 A759 R760 S765 L770 S771 P772 A773 S774 P777 L778 A779 K780 P781 S782 R783 D784 I785 I786 L787 Y791 I792 V795 R796 K797 E798 G801
F806 A807 T808 P809 E810 L813 E817 R818 A822 L823 N824 A825 P826 I827 K828 V829 A830 E833 T834 S835 V836 G837 R838 Y841 V842 N845 P846 A852 V853 A854 H855 G856 I857 V858 D859 L860 Q861 D862 V863 V864 T865 M869 G870 K871 R872 L873 E874 T875 S876 P877 G878 R879
I880 A883 R884 I885 A889 V890 K894 V895 L899 I900 Q901 L902 D903 Q906 E907 S910 T834 L911 K912 D913 L914 V915 Y916 Q917 A918 F919 L920 R921 L922 E925 K926 R929 D932 K935 Y936 Y937 G938 F939 T940 F941 S942 S945 G946 I947 T948 I949 G950 I951 D952 D953
E959 Y963 L964 D968 R969 K970 L971 L972 L983 T984 D985 R986 E987 R988 Y989 D990 Q991 I992 L993 Q994 L995 W996 T999 F1011 E1012 P1016 P1019 L1020 Y1021 V1022 M1023 A1024 Q1025 S1026 G1027 A1028 R1029 G1030 N1031 P1032 Q1033 Q1034 Q1037 G1040 L1041 R1042 M1045 Q1046 K1047
P1048 T1052 F1053 E1054 V1055 P1056 V1057 R1058 T1066 V1067 L1068 E1069 Y1070 F1071 I1072 S1073 S1074 H1075 G1076 A1077 L1086 R1087 T1088 A1089 D1090 S1091 G1092 Y1093 L1094 T1095 R1096 K1097 L1098 V1101 T1102 H1103 E1104 V1107 C1112 T1115 N1116 S1119 Q1124 P1125 D1126 E1127 V1128 S1131 L1132 R1133
L1134 R1135 K1136 D1139 I1140 E1141 A1142 Y1145 A1150 R1151 E1152 V1155 V1158 E1161 E1162 G1163 R1164 Y1165 L1166 S1167 M1168 D1169 D1170 V1171 H1172 L1173 L1174 I1175 V1186 P1187 V1188 R1189 S1190 P1191 L1192 T1193 C1194 V1200 C1201 Q1202 K1203 C1204 Y1205 D1208 L1209 S1210 R1213 P1214 V1215 S1216



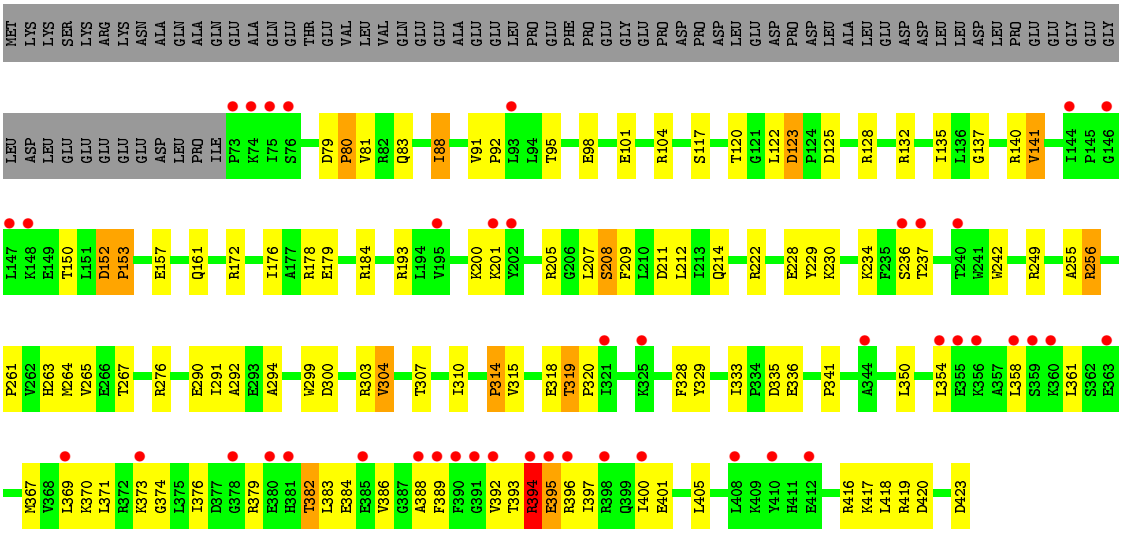
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



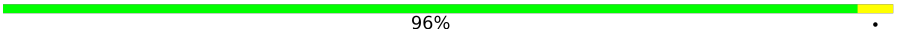
• Molecule 5: RNA polymerase sigma factor SigA

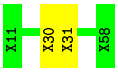
Chain F:



• Molecule 6: unknown protein

Chain Z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.51 – 2.71 48.50 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.51-2.71) 97.1 (48.50-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.265 , 0.286 0.265 , 0.286	Depositor DCC
R_{free} test set	7447 reflections (3.75%)	DCC
Wilson B-factor (Å^2)	51.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 89.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.086 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.875 for H, K, L 0.125 for -H-K, K, -L	Depositor
Outliers	1 of 206105 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	28419	wwPDB-VP
Average B, all atoms (Å^2)	121.0	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: G4P, PO4, MG, ZN

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	0.47	0/1848	0.64	0/2512
1	B	0.39	0/1896	0.57	0/2579
2	C	0.46	0/8997	0.65	0/12164
3	D	0.45	0/12073	0.65	2/16324 (0.0%)
4	E	0.44	0/783	0.63	0/1054
5	F	0.35	0/2890	0.55	0/3888
All	All	0.44	0/28487	0.63	2/38521 (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
3	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	95	LEU	CA-CB-CG	5.47	127.89	115.30
3	D	650	LEU	CA-CB-CG	5.43	127.79	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1126	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1816	0	1871	90	0
1	B	1863	0	1914	59	0
2	C	8829	0	8933	408	0
3	D	11864	0	12094	544	0
4	E	769	0	775	20	0
5	F	2844	0	2926	68	0
6	Z	240	0	50	1	0
7	A	5	0	0	0	0
8	C	1	0	0	0	0
8	D	3	0	0	0	0
9	D	2	0	0	0	0
10	D	36	0	11	1	0
11	A	15	0	0	0	0
11	B	2	0	0	2	0
11	C	54	0	0	4	0
11	D	62	0	0	7	0
11	E	9	0	0	1	0
11	F	5	0	0	0	0
All	All	28419	0	28574	1111	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 1111 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:1265:ALA:HA	3:D:1266:ARG:CB	1.60	1.29
3:D:1265:ALA:HA	3:D:1266:ARG:HB2	1.23	1.13
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.32	1.07
2:C:93:PRO:HA	2:C:117:HIS:HB2	1.36	1.06
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.41	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	229/315 (73%)	175 (76%)	40 (18%)	14 (6%)	2 2
1	B	236/315 (75%)	186 (79%)	45 (19%)	5 (2%)	9 21
2	C	1117/1119 (100%)	877 (78%)	187 (17%)	53 (5%)	3 5
3	D	1502/1524 (99%)	1160 (77%)	260 (17%)	82 (6%)	2 3
4	E	93/99 (94%)	76 (82%)	14 (15%)	3 (3%)	5 11
5	F	349/423 (82%)	286 (82%)	54 (16%)	9 (3%)	7 15
All	All	3526/3795 (93%)	2760 (78%)	600 (17%)	166 (5%)	3 5

5 of 166 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
2	C	42	VAL
2	C	263	ASP
2	C	272	ALA
2	C	738	ASP

5.3.2 Protein sidechains

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%)	171 (85%)	31 (15%)	3 8
1	B	206/273 (76%)	183 (89%)	23 (11%)	7 16
2	C	941/941 (100%)	816 (87%)	125 (13%)	5 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	1264/1279 (99%)	1111 (88%)	153 (12%)	6 13
4	E	83/87 (95%)	75 (90%)	8 (10%)	10 23
5	F	306/370 (83%)	283 (92%)	23 (8%)	17 37
All	All	3002/3223 (93%)	2639 (88%)	363 (12%)	6 13

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	900	ARG
3	D	344	ASP
4	E	37	ASN
2	C	999	HIS
3	D	48	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	889	HIS
3	D	442	ASN
4	E	33	HIS
3	D	33	ASN
3	D	463	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 8 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
7	PO4	A	401	-	4,4,4	0.78	0	6,6,6	0.23	0
10	G4P	D	1605	8	30,38,38	1.34	2 (6%)	35,61,61	1.58	4 (11%)

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
7	PO4	A	401	-	-	0/0/0/0	0/0/0/0
10	G4P	D	1605	8	-	0/23/43/43	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1605	G4P	C6-C5	4.01	1.49	1.41
10	D	1605	G4P	O6-C6	4.83	1.36	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	1605	G4P	N3-C2-N1	-4.38	121.60	127.56
10	D	1605	G4P	C5-C6-N1	-3.88	118.45	123.52
10	D	1605	G4P	C6-C5-C4	-2.32	118.21	120.86
10	D	1605	G4P	C6-N1-C2	4.01	120.58	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1605	G4P	1	0

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	231/315 (73%)	-0.02	8 (3%) 48 48	51, 78, 162, 212	1 (0%)
1	B	238/315 (75%)	0.53	31 (13%) 5 4	70, 149, 236, 260	0
2	C	1119/1119 (100%)	0.07	64 (5%) 27 26	53, 97, 222, 263	2 (0%)
3	D	1504/1524 (98%)	0.22	117 (7%) 16 14	52, 95, 245, 296	4 (0%)
4	E	95/99 (95%)	0.07	7 (7%) 17 16	58, 104, 192, 203	0
5	F	351/423 (82%)	0.60	44 (12%) 5 4	68, 124, 245, 277	2 (0%)
6	Z	0/48	-	-	-	-
All	All	3538/3843 (92%)	0.21	271 (7%) 16 15	51, 102, 233, 296	9 (0%)

The worst 5 of 271 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	391	GLY	25.7
3	D	1247	ALA	17.6
1	A	1	MET	14.6
5	F	390	PHE	13.7
1	A	3	ASP	13.7

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

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
7	PO4	A	401	5/5	0.95	0.31	5.45	143,144,148,149	0
8	MG	C	1201	1/1	0.90	0.22	2.19	131,131,131,131	0
10	G4P	D	1605	36/36	0.91	0.21	2.13	183,197,222,224	0
9	ZN	D	1603	1/1	0.96	0.11	-1.16	168,168,168,168	0
9	ZN	D	1602	1/1	0.60	0.08	-4.18	225,225,225,225	0
8	MG	D	1604	1/1	0.94	0.24	-	86,86,86,86	0
8	MG	D	1601	1/1	0.98	0.35	-	133,133,133,133	0
8	MG	D	1606	1/1	0.97	0.17	-	155,155,155,155	0

6.5 Other polymers

There are no such residues in this entry.