wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 01:19 AM EDT

PDB ID	:	2YU9
Title	:	RNA polymerase II elongation complex in 150 mm MG+2 with UTP
Authors	:	Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on	:	2007-04-06
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

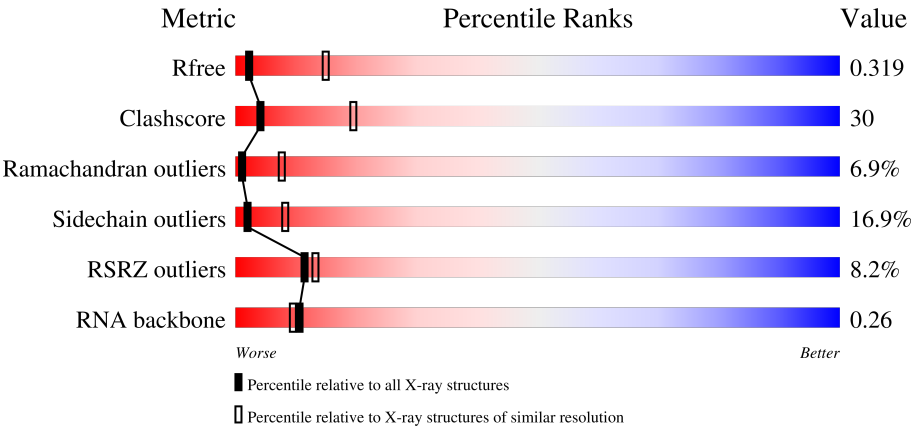
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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	R	10	70% 30%
2	T	28	43% 29% 43% 29%
3	N	14	64% 43% 43% 14%
4	A	1733	7% 41% 30% 9% • 19%

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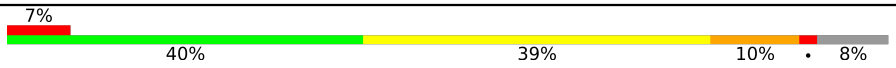
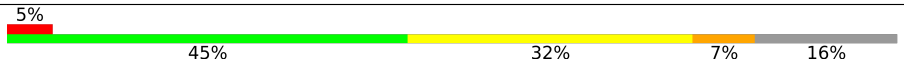
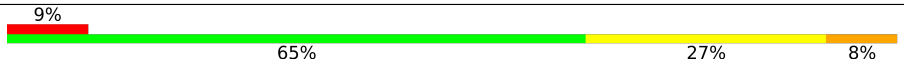
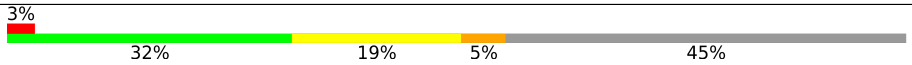
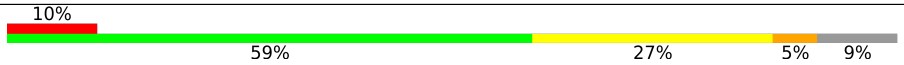
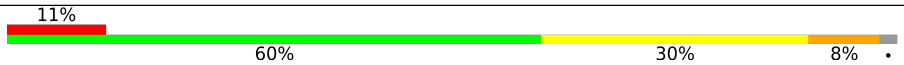
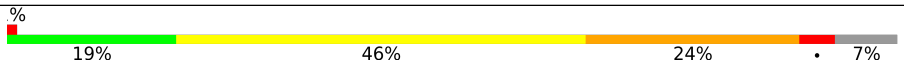
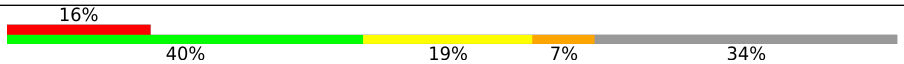
Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

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
16	UTP	A	2003[A]	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 29530 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 RNA chain called 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

- Molecule 2 is a DNA chain called 28-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 3 is a DNA chain called 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1411	Total	C	N	O	S	0	0	0
			11094	6994	1945	2094	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1121	Total	C	N	O	S	0	0	0
			8914	5643	1563	1653	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypep-

tide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

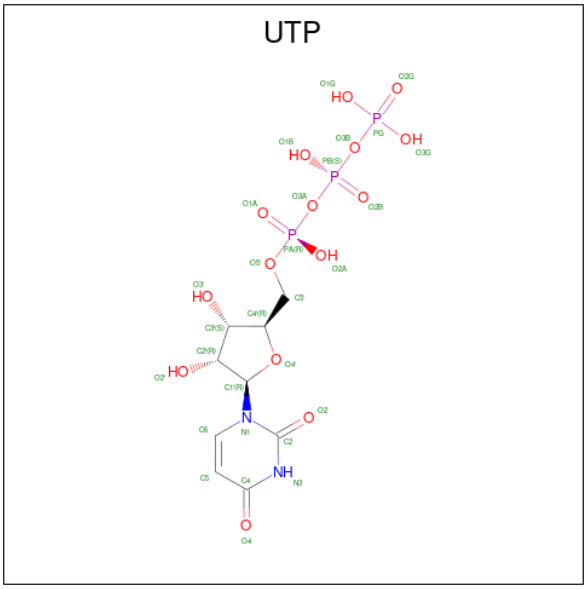
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	1	Total	Zn	0	0
			1	1		
14	C	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	J	1	Total	Zn	0	0
			1	1		
14	L	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



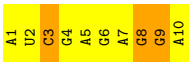
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	P	0	1
			58	18	4	30	6		

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.

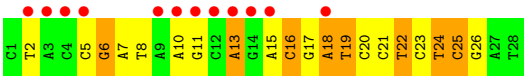
• Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'

Chain R:



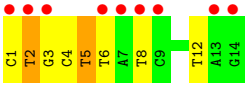
• Molecule 2: 28-MER DNA template strand

Chain T:



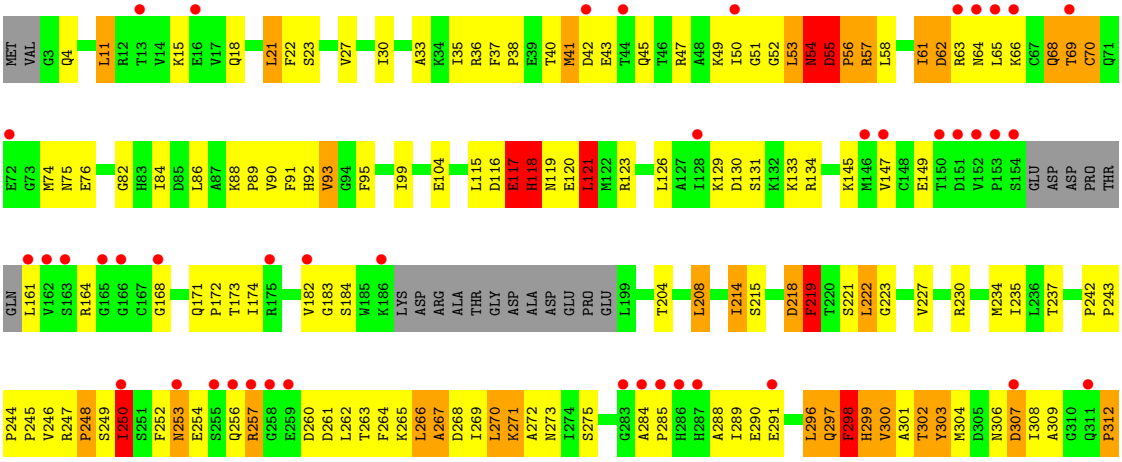
• Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'

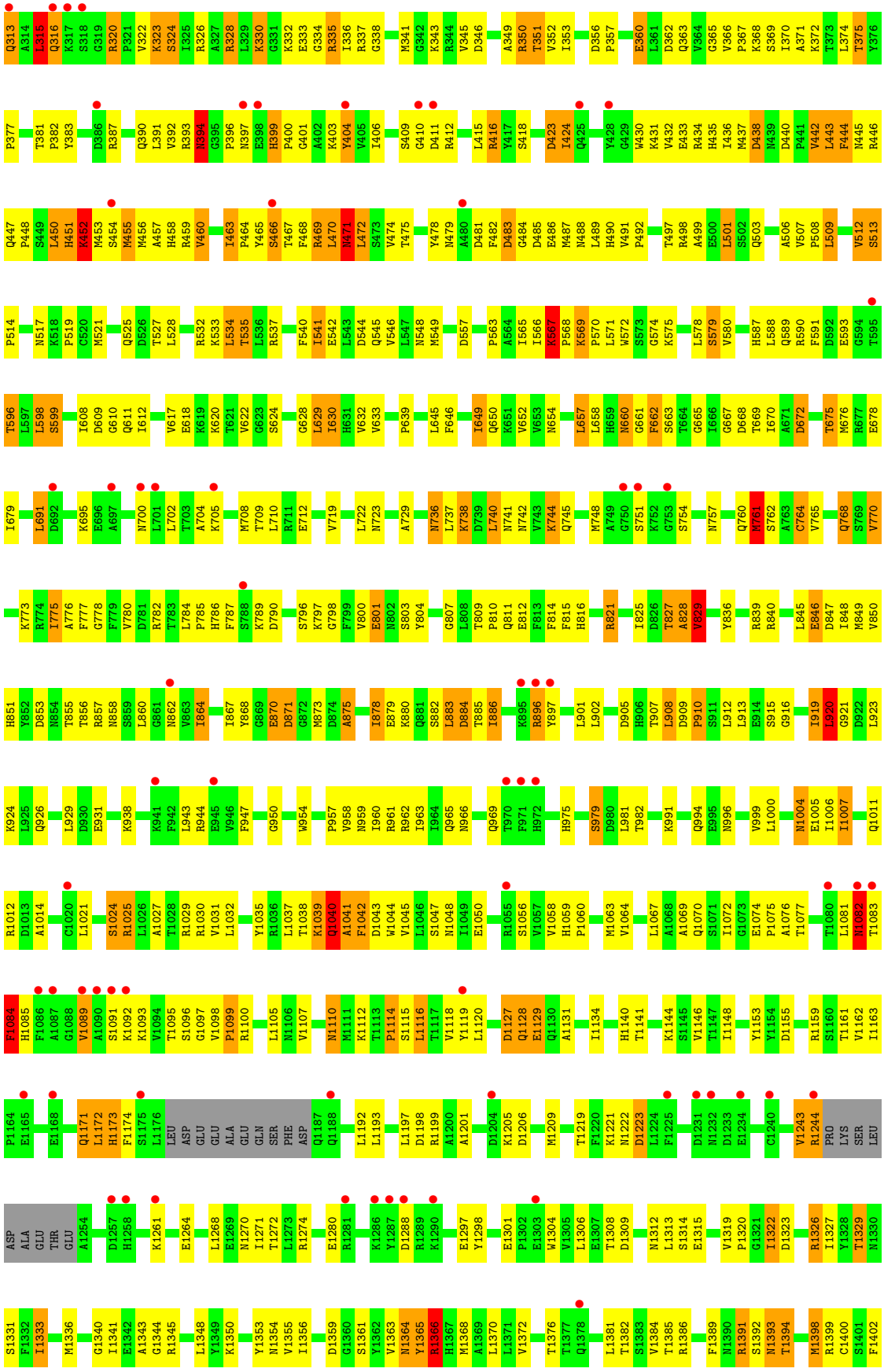
Chain N:

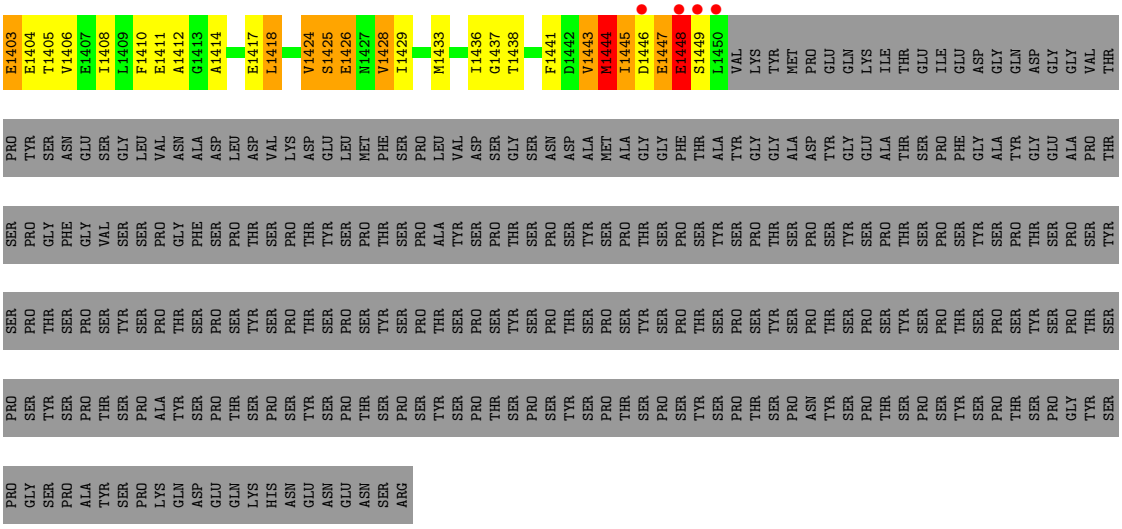


• Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A:

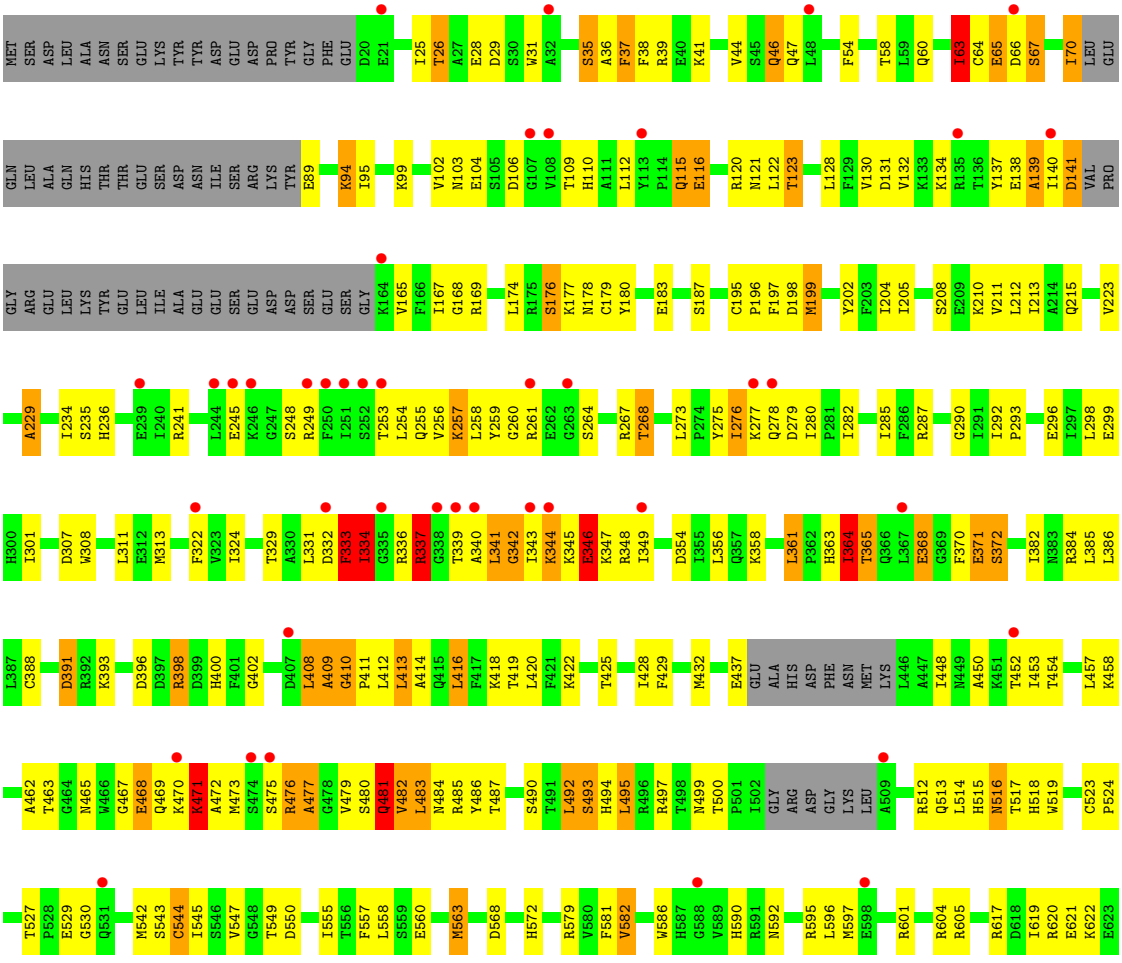


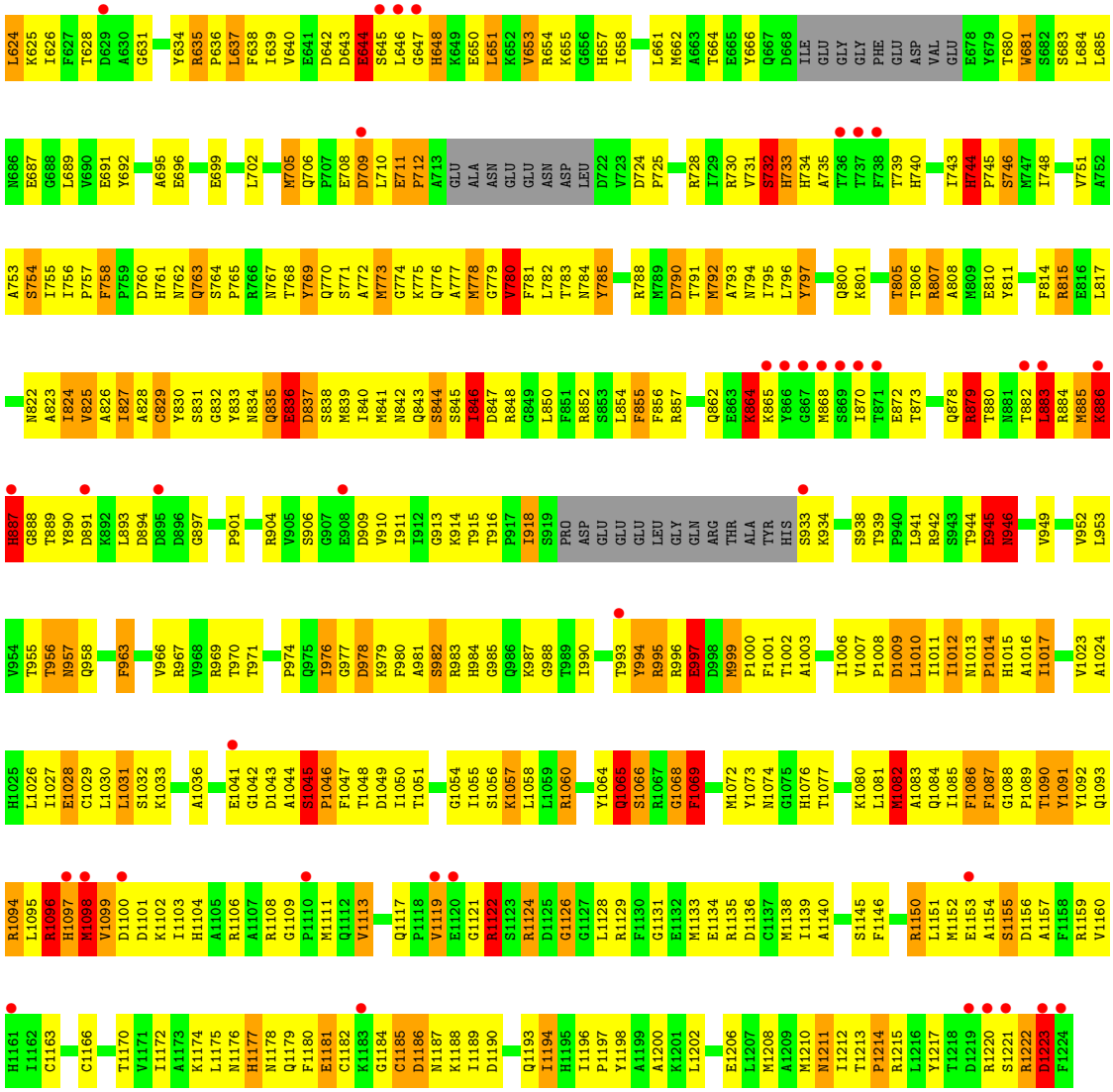

Q313 A314 L315 Q316 K317 S318 G319 R320 P321 V322 K323 S324 I325 R326 A327 R328 L329 K330 G331 K332 E333 G334 R335 I336 R337 G338 M341 G342 K343 R344 V345 D346 A349 R350 T351 V352 I353 D356 P357 E360 L361 D362 Q363 V364 G365 V366 P367 K368 S369 I370 A371 K372 T373 L374 T375 Y376
P377 T381 P382 Y383 D386 R387 Q390 L391 V392 R393 N394 G395 P396 N397 E398 H399 P400 G401 A402 K403 Y404 V405 I406 S409 G410 D411 R412 L415 R416 Y417 S418 A349 R350 T351 V352 I353 D423 I424 Q425 Y428 G429 W430 K431 V432 E433 R434 H435 I436 M437 D438 M439 D440 P441 V442 L443 F444 N445 R446
Q447 P448 S449 L450 H451 K452 M453 S454 M455 M456 A457 H458 R459 V460 I463 P464 Y465 S466 T467 F468 R469 L470 N471 L472 S473 V474 T475 Y478 N479 A480 D481 F482 D483 G484 D485 E486 M487 N488 L489 H490 V491 P492 T497 R498 A499 E500 L501 S502 Q503 A506 V507 P508 L509 V512 S513
P514 N517 K518 P519 G520 M521 Q525 D526 T527 L528 R532 K533 L534 T535 L536 R537 F540 I541 E542 L543 D544 Q545 V546 L547 N548 M549 D557 P563 A564 I565 I566 K567 P568 K569 P570 L571 W572 S573 G574 K575 L578 S579 V580 H587 L588 Q589 R590 F591 D592 L509 E593 G594 T595
T596 L597 L598 S599 I608 D609 G610 Q611 I612 V617 E618 K619 K620 T621 V622 G623 S624 G628 L629 I630 H631 V632 V633 P639 L645 F646 I649 Q650 K651 V652 V653 N654 L657 L658 H659 N660 G661 F662 S663 T664 G665 I666 G667 D668 T669 I670 A671 D672 T675 M676 R677 E678
I679 L691 D692 K695 E696 A697 N700 L701 L702 T703 A704 K705 M708 T709 L710 R711 E712 V719 L722 N723 A729 N736 L737 K738 D739 L740 N741 N742 V743 K744 Q745 M748 A749 G750 S751 K752 G753 S754 N757 Q760 R761 S762 A763 C764 V765 Q768 S769 V770
K773 R774 I775 A776 F777 G778 F779 V780 D781 R782 T783 L784 P785 H786 F787 S788 K789 D790 S796 K797 G798 F799 V800 E801 N802 S803 Y804 G807 L808 T809 P810 Q811 E812 F813 F814 F815 H816 R821 I825 D826 T827 A828 V829 Y836 R839 R840 L845 E846 D847 I848 M849 V850
H851 Y852 D853 N854 T855 T856 R857 N858 S859 L860 G861 N862 V863 I864 I867 Y868 G869 E870 D871 G872 M873 D874 A875 I878 E879 K880 Q881 S882 L883 D884 T885 I886 K895 R896 Y897 L901 L902 D905 H906 T907 L908 D909 P910 S911 L912 L913 E914 S915 G916 I919 L920 G921 D922 L923
K924 L925 Q926 L929 D930 E931 K938 K941 F942 L943 R944 E945 V946 F947 G950 W954 P957 V958 N959 I960 R961 R962 I963 I964 Q965 N966 Q969 T970 F971 H972 H975 S979 D980 L981 T982 L991 Q994 E995 N996 V999 L1000 N1004 E1005 I1006 I1007 Q1011
R1012 D1013 A1014 C1020 L1021 S1024 R1025 L1026 A1027 T1028 R1029 R1030 V1031 L1032 Y1035 R1036 L1037 T1038 K1039 Q1040 A1041 F1042 D1043 W1044 V1045 L1046 S1047 N1048 I1049 E1050 R1055 S1056 V1057 V1058 H1059 P1060 M1063 V1064 L1067 A1068 A1069 Q1070 S1071 I1072 G1073 E1074 P1075 A1076 T1077 T1080 L1081 N1082 T1083
F1084 H1085 F1086 A1087 G1088 V1089 A1090 S1091 K1092 K1093 V1094 T1095 S1096 G1097 V1098 P1099 R1100 L1105 R1106 V1107 N1110 M1111 K1112 T1113 P1114 S1115 L1116 T1117 V1118 Y1119 L1120 D1127 Q1128 E1129 Q1130 A1131 I1134 H1140 T1141 K1144 S1145 V1146 T1147 I1148 Y1153 Y1154 D1155 R1159 S1160 T1161 V1162 I1163
P1164 E1165 E1168 Q1171 L1172 H1173 F1174 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 L1192 L1193 L1197 D1198 R1199 A1200 A1201 D1204 K1205 D1206 M1209 T1219 F1220 K1221 N1222 D1223 L1224 F1225 D1231 N1232 D1233 E1234 C1240 V1243 R1244 PRO LYS SER LEU
ASP ALA GLU THR GLU A1254 D1257 H1258 K1261 E1264 L1268 E1269 N1270 I1271 T1272 L1273 R1274 E1280 R1281 K1286 Y1287 D1288 R1289 K1290 E1297 Y1298 E1301 P1302 E1303 W1304 V1305 L1306 E1307 T1308 D1309 N1312 L1313 S1314 E1315 V1319 P1320 G1321 I1322 D1323 R1326 I1327 Y1328 T1329 N1330
S1331 F1332 I1333 M1336 G1340 I1341 E1342 A1343 G1344 R1345 L1348 Y1349 K1350 Y1353 N1354 V1355 I1356 D1359 G1360 S1361 Y1362 V1363 N1364 Y1365 R1366 H1367 M1368 A1369 L1370 L1371 V1372 T1376 T1377 Q1378 L1381 T1382 S1383 V1384 T1385 R1386 F1389 N1390 R1391 S1392 N1393 T1394 M1398 R1399 C1400 S1401 F1402



• Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide

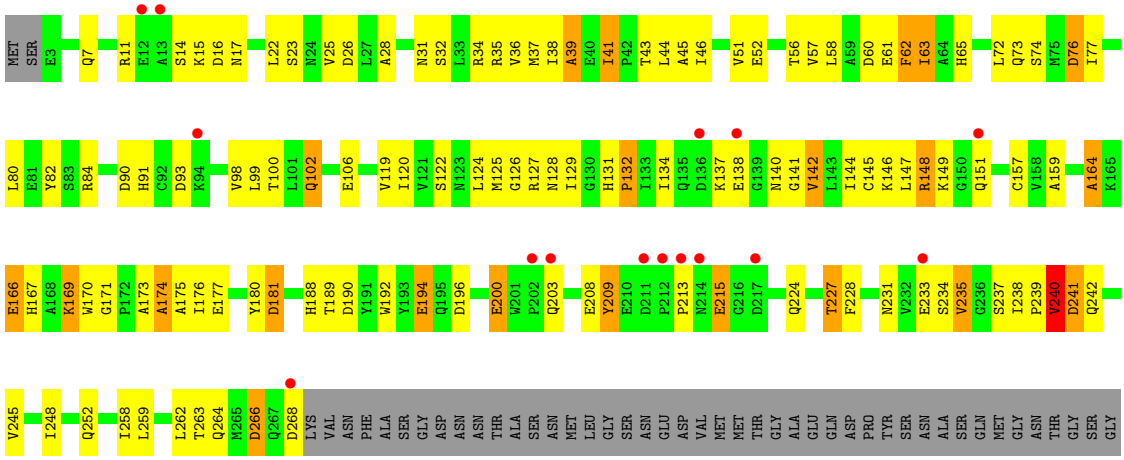
Chain B:





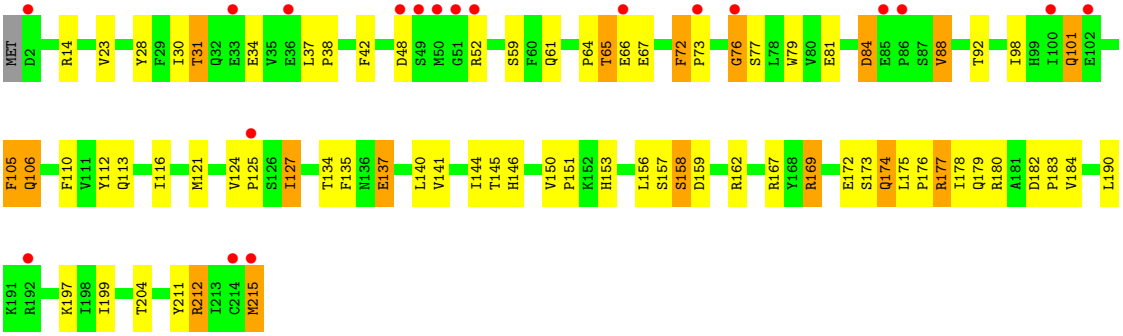
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:



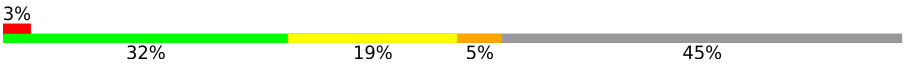
• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

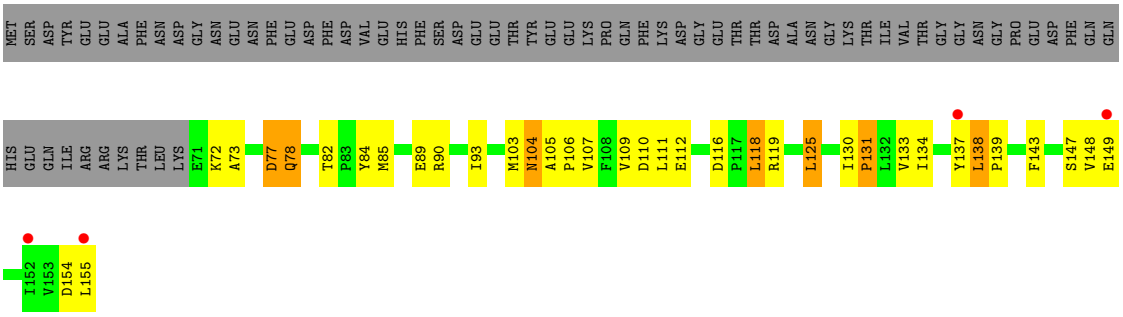
Chain E:



• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

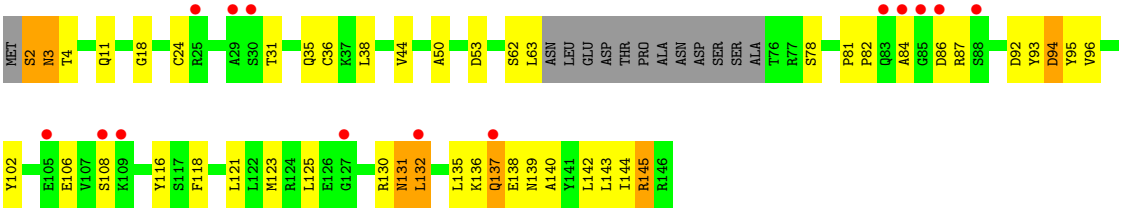
Chain F:





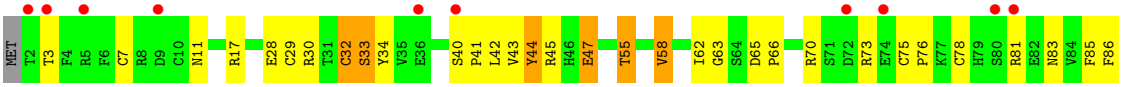
• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

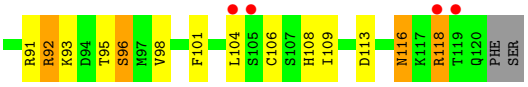
Chain H:



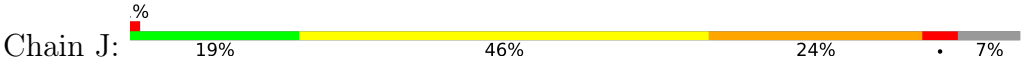
• Molecule 10: DNA-directed RNA polymerase II subunit 9

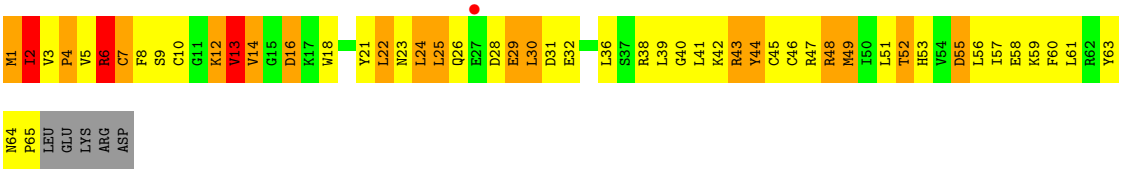
Chain I:



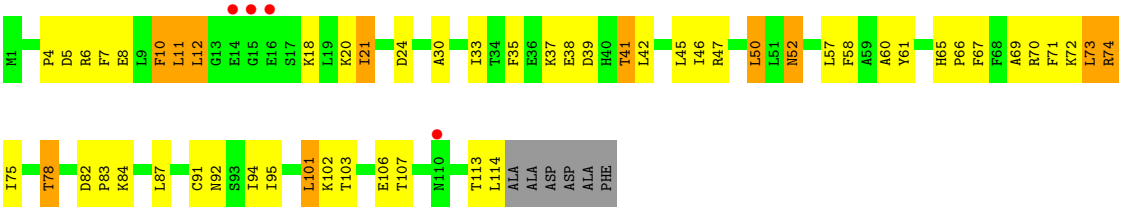


• Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

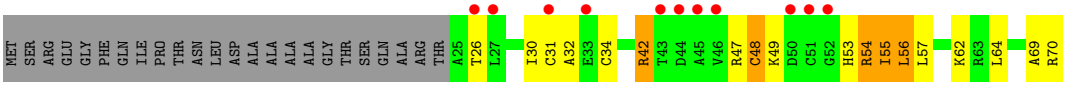




• Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



• Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.61Å 222.73Å 196.16Å 90.00° 101.87° 90.00°	Depositor
Resolution (Å)	19.98 – 3.40 19.97 – 3.40	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.98-3.40) 90.0 (19.97-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.283 , 0.344 0.271 , 0.319	Depositor DCC
R_{free} test set	2609 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å^2)	101.5	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 121.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29530	wwPDB-VP
Average B, all atoms (Å^2)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UTP, 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	R	0.58	0/243	1.05	1/378 (0.3%)
2	T	0.91	1/634 (0.2%)	1.72	18/975 (1.8%)
3	N	1.12	1/317 (0.3%)	1.59	6/488 (1.2%)
4	A	0.49	0/11292	0.66	0/15267
5	B	0.54	0/9087	0.68	0/12253
6	C	0.56	0/2133	0.68	0/2891
7	E	0.46	0/1788	0.61	0/2406
8	F	0.46	0/700	0.65	0/945
9	H	0.44	0/1086	0.66	0/1470
10	I	0.46	0/989	0.65	0/1331
11	J	0.50	0/541	0.65	0/727
12	K	0.53	0/937	0.64	0/1265
13	L	0.59	0/365	0.83	0/485
All	All	0.53	2/30112 (0.0%)	0.73	25/40881 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	18
5	B	0	20
6	C	0	1
9	H	0	1
11	J	0	4
All	All	0	44

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	12	DT	C5-C7	10.67	1.56	1.50
2	T	18	DA	O3'-P	7.41	1.70	1.61

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	25	DC	O4'-C1'-N1	13.75	117.62	108.00
3	N	1	DC	O4'-C1'-N1	10.87	115.61	108.00
2	T	16	DC	O4'-C1'-N1	10.29	115.21	108.00
2	T	25	DC	C1'-O4'-C4'	-10.21	99.89	110.10
2	T	25	DC	O4'-C4'-C3'	-9.01	100.60	106.00

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	117	GLU	Peptide
4	A	218	ASP	Peptide
4	A	222	LEU	Peptide
4	A	53	LEU	Peptide
4	A	54	ASN	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	R	216	0	109	59	0
2	T	566	0	316	44	0
3	N	284	0	161	3	0
4	A	11094	0	11178	663	0
5	B	8914	0	8953	727	0
6	C	2095	0	2051	120	0
7	E	1752	0	1776	52	0
8	F	688	0	707	23	0
9	H	1068	0	1040	38	0
10	I	971	0	927	30	0
11	J	532	0	542	121	0
12	K	919	0	929	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	363	0	386	10	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	A	58	0	22	12	0
All	All	29530	0	29097	1746	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 30.

The worst 5 of 1746 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)
16:A:2003[A]:UTP:C6	16:A:2003[A]:UTP:H5'2	1.44	1.52
9:H:2:SER:CB	9:H:3:ASN:HB2	1.35	1.50
4:A:1444:MET:CG	4:A:1445:ILE:HG13	1.49	1.42
9:H:2:SER:HB2	9:H:3:ASN:CB	1.52	1.40
4:A:1040:GLN:N	4:A:1041:ALA:HB3	1.43	1.31

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
4	A	1401/1733 (81%)	1052 (75%)	250 (18%)	99 (7%)	1 7
5	B	1105/1224 (90%)	836 (76%)	177 (16%)	92 (8%)	1 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	C	264/318 (83%)	197 (75%)	54 (20%)	13 (5%)	2 14
7	E	212/215 (99%)	184 (87%)	22 (10%)	6 (3%)	5 24
8	F	83/155 (54%)	70 (84%)	7 (8%)	6 (7%)	1 7
9	H	129/146 (88%)	99 (77%)	22 (17%)	8 (6%)	1 10
10	I	117/122 (96%)	88 (75%)	22 (19%)	7 (6%)	1 10
11	J	63/70 (90%)	49 (78%)	7 (11%)	7 (11%)	0 3
12	K	112/120 (93%)	96 (86%)	14 (12%)	2 (2%)	8 32
13	L	44/70 (63%)	26 (59%)	14 (32%)	4 (9%)	1 4
All	All	3530/4173 (85%)	2697 (76%)	589 (17%)	244 (7%)	1 8

5 of 244 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	68	GLN
4	A	93	VAL
4	A	117	GLU
4	A	118	HIS

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
4	A	1231/1520 (81%)	1016 (82%)	215 (18%)	2 7
5	B	972/1061 (92%)	799 (82%)	173 (18%)	2 6
6	C	234/274 (85%)	204 (87%)	30 (13%)	4 16
7	E	196/197 (100%)	173 (88%)	23 (12%)	5 20
8	F	75/137 (55%)	68 (91%)	7 (9%)	9 31
9	H	117/128 (91%)	102 (87%)	15 (13%)	4 16
10	I	113/116 (97%)	93 (82%)	20 (18%)	2 6
11	J	60/65 (92%)	40 (67%)	20 (33%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	K	99/102 (97%)	80 (81%)	19 (19%)	1 4
13	L	40/57 (70%)	32 (80%)	8 (20%)	1 3
All	All	3137/3657 (86%)	2607 (83%)	530 (17%)	2 8

5 of 530 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	I	7	CYS
10	I	92	ARG
9	H	145	ARG
12	K	113	THR
4	A	1350	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	1104	HIS
7	E	147	HIS
6	C	17	ASN
6	C	224	GLN
12	K	52	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	8	G
1	R	9	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 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	$\#\|Z\| > 2$
16	UTP	A	2003[B]	-	22,30,30	1.68	4 (18%)	27,47,47	1.47	4 (14%)
16	UTP	A	2003[A]	-	22,30,30	1.68	4 (18%)	27,47,47	1.47	3 (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
16	UTP	A	2003[B]	-	-	1/20/38/38	0/2/2/2
16	UTP	A	2003[A]	-	-	5/20/38/38	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2003[A]	UTP	C4-N3	4.24	1.40	1.33
16	A	2003[B]	UTP	C4-N3	4.24	1.40	1.33
16	A	2003[A]	UTP	C6-N1	3.78	1.40	1.35
16	A	2003[B]	UTP	C6-N1	3.75	1.40	1.35
16	A	2003[B]	UTP	PG-O2G	3.39	1.61	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	2003[A]	UTP	PB-O3B-PG	-3.75	119.95	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	2003[B]	UTP	PB-O3B-PG	-3.73	120.01	132.83
16	A	2003[A]	UTP	PB-O3A-PA	-3.73	120.03	132.83
16	A	2003[B]	UTP	PB-O3A-PA	-3.73	120.03	132.83
16	A	2003[B]	UTP	O1G-PG-O3B	2.45	112.86	104.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	2003[A]	UTP	C4'-C5'-O5'-PA
16	A	2003[A]	UTP	C2'-C1'-N1-C6
16	A	2003[A]	UTP	C3'-C4'-C5'-O5'
16	A	2003[A]	UTP	O4'-C4'-C5'-O5'
16	A	2003[B]	UTP	C4'-C5'-O5'-PA

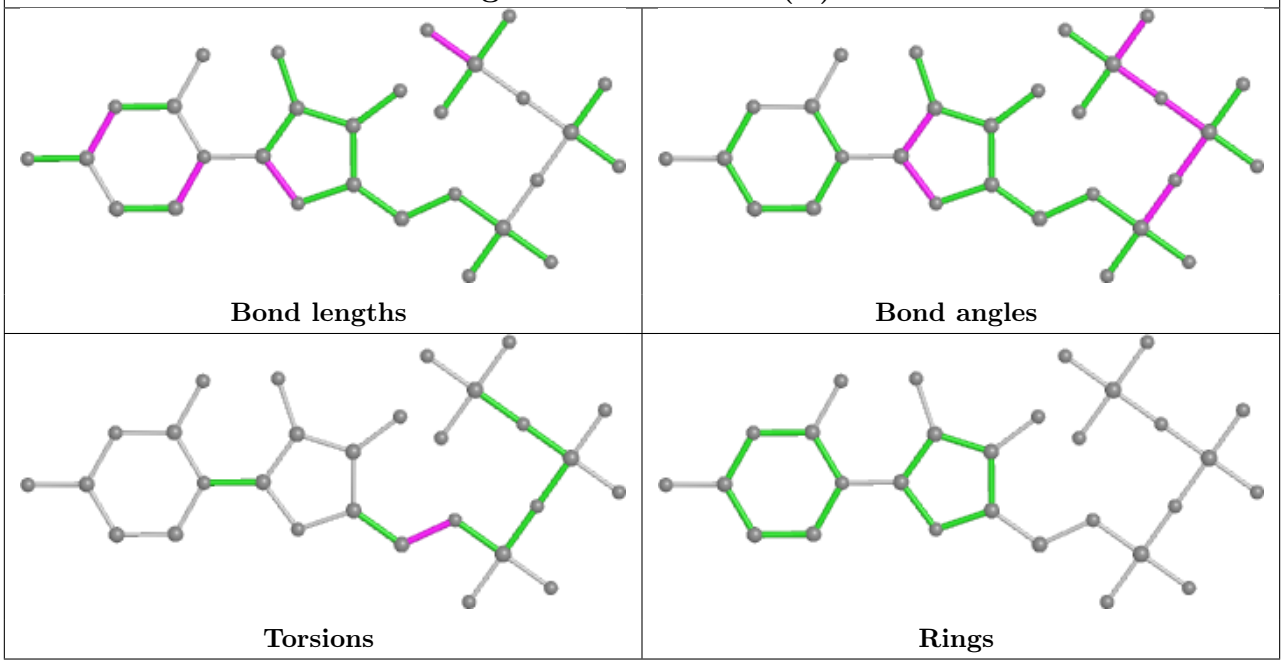
There are no ring outliers.

2 monomers are involved in 12 short contacts:

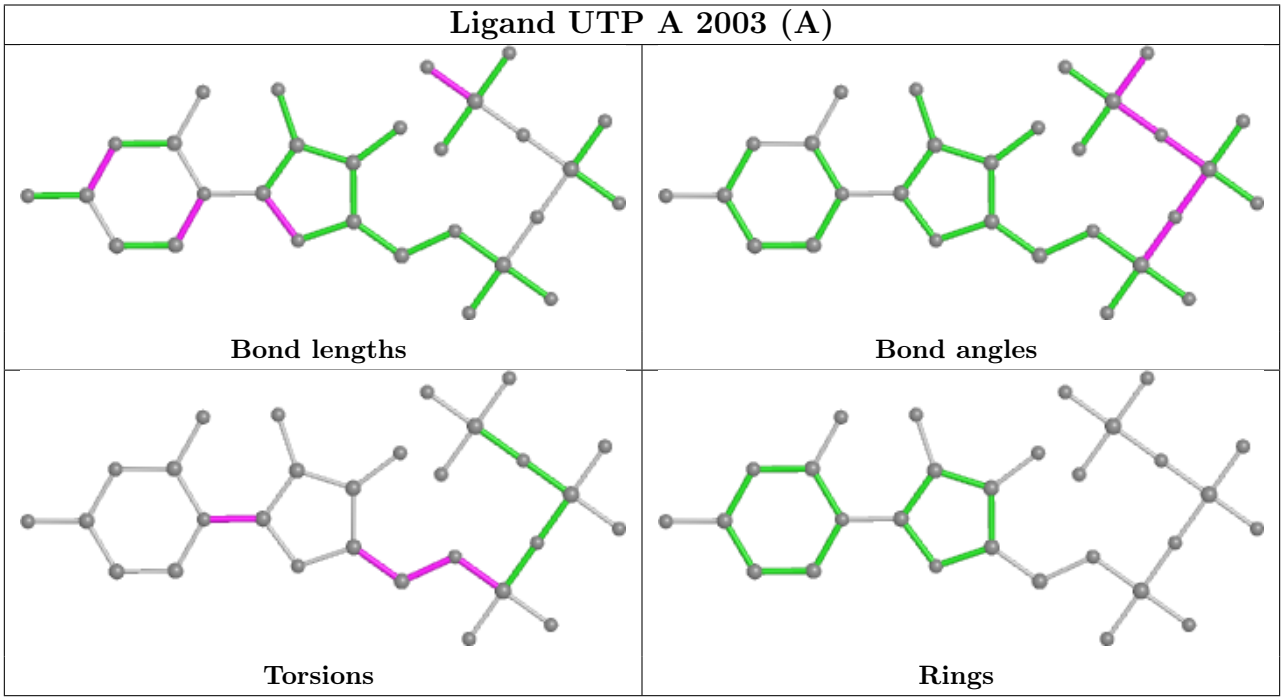
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2003[B]	UTP	3	0
16	A	2003[A]	UTP	9	0

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 UTP A 2003 (B)



Ligand UTP A 2003 (A)



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	R	10/10 (100%)	0.66	0 100 100	118, 142, 150, 153	0
2	T	28/28 (100%)	1.72	12 (42%) 0 0	138, 167, 200, 200	0
3	N	14/14 (100%)	2.74	9 (64%) 0 0	155, 184, 200, 200	0
4	A	1411/1733 (81%)	0.40	114 (8%) 12 13	101, 149, 166, 193	0
5	B	1121/1224 (91%)	0.34	81 (7%) 15 17	84, 141, 159, 176	0
6	C	266/318 (83%)	0.27	15 (5%) 24 25	109, 139, 155, 178	0
7	E	214/215 (99%)	0.57	19 (8%) 9 11	147, 163, 172, 177	0
8	F	85/155 (54%)	0.30	4 (4%) 31 31	144, 160, 173, 178	0
9	H	133/146 (91%)	0.54	14 (10%) 6 7	141, 154, 173, 182	0
10	I	119/122 (97%)	0.75	14 (11%) 4 5	134, 153, 168, 171	0
11	J	65/70 (92%)	0.04	1 (1%) 73 72	99, 120, 137, 144	0
12	K	114/120 (95%)	0.26	4 (3%) 44 43	130, 147, 166, 171	0
13	L	46/70 (65%)	1.20	11 (23%) 0 0	148, 174, 178, 178	0
All	All	3626/4225 (85%)	0.42	298 (8%) 11 13	84, 147, 169, 200	0

The worst 5 of 298 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	250	PHE	10.2
5	B	1221	SER	10.0
5	B	339	THR	8.9
4	A	1090	ALA	7.7
5	B	1224	PHE	7.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

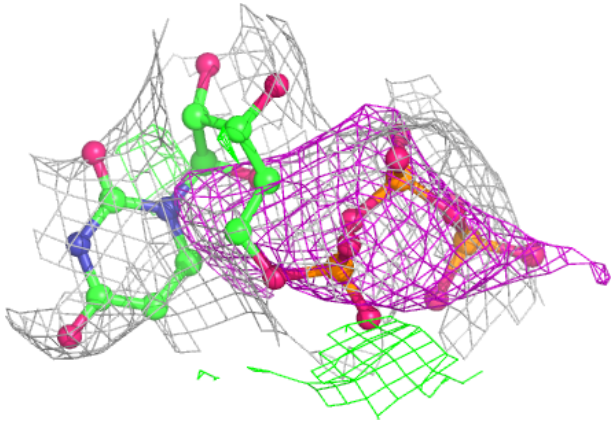
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

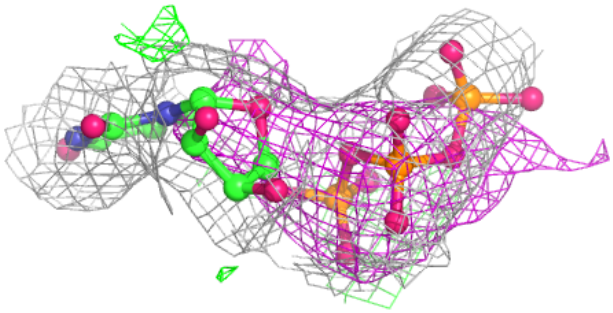
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	ZN	I	204	1/1	0.81	0.12	154,154,154,154	0
16	UTP	A	2003[A]	29/29	0.82	0.38	132,133,138,138	29
16	UTP	A	2003[B]	29/29	0.82	0.38	137,137,137,137	29
14	ZN	A	1734	1/1	0.87	0.25	157,157,157,157	0
14	ZN	I	203	1/1	0.90	0.10	141,141,141,141	0
15	MG	A	2001	1/1	0.91	0.15	124,124,124,124	0
14	ZN	A	1735	1/1	0.93	0.08	149,149,149,149	0
14	ZN	L	105	1/1	0.95	0.27	175,175,175,175	0
14	ZN	C	319	1/1	0.95	0.09	149,149,149,149	0
14	ZN	B	1307	1/1	0.96	0.19	142,142,142,142	0
15	MG	A	2002	1/1	0.96	0.33	59,59,59,59	0
14	ZN	J	101	1/1	0.98	0.07	109,109,109,109	0

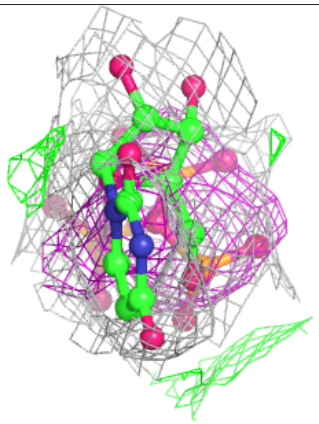
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UTP A 2003 (A):

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

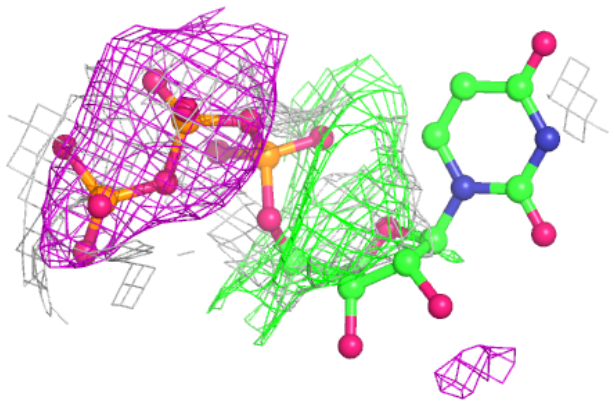


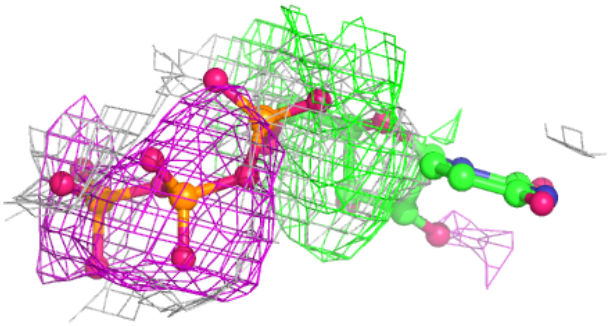


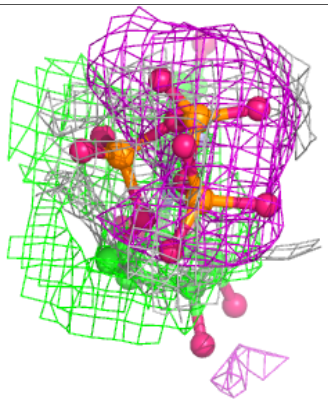


Electron density around UTP A 2003 (B):

$2mF_o$-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.