wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 03:30 AM EDT

PDB ID	:	3GTP
Title	:	Backtracked RNA polymerase II complex with 24mer RNA
Authors	:	Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on	:	2009-03-27
Resolution	:	3.90 Å(reported)

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

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

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

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

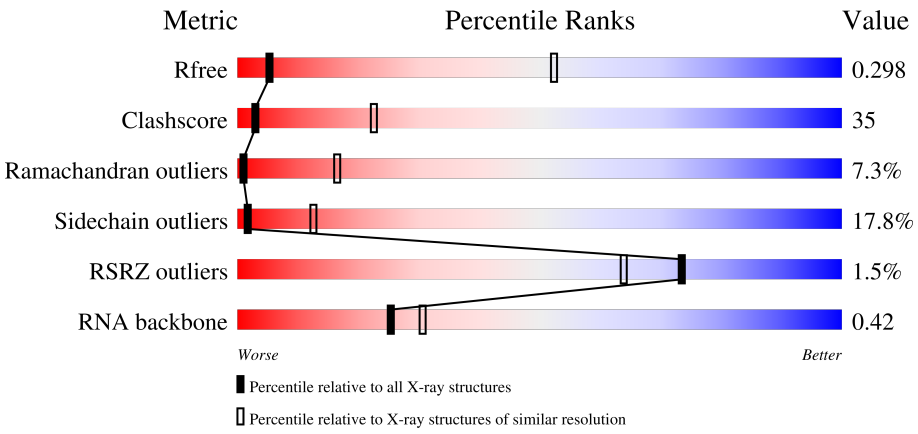
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	2% 31% 38% 11% • 20%
2	B	1224	% 34% 44% 10% • 10%
3	C	318	30% 42% 12% • 16%
4	E	215	2% 47% 41% 10% •

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Mol	Chain	Length	Quality of chain
5	F	155	26% 23% 5% 46%
6	H	146	2% 34% 42% 14% 9%
7	I	122	47% 40% 10%
8	J	70	27% 53% 11% 7%
9	K	120	42% 44% 8% 5%
10	L	70	% 26% 24% 14% 34%
11	R	24	8% 17% 17% 12% 46%
12	T	28	14% 61% 25%
13	N	14	7% 21% 57% 21%

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
14	ZN	J	101	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29279 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1395	10969	6917	1923	2068	61	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1106	8792	5568	1538	1631	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	84	679	434	115	127	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP *UP*GP*CP*AP*GP*AP*CP*GP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	R	13	280	126	55	87	12	0	0	0

- Molecule 12 is a DNA chain called DNA (28-MER).

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

- Molecule 13 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP *GP*TP*AP*G)-3').

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

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

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

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

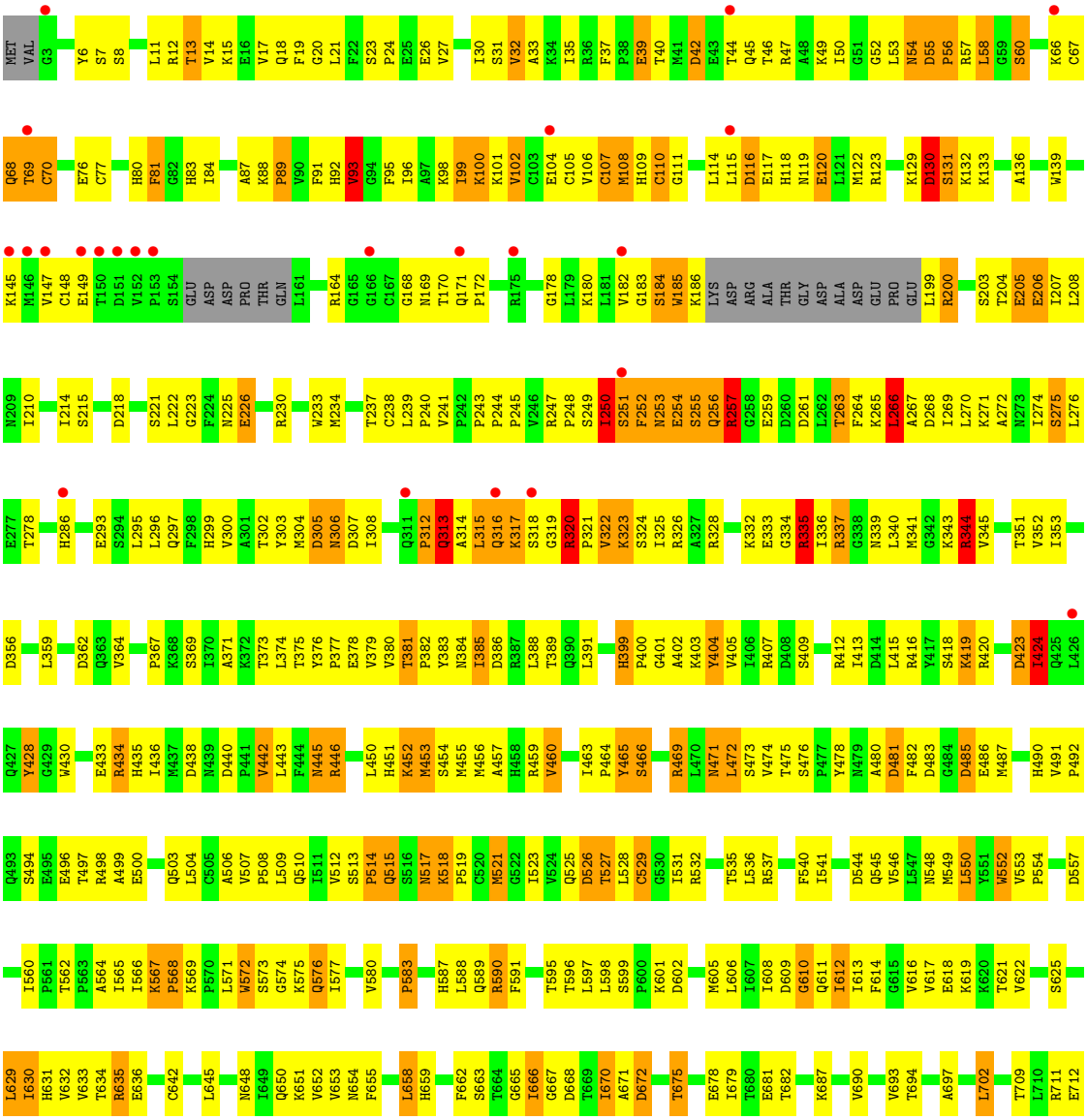
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	A	1	1	1	0	0

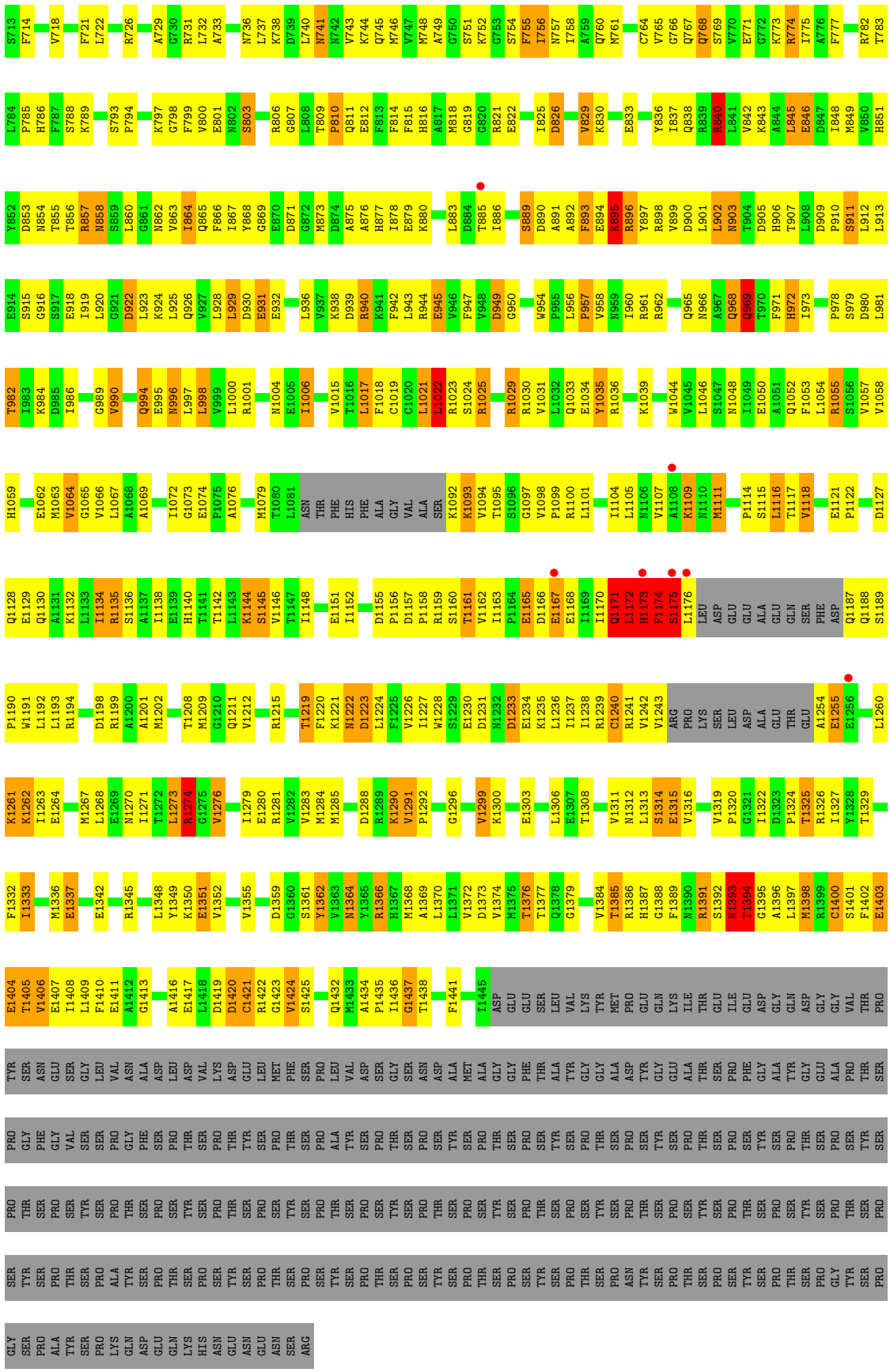
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A: 2% 31% 38% 11% • 20%

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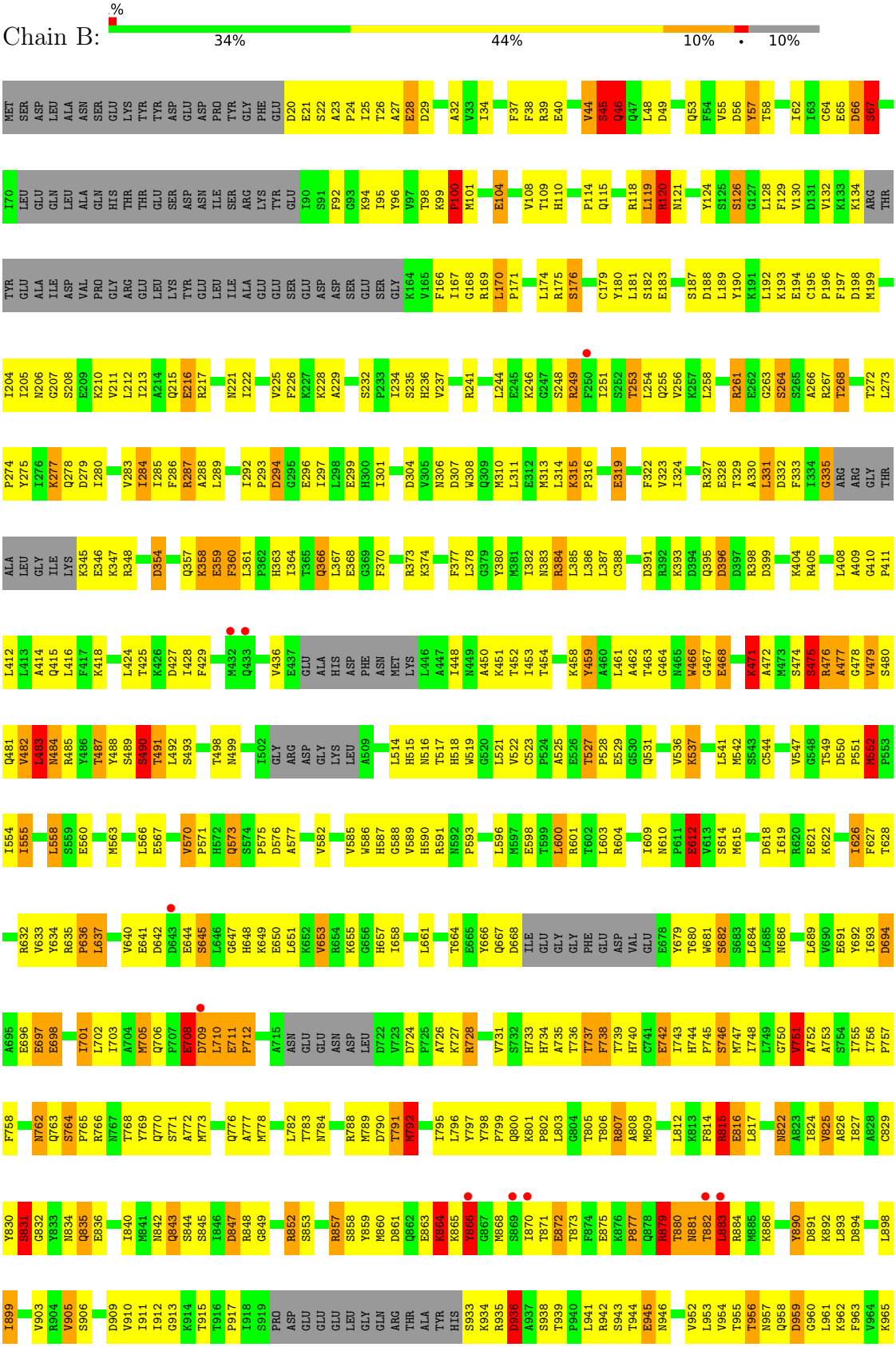
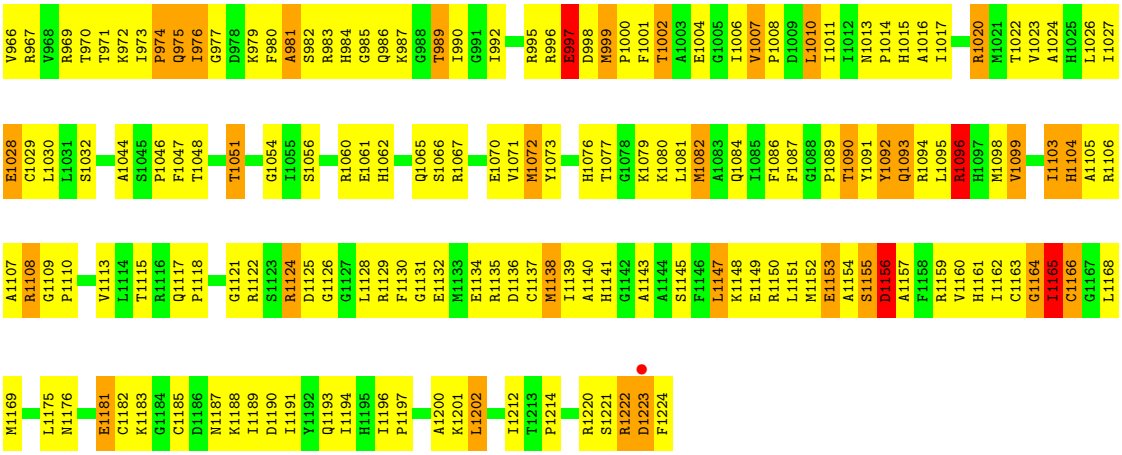
L784 P785 H786 F787 S788 K789 S793 P794 K797 G798 F799 V800 E801 N802 S803 R806 G807 L808 T809 P810 Q811 E812 F813 F814 F815 H816 A817 M818 G819 G820 R821 E822 I825 D826 V829 K830 E833 Y836 I837 Q838 R839 R840 L841 V842 K843 A844 L845 E846 D847 I848 M849 V850 H851
Y852 D853 N854 T855 T856 R857 N858 S859 L860 G861 N862 V863 I864 Q865 F866 I867 Y868 G869 E870 D871 G872 M873 D874 A875 A876 H877 I878 E879 K880 L883 D884 T885 I886 S889 D890 A891 A892 F893 E894 K895 R896 Y897 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908 D909 P910 S911 L912 L913
E914 S915 G916 S917 E918 I919 L920 G921 D922 L923 K924 L925 Q926 V927 L928 L929 D930 E931 E932 L936 V937 K938 D939 R940 K941 F942 L943 R944 E945 V946 F947 V948 D949 G950 W954 P955 L956 P957 V958 N959 I960 R961 R962 Q965 N966 A967 Q968 Q969 T970 F971 H972 I973 P978 S979 D980 L981
T982 I983 K984 D985 I986 G989 V990 Q994 E995 N996 L997 L998 V999 L1000 R1001 N1004 E1005 I1006 V1015 T1016 L1017 F1018 C1019 C1020 L1021 L1022 R1023 S1024 R1025 R1029 R1030 V1031 L1032 Q1033 E1034 Y1035 R1036 K1039 W1044 V1045 L1046 S1047 N1048 I1049 E1050 A1051 Q1052 F1053 L1054 R1055 S1056 V1057 V1058
H1059 E1062 M1063 V1064 G1065 V1066 L1067 A1068 A1069 I1072 G1073 E1074 P1075 A1076 M1079 T1080 L1081 ASN THR PHE HIS PHE ALA GLY VAL ALA SER K1092 K1093 V1094 T1095 S1096 G1097 V1098 P1099 R1100 L1101 I1104 L1105 N1106 V1107 A1108 K1109 N1110 M1111 P1114 S1115 L1116 T1117 V1118 E1121 P1122 D1127
Q1128 E1129 Q1130 A1131 K1132 L1133 I1134 R1135 S1136 A1137 I1138 E1139 H1140 T1141 T1142 L1143 K1144 S1145 V1146 T1147 I1148 E1151 I1152 D1155 P1156 D1157 P1158 R1159 S1160 T1161 V1162 I1163 P1164 E1165 D1166 E1167 E1168 I1169 I1170 Q1171 L1172 H1173 F1174 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189
P1190 W1191 L1192 L1193 R1194 D1198 R1199 A1200 A1201 M1202 T1208 M1209 G1210 Q1211 V1212 R1215 T1219 F1220 K1221 N1222 D1223 L1224 F1225 V1226 V1227 W1228 S1229 E1230 D1231 N1232 D1233 E1234 K1235 L1236 I1237 I1238 R1239 C1240 R1241 V1242 V1243 ARG PRO LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 L1260
K1261 K1262 I1263 E1264 M1267 L1268 E1259 N1270 I1271 T1272 L1273 R1274 G1275 V1276 I1279 E1280 R1281 V1282 V1283 M1284 M1285 D1288 R1289 K1290 V1291 P1292 G1296 V1299 K1300 E1303 L1306 E1307 T1308 V1311 N1312 L1313 S1314 E1315 V1316 V1319 P1320 G1321 I1322 D1323 P1324 T1325 R1326 I1327 Y1328 T1329
F1332 I1333 M1336 E1337 E1342 R1345 L1348 Y1349 K1350 E1351 V1352 V1355 D1359 G1360 S1361 Y1362 V1363 N1364 Y1365 R1366 H1367 M1368 A1369 L1370 L1371 V1372 D1373 V1374 M1375 T1376 T1377 Q1378 G1379 V1384 T1385 R1386 H1387 G1388 F1389 N1390 R1391 S1392 N1393 T1394 G1395 A1396 L1397 M1398 R1399 C1400 S1401 F1402 E1403
E1404 T1405 V1406 E1407 I1408 L1409 F1410 E1411 A1412 G1413 A1416 E1417 L1418 D1419 D1420 C1421 R1422 G1423 V1424 S1425 Q1432 M1433 A1434 P1435 I1436 G1437 T1438 F1441 I1445 ASP GLU GLU SER LEU VAL LYS TYR MET PRO GLU GLN LYS ILE THR GLU ILE GLU ASP GLY GLN ASP GLY GLU ALA PRO THR SER
TYR SER ASN GLU SER GLY LEU VAL ASN ALA ASP LEU ASP LEU MET PHE SER PRO LEU VAL ASP SER GLY SER ASN ASP ALA MET ALA GLY GLY PHE THR ALA TYR GLY GLY ALA ASP TYR GLY GLU ALA THR SER PRO GLY GLY GLU ALA PRO THR
PRO GLY PHE GLY VAL SER SER PRO PRO GLY PHE SER PRO SER PRO THR TYR SER TYR SER PRO PRO SER TYR SER PRO THR SER SER PRO PRO THR THR SER PRO SER TYR SER PRO SER SER TYR SER PRO SER PRO THR SER PRO SER TYR SER PRO SER PRO THR SER PRO SER TYR SER PRO SER PRO THR SER
PRO THR SER PRO SER TYR SER PRO PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO SER TYR SER PRO SER PRO SER PRO SER TYR SER PRO SER PRO SER PRO

• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

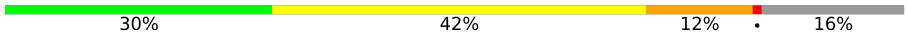
Chain B:

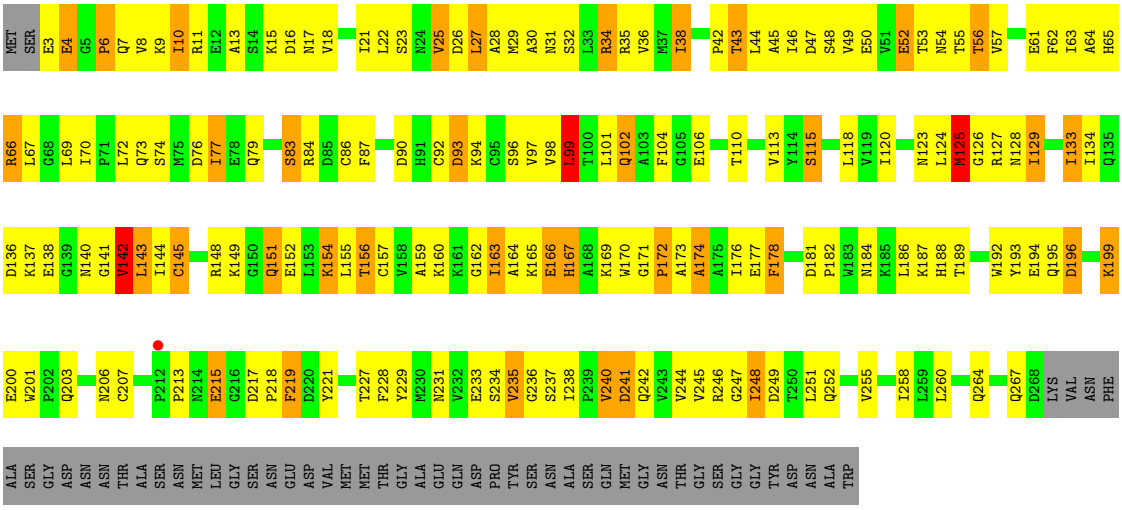




- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

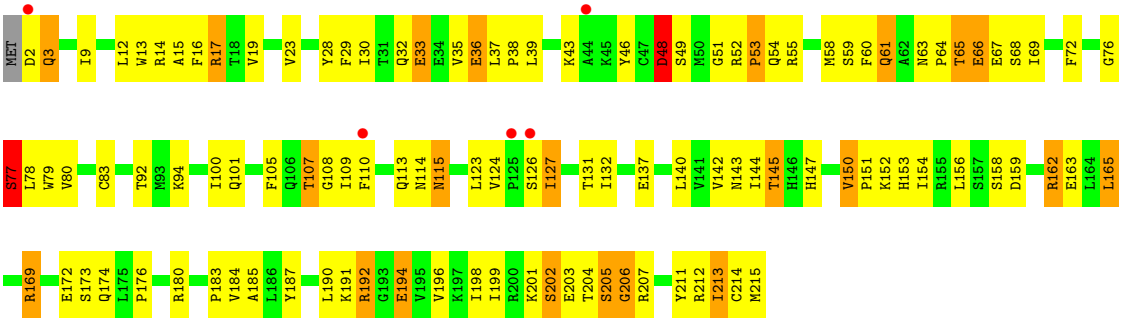
Chain C:





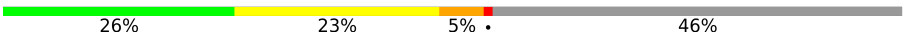
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

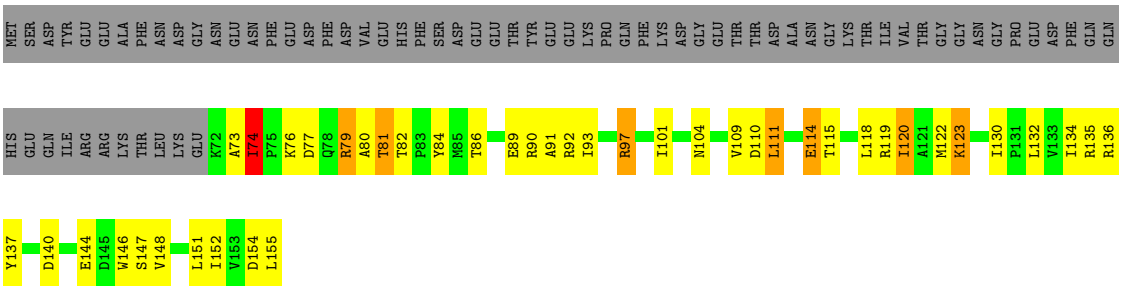
Chain E:



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

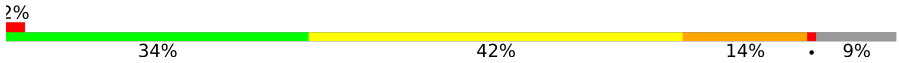
Chain F:

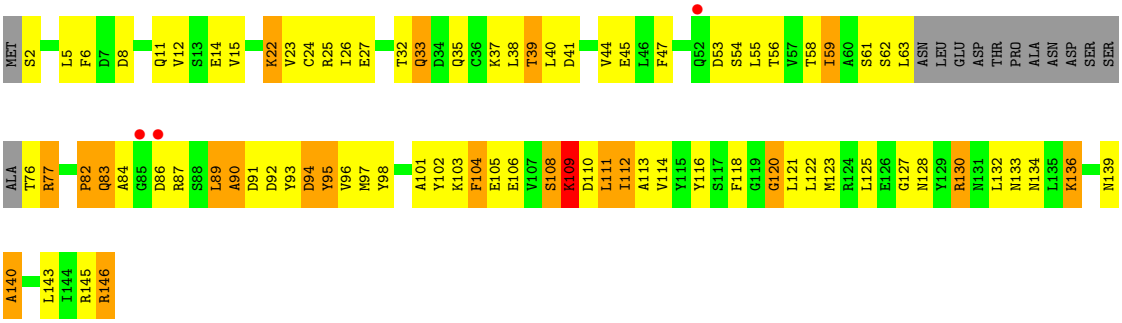




• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

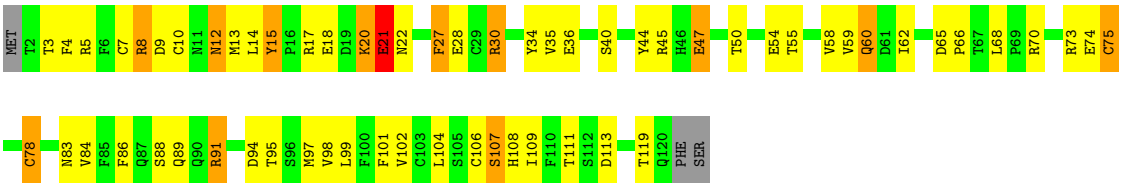
Chain H:





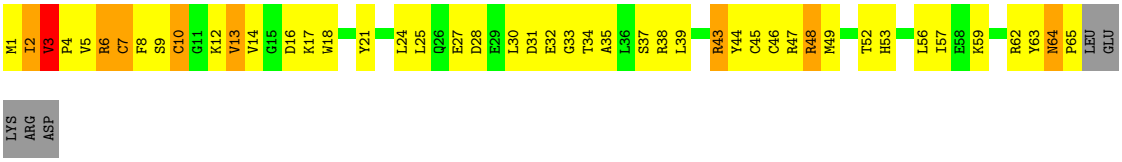
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

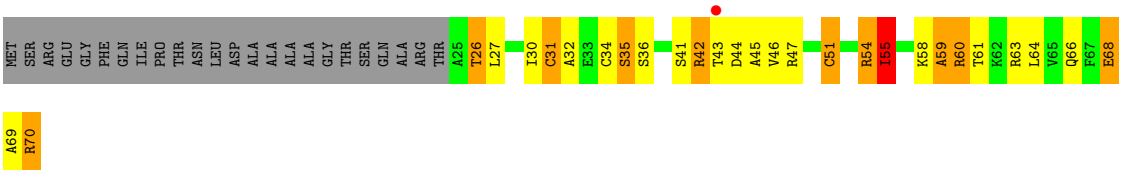


• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:

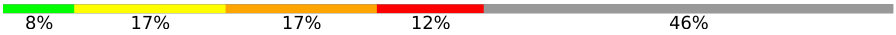
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



• Molecule 11: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*CP*AP*GP*AP*CP*GP*UP*UP*UP*UP*UP*U)-3')

Chain R:

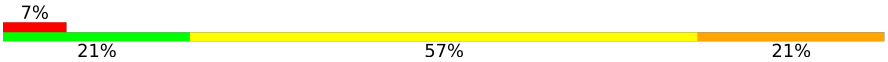


• Molecule 12: DNA (28-MER)

Chain T:

• Molecule 13: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.78Å 222.11Å 194.85Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 43.63 – 3.90	Depositor EDS
% Data completeness (in resolution range)	91.6 (50.00-3.90) 91.7 (43.63-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.266 , 0.299 0.269 , 0.298	Depositor DCC
R_{free} test set	3001 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	117.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	29279	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.06	51/11163 (0.5%)	0.84	14/15091 (0.1%)
2	B	1.12	54/8963 (0.6%)	0.86	12/12086 (0.1%)
3	C	1.06	8/2133 (0.4%)	0.85	2/2891 (0.1%)
4	E	1.10	11/1788 (0.6%)	0.77	1/2406 (0.0%)
5	F	1.00	3/691 (0.4%)	0.79	0/933
6	H	1.09	10/1086 (0.9%)	0.82	2/1470 (0.1%)
7	I	1.11	5/989 (0.5%)	0.94	4/1331 (0.3%)
8	J	1.12	1/541 (0.2%)	0.99	2/727 (0.3%)
9	K	1.08	2/937 (0.2%)	0.84	2/1265 (0.2%)
10	L	1.15	2/365 (0.5%)	0.93	0/485
11	R	1.35	3/314 (1.0%)	1.76	6/489 (1.2%)
12	T	2.13	19/634 (3.0%)	1.96	27/975 (2.8%)
13	N	2.23	6/317 (1.9%)	1.73	10/488 (2.0%)
All	All	1.14	175/29921 (0.6%)	0.92	82/40637 (0.2%)

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
1	A	0	1
6	H	0	1
All	All	0	2

The worst 5 of 175 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	12	DT	C5-C7	20.75	1.62	1.50
12	T	3	DA	P-O5'	20.57	1.80	1.59
12	T	3	DA	C4'-O4'	17.05	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	12	DT	N3-C4	12.54	1.48	1.38
1	A	833	GLU	CD-OE1	11.61	1.38	1.25

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1215	ARG	NE-CZ-NH2	-12.59	114.01	120.30
12	T	3	DA	O4'-C4'-C3'	-12.07	98.76	106.00
12	T	16	DC	O4'-C4'-C3'	-11.55	99.07	106.00
11	R	13	C	C1'-O4'-C4'	-10.90	101.18	109.90
2	B	287	ARG	NE-CZ-NH2	-10.47	115.06	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	523	ILE	Peptide
6	H	61	SER	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	10969	0	11070	870	0
2	B	8792	0	8825	673	0
3	C	2095	0	2051	163	0
4	E	1752	0	1776	90	0
5	F	679	0	701	39	0
6	H	1068	0	1040	97	0
7	I	971	0	928	46	0
8	J	532	0	544	79	0
9	K	919	0	929	71	0
10	L	363	0	387	24	0
11	R	280	0	143	19	0
12	T	566	0	314	20	0
13	N	284	0	161	5	0
14	A	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	L	1	0	0	1	0
15	A	1	0	0	0	0
All	All	29279	0	28869	2008	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 35.

The worst 5 of 2008 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)
6:H:104:PHE:CZ	6:H:136:LYS:HB3	1.37	1.55
7:I:109:ILE:CG1	7:I:109:ILE:CD1	1.84	1.53
2:B:100:PRO:CG	2:B:100:PRO:CB	1.75	1.48
1:A:256:GLN:CA	1:A:257:ARG:HB3	1.42	1.47
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.37	1.35

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	1383/1733 (80%)	1027 (74%)	248 (18%)	108 (8%)	1 15
2	B	1088/1224 (89%)	823 (76%)	195 (18%)	70 (6%)	1 19
3	C	264/318 (83%)	195 (74%)	51 (19%)	18 (7%)	1 18
4	E	212/215 (99%)	163 (77%)	35 (16%)	14 (7%)	1 19
5	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	H	129/146 (88%)	94 (73%)	24 (19%)	11 (8%)	1 13
7	I	117/122 (96%)	83 (71%)	23 (20%)	11 (9%)	0 12
8	J	63/70 (90%)	50 (79%)	9 (14%)	4 (6%)	1 19
9	K	112/120 (93%)	86 (77%)	21 (19%)	5 (4%)	2 25
10	L	44/70 (63%)	20 (46%)	16 (36%)	8 (18%)	0 2
All	All	3494/4173 (84%)	2603 (74%)	637 (18%)	254 (7%)	1 16

5 of 254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	68	GLN
1	A	69	THR
1	A	117	GLU

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	1218/1520 (80%)	976 (80%)	242 (20%)	1 9
2	B	960/1061 (90%)	797 (83%)	163 (17%)	2 14
3	C	234/274 (85%)	191 (82%)	43 (18%)	1 11
4	E	196/197 (100%)	168 (86%)	28 (14%)	3 20
5	F	74/137 (54%)	67 (90%)	7 (10%)	8 33
6	H	117/128 (91%)	93 (80%)	24 (20%)	1 8
7	I	113/116 (97%)	97 (86%)	16 (14%)	3 20
8	J	60/65 (92%)	49 (82%)	11 (18%)	1 11
9	K	99/102 (97%)	88 (89%)	11 (11%)	6 27
10	L	40/57 (70%)	32 (80%)	8 (20%)	1 8
All	All	3111/3657 (85%)	2558 (82%)	553 (18%)	2 12

5 of 553 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	127	ILE
5	F	74	ILE
4	E	110	PHE
7	I	95	THR
1	A	1171	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1015	HIS
3	C	203	GLN
2	B	1065	GLN
2	B	1211	ASN
4	E	61	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	12/24 (50%)	5 (41%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	10	A
11	R	11	U
11	R	12	G
11	R	13	C

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	1395/1733 (80%)	-0.19	31 (2%)	62	51	80, 126, 198, 230	0
2	B	1106/1224 (90%)	-0.21	11 (0%)	82	75	79, 120, 169, 188	0
3	C	266/318 (83%)	-0.33	1 (0%)	92	87	89, 116, 158, 167	0
4	E	214/215 (99%)	-0.22	5 (2%)	60	50	113, 165, 202, 206	0
5	F	84/155 (54%)	-0.49	0	100	100	110, 133, 152, 159	0
6	H	133/146 (91%)	-0.08	3 (2%)	60	50	137, 155, 178, 180	0
7	I	119/122 (97%)	-0.29	0	100	100	126, 147, 167, 181	0
8	J	65/70 (92%)	-0.35	0	100	100	86, 105, 134, 141	0
9	K	114/120 (95%)	-0.36	0	100	100	96, 118, 135, 139	0
10	L	46/70 (65%)	-0.15	1 (2%)	62	51	118, 175, 189, 193	0
11	R	13/24 (54%)	-0.32	0	100	100	97, 128, 191, 203	0
12	T	28/28 (100%)	-0.13	0	100	100	111, 219, 343, 346	0
13	N	14/14 (100%)	0.16	1 (7%)	16	11	308, 330, 332, 333	0
All	All	3597/4239 (84%)	-0.22	53 (1%)	73	64	79, 127, 194, 346	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	126	SER	4.8
1	A	1176	LEU	4.6
2	B	869	SER	4.5
13	N	1	DC	4.2
2	B	643	ASP	3.9

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
15	MG	A	1736	1/1	0.89	0.11	97,97,97,97	0
14	ZN	A	1735	1/1	0.94	0.08	177,177,177,177	0
14	ZN	L	105	1/1	0.97	0.09	183,183,183,183	0
14	ZN	A	1734	1/1	0.97	0.08	181,181,181,181	0
14	ZN	I	204	1/1	0.98	0.04	148,148,148,148	0
14	ZN	I	203	1/1	0.99	0.10	139,139,139,139	0
14	ZN	B	1307	1/1	0.99	0.06	156,156,156,156	0
14	ZN	C	319	1/1	1.00	0.07	107,107,107,107	0
14	ZN	J	101	1/1	1.00	0.13	109,109,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.