# W O R L D W I D E
# wwPDB
## PROTEIN DATA BANK

# wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 02:23 AM EDT

|  |  |  |
|---|---|---|
| PDB ID | : | 4IQJ |
| Title | : | Structure of PolIIIalpha-Tauc-DNA complex suggests an atomic model of the replisome |
| Authors | : | Liu, B.; Lin, J.; Steitz, T. |
| Deposited on | : | 2013-01-11 |
| Resolution | : | 3.20 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:

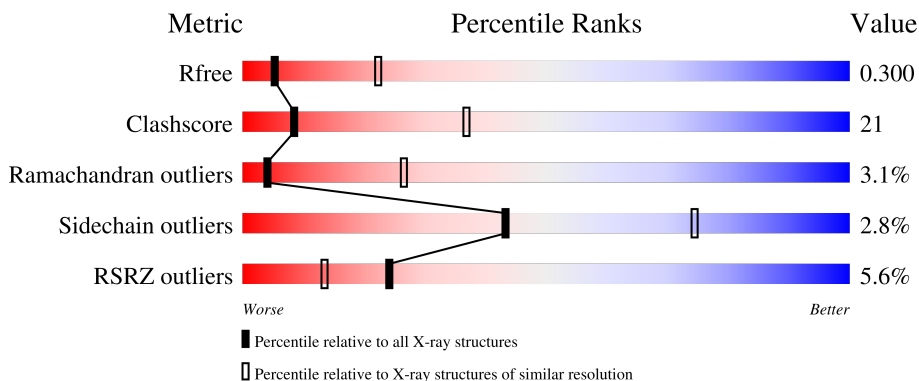|  |  |  |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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 | Percentile Ranks | Value |
|--------|------------------|-------|
| Rfree | | 0.300 |
| Clashscore | | 21 |
| Ramachandran outliers | | 3.1% |
| Sidechain outliers | | 2.8% |
| RSRZ outliers | | 5.6% |

*Worse* — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|--------|--------------------------|-----------------------------------------------------|
| $R_{free}$ | 130704 | 1133 (3.20-3.20) |
| Clashscore | 141614 | 1253 (3.20-3.20) |
| Ramachandran outliers | 138981 | 1234 (3.20-3.20) |
| Sidechain outliers | 138945 | 1233 (3.20-3.20) |
| RSRZ outliers | 127900 | 1095 (3.20-3.20) |

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 | E | 20 | 5% / 90% 10% |
| 1 | G | 20 | 15% / 75% 20% 5% |
| 1 | K | 20 | 15% / 90% 10% |
| 2 | F | 28 | 18% / 50% 14% 7% 29% |
| 2 | H | 28 | 25% / 82% 11% • • |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | J | 28 | 29% · 71% · 11% · 18% |
| 2 | L | 28 | 14% · 79% · 7% · 14% |
| 3 | I | 21 | 24% · 71% · 19% · 10% |
| 4 | A | 1220 | 4% · 75% · 19% · 5% |
| 4 | B | 1220 | 4% · 75% · 19% |
| 4 | C | 1220 | 4% · 74% · 20% |
| 4 | D | 1220 | 3% · 72% · 23% |
| 5 | M | 177 | 17% · 28% · 31% · 15% · 22% |
| 5 | N | 177 | 8% · 35% · 31% · 9% · 24% |
| 5 | O | 177 | 11% · 29% · 31% · 13% · 24% |
| 5 | P | 177 | 12% · 25% · 32% · 14% · 6% · 22% |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3 | DOC | I | 21 | - | - | - | X |

## 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 45265 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 DNA chain called DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP *GP*CP*CP*AP*GP*TP*GP*CP*CP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | E | 20 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 411 | 193 | 83 | 115 | 20 | | | |
| 1 | G | 20 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 411 | 193 | 83 | 115 | 20 | | | |
| 1 | K | 20 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 411 | 193 | 83 | 115 | 20 | | | |

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP* GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | F | 20 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 409 | 194 | 70 | 125 | 20 | | | |
| 2 | H | 27 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 551 | 264 | 87 | 173 | 27 | | | |
| 2 | J | 23 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 471 | 224 | 79 | 145 | 23 | | | |
| 2 | L | 24 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 491 | 234 | 81 | 152 | 24 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | I | 21 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 429 | 202 | 86 | 120 | 21 | | | |

- Molecule 4 is a protein called DNA polymerase III subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 4 | A | 1164 | Total 9280 | C 5918 | N 1620 | O 1714 | S 28 | 0 | 0 | 0 |
| 4 | B | 1167 | Total 9295 | C 5926 | N 1623 | O 1716 | S 30 | 0 | 0 | 0 |
| 4 | C | 1166 | Total 9293 | C 5930 | N 1621 | O 1714 | S 28 | 0 | 0 | 0 |
| 4 | D | 1185 | Total 9445 | C 6026 | N 1651 | O 1738 | S 30 | 0 | 0 | 0 |

- Molecule 5 is a protein called DNA polymerase III subunit gamma/tau.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 5 | M | 138 | Total 1103 | C 702 | N 203 | O 197 | S 1 | 0 | 0 | 0 |
| 5 | N | 135 | Total 1078 | C 687 | N 200 | O 190 | S 1 | 0 | 0 | 0 |
| 5 | O | 135 | Total 1078 | C 687 | N 200 | O 190 | S 1 | 0 | 0 | 0 |
| 5 | P | 138 | Total 1093 | C 695 | N 203 | O 194 | S 1 | 0 | 0 | 0 |

There are 40 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| M | 367 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| M | 368 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| M | 369 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| M | 370 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| M | 371 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| M | 372 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| M | 373 | LYS | GLU | conflict | UNP A0A0M9ACL9 |
| M | 541 | MET | - | expression tag | UNP A0A0M9ACL9 |
| M | 542 | PRO | - | expression tag | UNP A0A0M9ACL9 |
| M | 543 | PRO | - | expression tag | UNP A0A0M9ACL9 |
| N | 367 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| N | 368 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| N | 369 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| N | 370 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| N | 371 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| N | 372 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| N | 373 | LYS | GLU | conflict | UNP A0A0M9ACL9 |
| N | 541 | MET | - | expression tag | UNP A0A0M9ACL9 |
| N | 542 | PRO | - | expression tag | UNP A0A0M9ACL9 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| N | 543 | PRO | - | expression tag | UNP A0A0M9ACL9 |
| O | 367 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| O | 368 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| O | 369 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| O | 370 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| O | 371 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| O | 372 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| O | 373 | LYS | GLU | conflict | UNP A0A0M9ACL9 |
| O | 541 | MET | - | expression tag | UNP A0A0M9ACL9 |
| O | 542 | PRO | - | expression tag | UNP A0A0M9ACL9 |
| O | 543 | PRO | - | expression tag | UNP A0A0M9ACL9 |
| P | 367 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| P | 368 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| P | 369 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| P | 370 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| P | 371 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| P | 372 | HIS | - | expression tag | UNP A0A0M9ACL9 |
| P | 373 | LYS | GLU | conflict | UNP A0A0M9ACL9 |
| P | 541 | MET | - | expression tag | UNP A0A0M9ACL9 |
| P | 542 | PRO | - | expression tag | UNP A0A0M9ACL9 |
| P | 543 | PRO | - | expression tag | UNP A0A0M9ACL9 |

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6 | A | 3 | Total 3 | Zn 3 | 0 | 0 |
| 6 | B | 3 | Total 3 | Zn 3 | 0 | 0 |
| 6 | C | 3 | Total 3 | Zn 3 | 0 | 0 |
| 6 | D | 3 | Total 3 | Zn 3 | 0 | 0 |

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 7 | A | 1 | Total 1 | Mg 1 | 0 | 0 |
| 7 | B | 1 | Total 1 | Mg 1 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

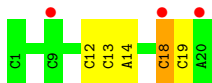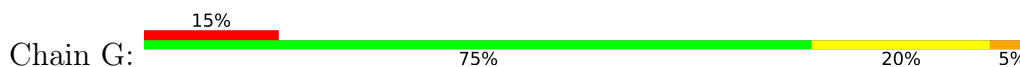| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 7 | C | 1 | Total<br>1 | Mg<br>1 | 0 | 0 |
| 7 | D | 1 | Total<br>1 | Mg<br>1 | 0 | 0 |

# 3  Residue-property plots ⓘ

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 (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*T P*GP*CP*CP*A)-3')

Chain E:

5%
90%          10%

C1  G11  G15  A20

• Molecule 1: DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*T P*GP*CP*CP*A)-3')

Chain G:

15%
75%          20%     5%

C1  C9  C12 C13 A14  C18 C19 A20

• Molecule 1: DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*T P*GP*CP*CP*A)-3')

Chain K:

15%
90%          10%

C1  C12  T16 G17  A20

• Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP *GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3')

Chain F:

18%
50%          14%   7%      29%

DT DT DT DT DT DT DT DG  T9 G10 G11 C12 A13 C14  C18  T24 T25 T26 C27 G28

• Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP *GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3')

Chain H:

25%
82%          11%   •   •

• Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP *GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3')



Chain J:



• Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP *GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3')



Chain L:
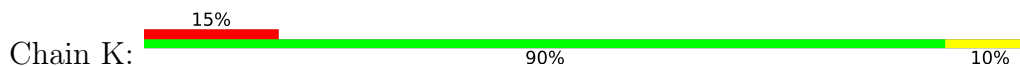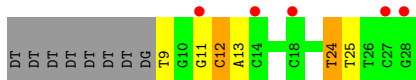


• Molecule 3: DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*T P*GP*CP*CP*AP*(DOC))-3')



Chain I:
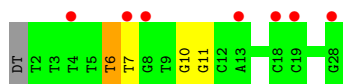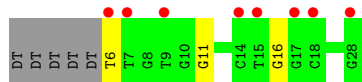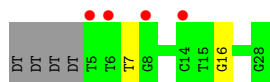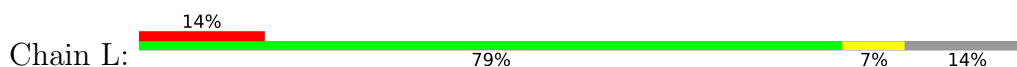


• Molecule 4: DNA polymerase III subunit alpha



Chain A:

Q746 I747 K771 V774 E775 V785 A788 K789 G792 V793 P794 E795 E796 L805 A820 Y821 V837 E838 A842 V854 A855 I858 I866 E885 R909 G912 K916 S917 L918 V930 L935 V939 K940 A941 L944 A951 R952 L953

L960 T967 R968 E969 R970 G971 G974 L975 V976 F979 A980 E981 V982 E983 P986 L987 A990 S991 P992 L993 D994 A1005 I1008 H1013 P1014 V1015 L1016 R1022 E1023 V1024 A1025 I1029 L1032 S1033 E1034 G1041 L1047 S1048 G1049 M1050 V1051 V1054 VAL ARG LYS

PRO THR ARG SER GLY MET ALA R1067 A1076 L1077 V1080 V1081 F1082 E1087 G1088 P1091 K1092 L1093 K1094 E1095 D1096 I1097 P1098 L1099 E1106 LYS GLY GLU GLU LEU R1112 V1113 L1114 V1118 W1119 T1120 L1121 E1122 E1123 V1124 L1125 E1126 A1127 P1128 K1129 L1131 L1132 V1133 E1134 V1135

L1139 L1140 D1141 E1142 K1143 L1152 L1159 P1160 V1161 Y1162 L1163 R1164 V1165 P1168 E1171 A1172 L1173 L1176 R1177 E1178 V1179 R1180 VAL G1182 L1189 E1190 A1191 E1192 G1193 Y1194 Y1197 L1198 V1199 P1200 D1201 R1202 E1203 V1204 F1205 L1206 N1209 G1210 G1211 K1214 E1215 E1216 V1217 V1218 P1219 F1220

• Molecule 4: DNA polymerase III subunit alpha

Chain B:



MET GLY SER LYS L5 H11 L28 V32 L42 I69 R83 LYS ARG GLY LYS GLY LEU ASP GLY G92 L98 L99 R111 L132 A136 S143 I154 L170 I179 L186 V195 L196 K197 A200 L205 G206 M207 D212 D220 A221

R222 V226 L227 L228 A229 I230 K233 T234 T235 L236 D237 D238 P239 W242 P245 V251 N273 L285 K290 M291 P296 R297 L300 P301 E302 G303 R304 Q308 Y309 L310 L313 L319 R325 A329 F330 Y331 R332 V334 L335 R336 L337 L338 GLY THR

MET PRO PRO HIS GLY D346 L350 A351 E352 A353 L354 A355 R356 V357 E358 E359 W362 E363 E364 L365 R366 LYS ARG LEU PRO LEU GLU GLY VAL ARG E377 Y389 V393 F399 P400 F403 L404 I405 V406 Q407 I410 V420 G421 R424 A428 V436 T439

L449 F453 I464 Y484 A490 T494 PHE GLY SER LEU A499 K505 D506 V507 A508 R509 V510 TYR GLY I513 P514 H515 K516 K517 E520 L521 A522 I525 P526 VAL GLN PHE GLY LYS P532 L535 Q536 E537 A538 ILE GLN VAL VAL PRO E544 M549 I559 E560

V561 N569 R570 H571 V574 V580 I581 L586 T587 V590 P591 L592 D595 Q596 E597 G598 R599 P600 V601 T602 Q603 Y604 L615 K616 M617 L620 G621 L622 L625 R633 L670 M675 V679 I690 I691 A692 L693 V694 S695 L696 Y697 G700 P701 M702

I705 H713 G714 Q715 V718 F723 A726 L734 V742 Y743 Q746 I747 A755 L759 K772 R773 V774 E775 F784 L805 L823 Q827 M840 A861 R862 A863 V868 E885 E886 I887 G898 G913 L922 L938 V939 K940 A941 G942

A943 L944 A951 R952 A964 E969 S973 G974 L975 V976 G977 L978 F979 A980 E981 V982 S991 P992 L993 D994 E995 I996 T997 A1005 L1006 G1007 I1008 H1013 P1014 V1015 L1016 R1017 Y1018 L1021 R1022 E1023 V1024 A1025 S1026 C1027 T1028 I1029 L1032 L1039 V1045 L1046 L1047 S1048 G1049

M1050 V1051 E1052 E1053 V1054 V1055 R1056 K1057 P1058 T1059 ARG SER GLY G1063 M1064 M1065 A1066 R1067 F1068 T1069 A1076 L1077 V1080 V1081 F1082 G1083 R1084 A1085 Y1086 E1087 G1088 V1089 S1090 P1091 K1092 L1093 K1094 E1095 D1096 I1097 P1098 L1099 L1100 E1106 LYS GLY GLU GLU LEU R1112 V1113 L1114 V1118 W1119 T1120 L1121

E1122 E1123 K1129 A1130 L1131 A1138 L1139 E1142 K1143 G1144 V1145 A1146 R1147 L1148 L1151 L1152 L1159 R1164 V1165 F1169 G1170 L1173 L1176 V1181 G1182 E1183 A1184 A1185 L1189 Q1207 G1208 G1211 G1212 P1213 E1216 V1217 V1218 P1219 F1220
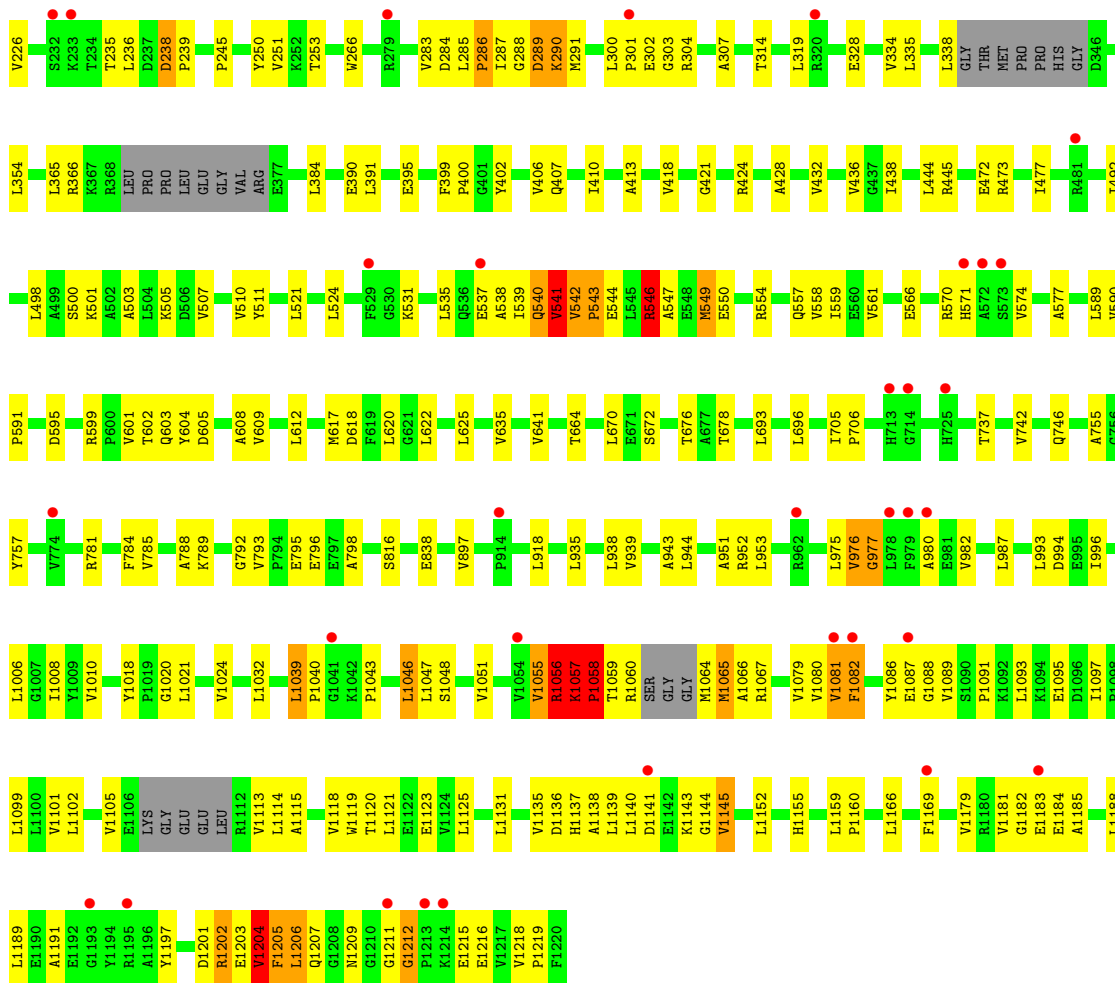
• Molecule 4: DNA polymerase III subunit alpha

Chain C:



• Molecule 4: DNA polymerase III subunit alpha

Chain D:

• Molecule 5: DNA polymerase III subunit gamma/tau



Chain M:



• Molecule 5: DNA polymerase III subunit gamma/tau



Chain N:

V443 E444 E445 V449 L450 E451 K452 K453 S454 L455 S456 GLY ALA SER PRO PRO PRO PRO THR LYS PRO VAL PRO PRO ARG GLU ALA PRO PRO GLU PRO GLU PRO PRO VAL ALA ALA PRO PRO GLU PRO GLU PRO PRO GLU PRO LEU GLU ASP P490 P491 W492 E493 A494 E495 E496 G497 E498 D499 E503 L504 R505 R506

L507 A508 R509 L510 L511 G512 L515 L516 W517 V518 R519 K520 P521 K522 A523 P524 E525 A526 E527 E528 P529 V530 S531 E532 D533 G534 I535 G536 I540 M541 P542 P543

• Molecule 5: DNA polymerase III subunit gamma/tau

Chain O:

11%

29% 31% 13% • 24%

H367 H368 H369 H370 K373 A374 Q378 D379 L380 A381 E382 G383 W384 R385 A386 F387 L388 E389 A390 L391 K392 P393 T394 L395 R396 A397 F398 V399 R400 E401 A402 R403 L406 E407 G408 K409 T410 L411 V412 L413 R414 F415 P416 H422 H423 LYS LYS ALA GLU GLU GLN LYS ALA HIS L433 L434

P435 L436 A437 Q440 F441 G442 V443 E444 E445 L446 A447 F448 V449 L450 E451 K452 K453 S454 L455 S456 GLY ALA SER PRO PRO PRO PRO THR LYS PRO VAL PRO PRO ARG GLU ALA PRO PRO VAL ALA ALA PRO PRO GLU PRO GLU PRO PRO GLU PRO LEU GLU ASP P490 P491 W492 E493 A494 E495

D499 P500 S501 E502 E503 L504 R505 R506 L507 A508 R509 L510 R514 V518 R519 K520 P521 K522 A523 P524 E527 E528 P529 V530 S531 I540 M541 P542 P543

• Molecule 5: DNA polymerase III subunit gamma/tau

Chain P:

12%

25% 32% 14% 6% 22%

H367 H368 K373 A374 G375 E376 A377 Q378 D379 L380 A381 E382 R385 A386 F387 L388 E389 A390 L391 K392 P393 T394 L395 R396 A397 F398 V399 P404 E407 G408 K409 T410 L411 V412 L413 R414 F415 P416 E417 S418 F421 H422 H423 LYS LYS ALA GLU GLU GLN LYS ALA HIS L433 L434 P435

Q440 F441 L446 V449 L450 E451 K452 K453 S454 L455 S456 G457 A458 S459 PRO PRO PRO PRO THR LYS PRO VAL PRO PRO ARG GLU ALA PRO PRO VAL ALA ALA PRO PRO GLU PRO GLU PRO PRO LEU GLU ASP P490 P491 W492 E493 A494 E495 E496 G497 E498 D499 P500 S501 E502

E503 L504 R505 R506 L507 A508 R509 L510 L511 G512 G513 R514 L515 L516 W517 V518 R519 K520 P521 K522 A523 P524 E525 A526 E527 E528 P529 V530 S531 E532 D533 G534 I535 G536 G537 N538 G539 I540 M541 P542 P543

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 188.53Å 94.97Å 204.08Å<br>90.00° 89.97° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.20<br>20.00 – 3.20 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 96.0 (20.00-3.20)<br>96.0 (20.00-3.20) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.04 | Depositor |
| $< I/\sigma(I) >$ [1] | 15.90 (at 3.22Å) | Xtriage |
| Refinement program | REFMAC 5.5.0109 | Depositor |
| R, $R_{free}$ | 0.264 , 0.305<br>0.258 , 0.300 | Depositor<br>DCC |
| $R_{free}$ test set | 5710 reflections (4.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 99.9 | Xtriage |
| Anisotropy | 0.095 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.26 , 77.2 | EDS |
| L-test for twinning[2] | $< |L| > = 0.43, < L^2 > = 0.25$ | Xtriage |
| Estimated twinning fraction | 0.018 for h,-k,-l | Xtriage |
| $F_o,F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 45265 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 151.0 | 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: DOC, 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 | E | 0.31 | 0/462 | 0.78 | 0/710 |
| 1 | G | 0.34 | 0/462 | 0.81 | 1/710 (0.1%) |
| 1 | K | 0.30 | 0/462 | 0.80 | 1/710 (0.1%) |
| 2 | F | 0.31 | 0/456 | 0.88 | 2/702 (0.3%) |
| 2 | H | 0.41 | 0/613 | 0.84 | 1/945 (0.1%) |
| 2 | J | 0.34 | 0/525 | 0.85 | 1/809 (0.1%) |
| 2 | L | 0.38 | 0/547 | 0.80 | 0/843 |
| 3 | I | 0.33 | 0/462 | 0.80 | 1/710 (0.1%) |
| 4 | A | 0.50 | 2/9466 (0.0%) | 0.60 | 5/12781 (0.0%) |
| 4 | B | 0.50 | 1/9480 (0.0%) | 0.61 | 2/12800 (0.0%) |
| 4 | C | 0.51 | 3/9481 (0.0%) | 0.61 | 3/12805 (0.0%) |
| 4 | D | 0.52 | 1/9638 (0.0%) | 0.62 | 10/13019 (0.1%) |
| 5 | M | 0.85 | 7/1133 (0.6%) | 1.06 | 11/1528 (0.7%) |
| 5 | N | 0.63 | 0/1108 | 0.80 | 3/1493 (0.2%) |
| 5 | O | 0.69 | 0/1108 | 0.87 | 5/1493 (0.3%) |
| 5 | P | 0.82 | 2/1123 (0.2%) | 1.05 | 7/1513 (0.5%) |
| All | All | 0.53 | 16/46526 (0.0%) | 0.67 | 53/63571 (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 | 1 |
| 4 | B | 0 | 1 |
| 4 | C | 0 | 3 |
| 4 | D | 0 | 4 |
| 5 | M | 0 | 7 |
| 5 | N | 0 | 1 |
| 5 | O | 0 | 2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|--------------------|--------------------|
| 5 | P | 0 | 7 |
| All | All | 0 | 26 |

The worst 5 of 16 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 5 | P | 543 | PRO | N-CD | 5.93 | 1.56 | 1.47 |
| 5 | M | 524 | PRO | N-CD | 5.75 | 1.55 | 1.47 |
| 5 | M | 416 | PRO | N-CD | 5.70 | 1.55 | 1.47 |
| 4 | A | 31 | TRP | CD2-CE2 | 5.58 | 1.48 | 1.41 |
| 4 | D | 1058 | PRO | N-CD | 5.57 | 1.55 | 1.47 |

The worst 5 of 53 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 4 | B | 212 | ASP | CB-CG-OD1 | 9.95 | 127.25 | 118.30 |
| 2 | F | 24 | DT | P-O3'-C3' | 9.83 | 131.50 | 119.70 |
| 5 | P | 541 | MET | C-N-CD | 8.76 | 146.79 | 128.40 |
| 5 | P | 415 | PHE | C-N-CD | 8.45 | 146.15 | 128.40 |
| 5 | M | 541 | MET | C-N-CD | 8.39 | 146.02 | 128.40 |

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 4 | A | 570 | ARG | Peptide |
| 4 | B | 1084 | ARG | Sidechain |
| 4 | C | 1080 | VAL | Peptide |
| 4 | C | 972 | ARG | Mainchain |
| 4 | C | 974 | GLY | Peptide |

## 5.2 Too-close contacts ⓘ

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 | E | 411 | 0 | 222 | 2 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | G | 411 | 0 | 222 | 5 | 0 |
| 1 | K | 411 | 0 | 222 | 1 | 0 |
| 2 | F | 409 | 0 | 227 | 5 | 0 |
| 2 | H | 551 | 0 | 310 | 4 | 0 |
| 2 | J | 471 | 0 | 262 | 2 | 0 |
| 2 | L | 491 | 0 | 274 | 2 | 0 |
| 3 | I | 429 | 0 | 233 | 5 | 0 |
| 4 | A | 9280 | 0 | 9298 | 227 | 2 |
| 4 | B | 9295 | 0 | 9323 | 298 | 3 |
| 4 | C | 9293 | 0 | 9318 | 274 | 0 |
| 4 | D | 9445 | 0 | 9488 | 387 | 2 |
| 5 | M | 1103 | 0 | 1085 | 176 | 0 |
| 5 | N | 1078 | 0 | 1065 | 134 | 1 |
| 5 | O | 1078 | 0 | 1065 | 143 | 0 |
| 5 | P | 1093 | 0 | 1078 | 208 | 2 |
| 6 | A | 3 | 0 | 0 | 0 | 0 |
| 6 | B | 3 | 0 | 0 | 0 | 0 |
| 6 | C | 3 | 0 | 0 | 0 | 0 |
| 6 | D | 3 | 0 | 0 | 0 | 0 |
| 7 | A | 1 | 0 | 0 | 0 | 0 |
| 7 | B | 1 | 0 | 0 | 0 | 0 |
| 7 | C | 1 | 0 | 0 | 0 | 0 |
| 7 | D | 1 | 0 | 0 | 0 | 0 |
| All | All | 45265 | 0 | 43692 | 1851 | 7 |

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 21.

The worst 5 of 1851 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) |
|--------|--------|--------------------------|-------------------|
| 5:P:528:GLU:CG | 5:P:529:PRO:HD3 | 1.29 | 1.53 |
| 5:O:387:PHE:CE2 | 5:O:441:PHE:CE2 | 2.03 | 1.47 |
| 4:D:1080:VAL:HG11 | 4:D:1082:PHE:CE2 | 1.50 | 1.45 |
| 5:P:523:ALA:CB | 5:P:524:PRO:HA | 1.38 | 1.43 |
| 4:D:1080:VAL:HA | 4:D:1081:VAL:CG2 | 1.47 | 1.41 |

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:175:ASP:OD1 | 5:P:414:ARG:NH1[2_655] | 1.84 | 0.36 |
| 4:A:115:ARG:NE | 4:A:976:VAL:CG1[2_555] | 1.90 | 0.30 |
| 4:A:115:ARG:NH2 | 4:A:976:VAL:CG2[2_555] | 1.95 | 0.25 |
| 4:B:363:GLU:OE2 | 4:B:969:GLU:OE2[1_545] | 2.01 | 0.19 |
| 4:D:160:ASP:N | 5:N:454:SER:OG[1_545] | 2.01 | 0.19 |

## 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 | |
|---|---|---|---|---|---|---|---|
| 4 | A | 1146/1220 (94%) | 1036 (90%) | 87 (8%) | 23 (2%) | 7 | 38 |
| 4 | B | 1147/1220 (94%) | 1051 (92%) | 76 (7%) | 20 (2%) | 9 | 42 |
| 4 | C | 1148/1220 (94%) | 1056 (92%) | 79 (7%) | 13 (1%) | 14 | 51 |
| 4 | D | 1173/1220 (96%) | 1062 (90%) | 94 (8%) | 17 (1%) | 11 | 46 |
| 5 | M | 132/177 (75%) | 84 (64%) | 31 (24%) | 17 (13%) | 0 | 1 |
| 5 | N | 129/177 (73%) | 76 (59%) | 28 (22%) | 25 (19%) | 0 | 0 |
| 5 | O | 129/177 (73%) | 77 (60%) | 28 (22%) | 24 (19%) | 0 | 0 |
| 5 | P | 132/177 (75%) | 80 (61%) | 33 (25%) | 19 (14%) | 0 | 1 |
| All | All | 5136/5588 (92%) | 4522 (88%) | 456 (9%) | 158 (3%) | 4 | 26 |

5 of 158 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | A | 506 | ASP |
| 4 | A | 1081 | VAL |
| 4 | A | 1201 | ASP |
| 4 | A | 1204 | VAL |
| 4 | B | 301 | PRO |

#### 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 | 965/1009 (96%) | 958 (99%) | 7 (1%) | 84 | 94 |
| 4 | B | 968/1009 (96%) | 946 (98%) | 22 (2%) | 50 | 78 |
| 4 | C | 968/1009 (96%) | 949 (98%) | 19 (2%) | 55 | 80 |
| 4 | D | 984/1009 (98%) | 961 (98%) | 23 (2%) | 50 | 78 |
| 5 | M | 112/144 (78%) | 102 (91%) | 10 (9%) | 9 | 35 |
| 5 | N | 109/144 (76%) | 104 (95%) | 5 (5%) | 27 | 63 |
| 5 | O | 109/144 (76%) | 97 (89%) | 12 (11%) | 6 | 26 |
| 5 | P | 110/144 (76%) | 89 (81%) | 21 (19%) | 1 | 8 |
| All | All | 4325/4612 (94%) | 4206 (97%) | 119 (3%) | 43 | 74 |

5 of 119 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 976 | VAL |
| 5 | P | 522 | LYS |
| 5 | M | 395 | LEU |
| 5 | P | 520 | LYS |
| 5 | P | 543 | PRO |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 411 | ASN |
| 4 | D | 799 | ASN |
| 5 | O | 369 | HIS |
| 4 | D | 540 | GLN |
| 4 | D | 896 | ASN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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 | $\#|Z| > 2$ |
| 3 | DOC | I | 21 | 3,2 | 16,19,20 | 1.02 | 1 (6%) | 20,26,29 | 1.37 | 4 (20%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 3 | DOC | I | 21 | 3,2 | - | 1/7/18/19 | 0/2/2/2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 3 | I | 21 | DOC | C6-C5 | 2.16 | 1.40 | 1.35 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 3 | I | 21 | DOC | C3'-C2'-C1' | 2.96 | 106.20 | 102.78 |
| 3 | I | 21 | DOC | O4'-C1'-N1 | 2.44 | 112.22 | 107.86 |
| 3 | I | 21 | DOC | O4'-C4'-C3' | 2.35 | 108.71 | 104.80 |
| 3 | I | 21 | DOC | O2-C2-N3 | -2.28 | 118.62 | 122.33 |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 3 | I | 21 | DOC | C3'-C4'-C5'-O5' |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | I | 21 | DOC | 1 | 0 |

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 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 ⓘ

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 | E | 20/20 (100%) | 0.86 | 1 (5%) | 28 | 16 | 159, 177, 203, 209 | 0 |
| 1 | G | 20/20 (100%) | 0.82 | 3 (15%) | 2 | 1 | 160, 175, 204, 216 | 0 |
| 1 | K | 20/20 (100%) | 0.94 | 3 (15%) | 2 | 1 | 157, 168, 206, 213 | 0 |
| 2 | F | 20/28 (71%) | 1.38 | 5 (25%) | 0 | 0 | 165, 187, 208, 217 | 0 |
| 2 | H | 27/28 (96%) | 1.25 | 7 (25%) | 0 | 0 | 145, 168, 184, 186 | 0 |
| 2 | J | 23/28 (82%) | 1.60 | 8 (34%) | 0 | 0 | 148, 171, 192, 201 | 0 |
| 2 | L | 24/28 (85%) | 1.41 | 4 (16%) | 1 | 1 | 150, 176, 197, 204 | 0 |
| 3 | I | 20/21 (95%) | 1.42 | 5 (25%) | 0 | 0 | 198, 224, 252, 255 | 0 |
| 4 | A | 1164/1220 (95%) | 0.19 | 50 (4%) | 35 | 22 | 109, 140, 177, 212 | 0 |
| 4 | B | 1167/1220 (95%) | 0.21 | 48 (4%) | 37 | 24 | 107, 140, 174, 218 | 0 |
| 4 | C | 1166/1220 (95%) | 0.22 | 46 (3%) | 39 | 25 | 108, 148, 176, 203 | 0 |
| 4 | D | 1185/1220 (97%) | 0.16 | 39 (3%) | 46 | 30 | 111, 145, 175, 230 | 0 |
| 5 | M | 138/177 (77%) | 1.09 | 30 (21%) | 0 | 0 | 159, 176, 196, 209 | 0 |
| 5 | N | 135/177 (76%) | 0.87 | 14 (10%) | 6 | 4 | 143, 169, 187, 203 | 0 |
| 5 | O | 135/177 (76%) | 1.03 | 19 (14%) | 2 | 2 | 155, 181, 206, 227 | 0 |
| 5 | P | 138/177 (77%) | 0.95 | 22 (15%) | 1 | 1 | 139, 177, 202, 226 | 0 |
| All | All | 5402/5781 (93%) | 0.31 | 304 (5%) | 24 | 13 | 107, 147, 186, 255 | 0 |

The worst 5 of 304 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | P | 446 | LEU | 9.6 |
| 4 | D | 714 | GLY | 6.0 |
| 4 | D | 1087 | GLU | 5.8 |
| 4 | D | 978 | LEU | 5.4 |
| 4 | B | 1085 | ALA | 5.3 |

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

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($\text{Å}^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|-------------------------|-------|
| 3 | DOC | I | 21 | 18/19 | 0.77 | 0.44 | 173,185,229,232 | 0 |

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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($\text{Å}^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|-------------------------|-------|
| 6 | ZN | C | 1301 | 1/1 | 0.76 | 0.14 | 197,197,197,197 | 0 |
| 7 | MG | C | 1304 | 1/1 | 0.79 | 0.07 | 177,177,177,177 | 0 |
| 6 | ZN | D | 1302 | 1/1 | 0.83 | 0.16 | 159,159,159,159 | 0 |
| 6 | ZN | C | 1303 | 1/1 | 0.83 | 0.20 | 179,179,179,179 | 0 |
| 7 | MG | B | 1304 | 1/1 | 0.84 | 0.27 | 132,132,132,132 | 0 |
| 6 | ZN | A | 1302 | 1/1 | 0.85 | 0.20 | 168,168,168,168 | 0 |
| 7 | MG | A | 1304 | 1/1 | 0.85 | 0.17 | 156,156,156,156 | 0 |
| 6 | ZN | B | 1302 | 1/1 | 0.88 | 0.15 | 141,141,141,141 | 0 |
| 6 | ZN | C | 1302 | 1/1 | 0.89 | 0.11 | 158,158,158,158 | 0 |
| 6 | ZN | B | 1303 | 1/1 | 0.90 | 0.21 | 166,166,166,166 | 0 |
| 6 | ZN | D | 1303 | 1/1 | 0.91 | 0.14 | 176,176,176,176 | 0 |
| 6 | ZN | A | 1301 | 1/1 | 0.91 | 0.17 | 187,187,187,187 | 0 |
| 6 | ZN | D | 1301 | 1/1 | 0.93 | 0.11 | 233,233,233,233 | 0 |
| 6 | ZN | A | 1303 | 1/1 | 0.94 | 0.10 | 141,141,141,141 | 0 |
| 6 | ZN | B | 1301 | 1/1 | 0.95 | 0.14 | 163,163,163,163 | 0 |
| 7 | MG | D | 1304 | 1/1 | 0.95 | 0.28 | 139,139,139,139 | 0 |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.