



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:19 AM GMT

PDB ID : 3DXJ
Title : Crystal structure of thermus thermophilus rna polymerase holoenzyme in complex with the antibiotic myxopyronin
Authors : Das, K.; Arnold, E.
Deposited on : 2008-07-24
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

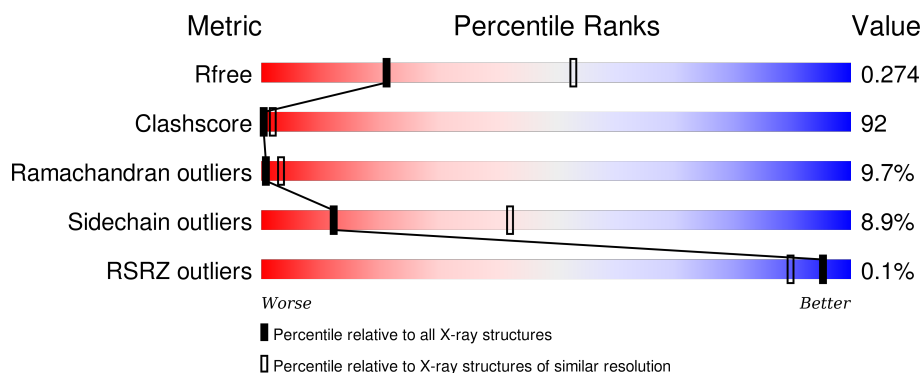
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



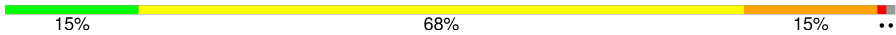
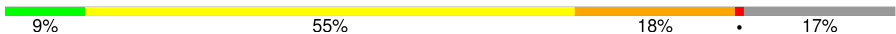
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1578 (3.00-3.00) |
| Clashscore | 102246 | 1912 (3.00-3.00) |
| Ramachandran outliers | 100387 | 1853 (3.00-3.00) |
| Sidechain outliers | 100360 | 1856 (3.00-3.00) |
| RSRZ outliers | 91569 | 1592 (3.00-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 315 | |
| 1 | B | 315 | |
| 1 | K | 315 | |
| 1 | L | 315 | |
| 2 | C | 1119 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | M | 1119 |  |
| 3 | D | 1524 |  |
| 3 | N | 1524 |  |
| 4 | E | 99 |  |
| 4 | O | 99 |  |
| 5 | F | 423 |  |
| 5 | P | 423 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 8 | ZN | D | 1525 | - | - | - | X |
| 8 | ZN | D | 1526 | - | - | - | X |
| 8 | ZN | N | 1525 | - | - | - | X |
| 9 | NE6 | D | 1529 | X | - | - | - |
| 9 | NE6 | N | 1528 | X | - | - | X |

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 56149 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1816 | 1159 | 315 | 339 | 3 | | | |
| 1 | B | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1902 | 1212 | 328 | 359 | 3 | | | |
| 1 | K | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1816 | 1159 | 315 | 339 | 3 | | | |
| 1 | L | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1902 | 1212 | 328 | 359 | 3 | | | |

- Molecule 2 is a protein called BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M.

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

- Molecule 3 is a protein called BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N.

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

- Molecule 4 is a protein called BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O.

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

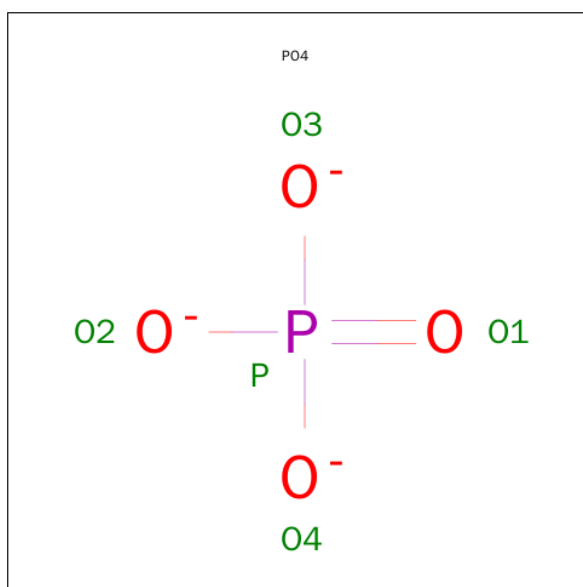
There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|------------|
| E | 61 | GLU | VAL | VARIANT | UNP Q8RQE7 |
| E | 92 | ILE | LEU | VARIANT | UNP Q8RQE7 |
| E | 95 | GLY | VAL | VARIANT | UNP Q8RQE7 |
| O | 61 | GLU | VAL | VARIANT | UNP Q8RQE7 |
| O | 92 | ILE | LEU | VARIANT | UNP Q8RQE7 |
| O | 95 | GLY | VAL | VARIANT | UNP Q8RQE7 |

- Molecule 5 is a protein called RNA polymerase principal sigma factor (RpoD); CHAIN F, P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | F | 349 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2829 | 1785 | 513 | 527 | 4 | | | |
| 5 | P | 349 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2829 | 1785 | 513 | 527 | 4 | | | |

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6 | A | 1 | Total O P 5 4 1 | 0 | 0 |
| 6 | D | 1 | Total O P 5 4 1 | 0 | 0 |

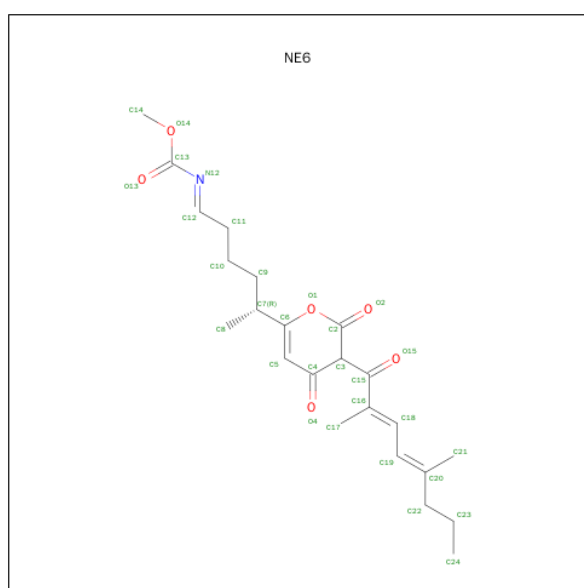
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

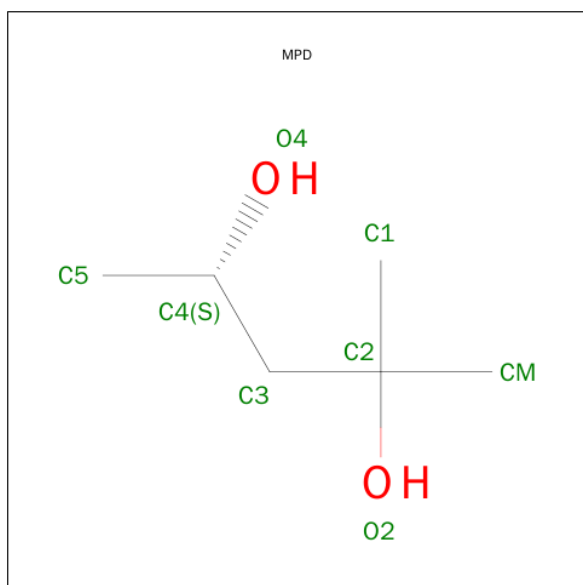
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8 | D | 2 | Total Zn 2 2 | 0 | 0 |
| 8 | N | 2 | Total Zn 2 2 | 0 | 0 |

- Molecule 9 is METHYL [(1E,5R)-5-{(3S)-3-[(2E,4E)-2,5-DIMETHYLOCTA-2,4-DIENOYL]-2,4-DIOXO-3,4-DIHYDRO-2H-PYRAN-6-YL}HEXYLIDENE]CARBAMATE (three-letter code: NE6) (formula: C₂₃H₃₁NO₆).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 9 | D | 1 | Total | C | N | O | 0 | 0 |
| | | | 30 | 23 | 1 | 6 | | |
| 9 | N | 1 | Total | C | N | O | 0 | 0 |
| | | | 30 | 23 | 1 | 6 | | |

- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10 | C | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 10 | C | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 10 | M | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 11 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11 | A | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 11 | B | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 11 | C | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 11 | D | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |

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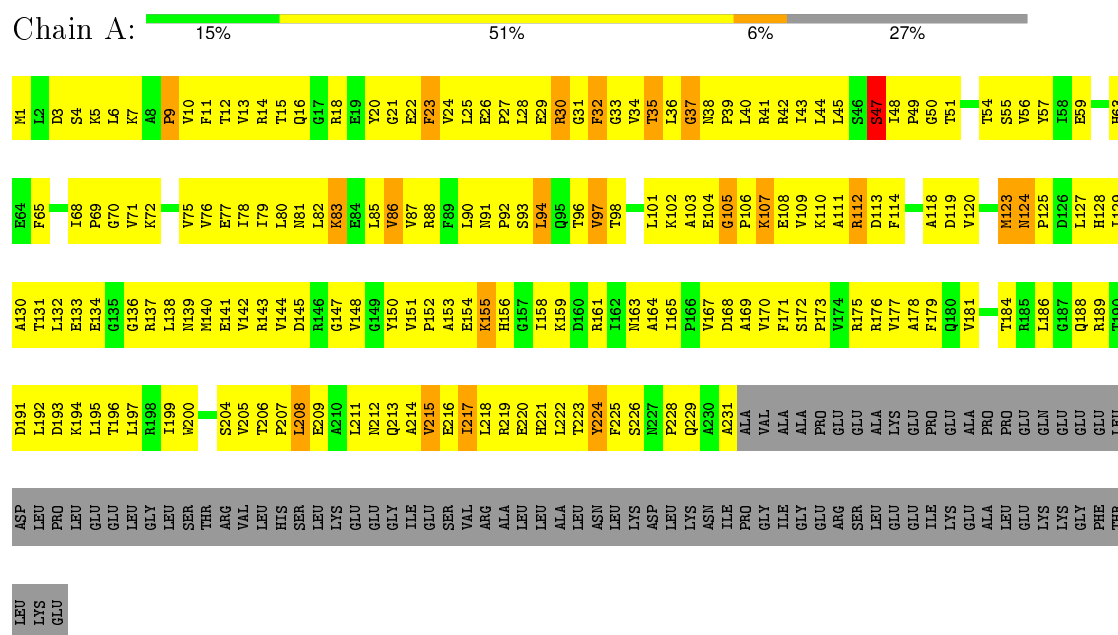
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 11 | F | 1 | Total 1 | O 1 | 0 | 0 |
| 11 | M | 5 | Total 5 | O 5 | 0 | 0 |
| 11 | N | 4 | Total 4 | O 4 | 0 | 0 |
| 11 | O | 1 | Total 1 | O 1 | 0 | 0 |

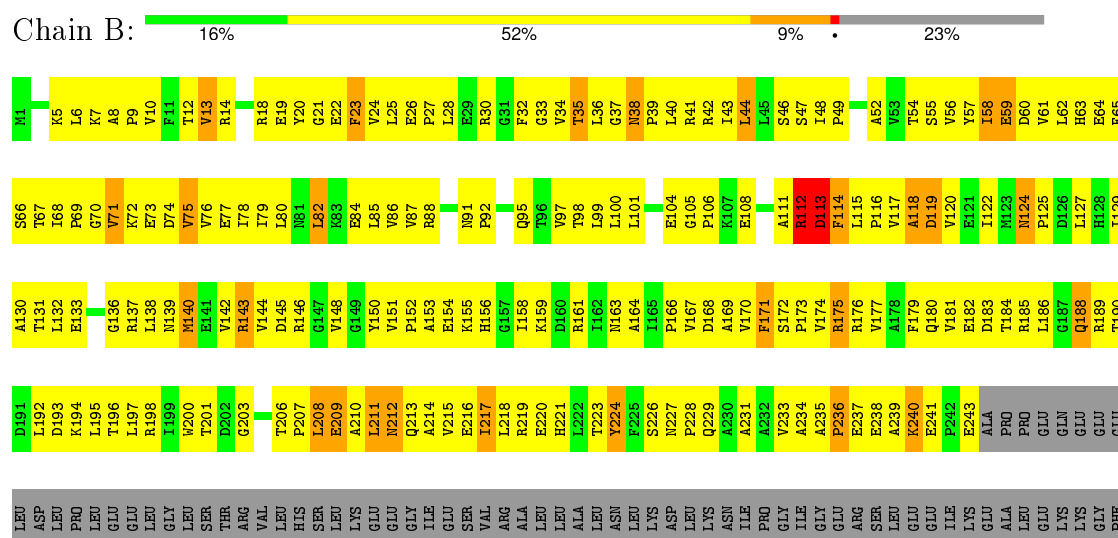
3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L



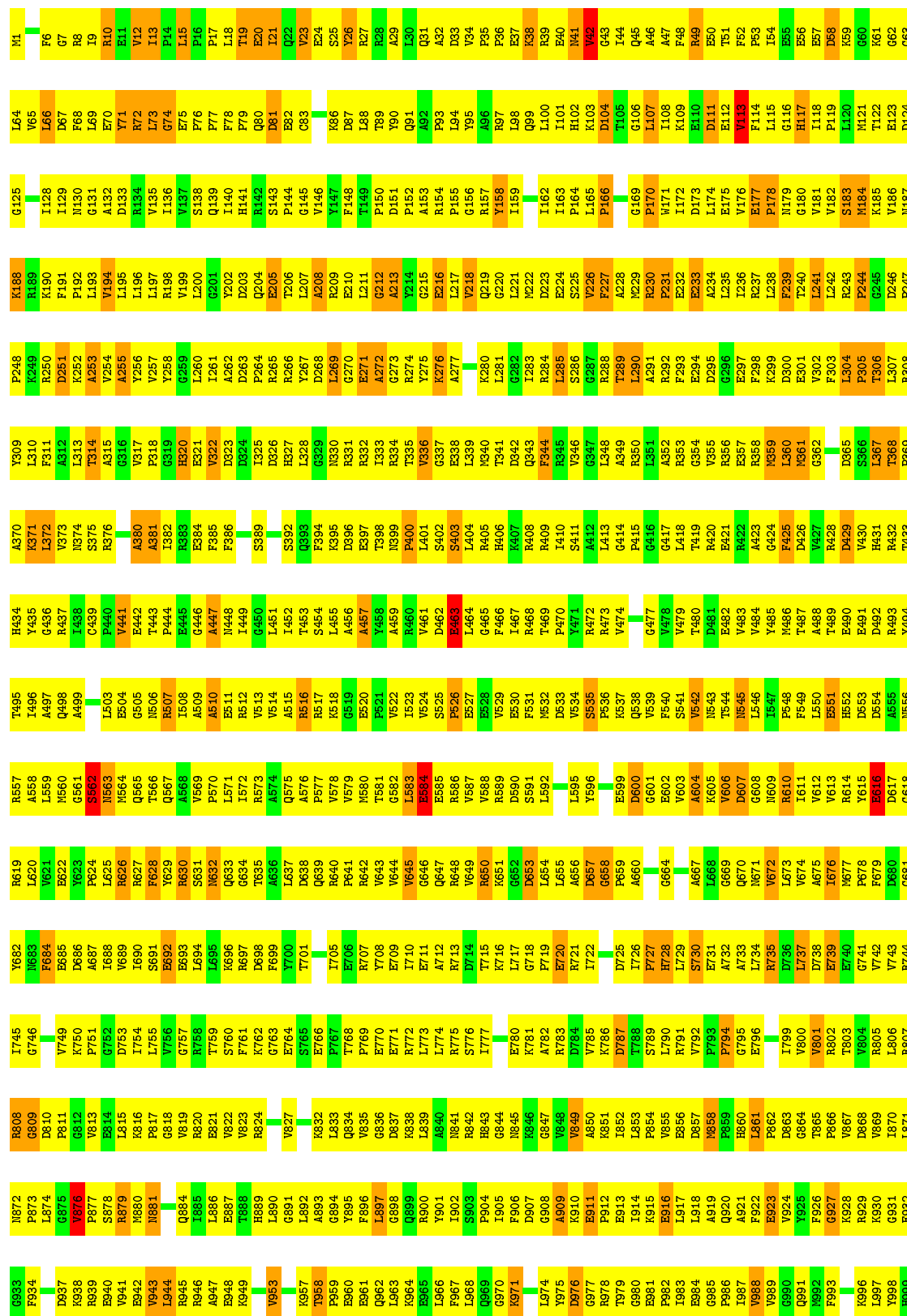
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L



| | | | | | | | | | | | | | | | | | |
|-------|------|-------|-------|------|-------|------|------|------|------|------|------|------|------|------|------|------|-----|
| H1064 | K938 | V1001 | H1066 | K939 | E1002 | V143 | D880 | G618 | A555 | R493 | R432 | L372 | L310 | P248 | N187 | D124 | G62 |
| A1065 | R939 | E1002 | A1065 | R939 | E1002 | | G681 | R619 | M556 | R494 | T433 | V373 | F311 | K249 | K188 | | G63 |
| A1066 | E940 | D1003 | E1067 | R940 | E1003 | A747 | N683 | E622 | A557 | T495 | H434 | N374 | A312 | R250 | R189 | F127 | L64 |
| E1068 | E941 | K1004 | E1068 | R941 | E1004 | E748 | N683 | E622 | A558 | T495 | H434 | N374 | A312 | D251 | K190 | | V65 |
| A1069 | E942 | M1005 | E1069 | R942 | M1005 | E749 | E685 | E624 | L559 | A497 | G436 | R376 | T314 | F191 | F191 | I129 | L66 |
| L1070 | L944 | M1006 | L1070 | L944 | M1006 | K750 | E686 | L625 | M560 | A499 | R437 | P377 | A315 | A253 | P192 | M130 | D67 |
| L1071 | L945 | M1007 | L1071 | L945 | M1007 | P751 | D686 | L625 | M560 | A499 | L438 | L378 | G316 | V254 | L193 | G131 | F68 |
| K1072 | R946 | S1009 | K1072 | R946 | S1009 | G752 | A687 | R626 | M564 | M500 | C439 | E379 | F317 | | L194 | A132 | L69 |
| E1073 | R947 | T1010 | E1073 | R947 | T1010 | D753 | G688 | R627 | Q565 | T501 | P440 | A380 | F318 | V257 | L195 | A132 | E70 |
| E1074 | R948 | E1011 | E1074 | R948 | E1011 | L754 | G689 | F628 | T566 | F502 | V441 | A381 | | G259 | L196 | R134 | R71 |
| P1075 | R949 | P1012 | P1075 | R949 | P1012 | L755 | G690 | E629 | V569 | L503 | E442 | L382 | E321 | L260 | L197 | V135 | R72 |
| V1076 | T888 | V1013 | V1076 | T888 | V1013 | G757 | E692 | R630 | P570 | E504 | T443 | R363 | V322 | L261 | L198 | I136 | L73 |
| P1077 | T888 | S1014 | P1077 | T888 | S1014 | G758 | E693 | R631 | P570 | E505 | R364 | R364 | D323 | L261 | L199 | V137 | G74 |
| L1078 | T889 | E1015 | L1078 | T889 | E1015 | R759 | E694 | R632 | L571 | M506 | P444 | F365 | G324 | A262 | L200 | S138 | E75 |
| P1079 | T890 | E1016 | P1079 | T890 | E1016 | G760 | E695 | R633 | L572 | R507 | G447 | F366 | I325 | D263 | Y202 | Q139 | P77 |
| P1082 | T891 | T1017 | P1082 | T891 | T1017 | F761 | G696 | T635 | A574 | F508 | A447 | F366 | I326 | P264 | Y202 | H141 | F78 |
| E1083 | T892 | Q1018 | E1083 | T892 | Q1018 | G762 | G697 | T636 | A575 | F509 | L449 | S369 | L328 | R266 | Q204 | R142 | P79 |
| S1084 | T893 | E1019 | S1084 | T893 | E1019 | G763 | G698 | L637 | A576 | F510 | G450 | Q390 | G329 | Y267 | E205 | S143 | O80 |
| F1085 | T894 | E1020 | F1085 | T894 | E1020 | E764 | G699 | L638 | P577 | F511 | L451 | L391 | R330 | D268 | E206 | S144 | D81 |
| R1086 | T895 | E1021 | R1086 | T895 | E1021 | G765 | G700 | L639 | P578 | F512 | L452 | L392 | R331 | L269 | L207 | G145 | E82 |
| V1087 | T896 | E1022 | V1087 | T896 | E1022 | E766 | G701 | L640 | V579 | F513 | T453 | Q393 | R332 | G270 | A208 | F148 | R84 |
| L1088 | T897 | E1023 | L1088 | T897 | E1023 | E767 | G702 | P641 | M580 | F514 | S454 | F394 | R333 | E271 | R209 | | |
| V1089 | T898 | E1024 | V1089 | T898 | E1024 | E768 | H704 | R642 | T581 | F515 | L455 | K395 | R334 | A272 | G210 | G273 | |
| E1090 | T899 | E1025 | E1090 | T899 | E1025 | E769 | H705 | R643 | T582 | F516 | L456 | K396 | R335 | G274 | L211 | G273 | |
| E1091 | T900 | E1026 | E1091 | T900 | E1026 | E770 | H706 | R644 | L583 | G519 | A457 | S403 | R336 | R274 | E205 | S145 | |
| E1092 | T901 | E1027 | E1092 | T901 | E1027 | E771 | H707 | R645 | E584 | E520 | T458 | L404 | G337 | Y275 | E206 | P144 | |
| E1093 | T902 | E1028 | E1093 | T902 | E1028 | E772 | H708 | R646 | E585 | E521 | T459 | R405 | G338 | Y276 | E207 | P145 | |
| E1094 | T903 | E1029 | E1094 | T903 | E1029 | E773 | H709 | R647 | E586 | E522 | T460 | R406 | G339 | A277 | E208 | A152 | |
| E1095 | T904 | E1030 | E1095 | T904 | E1030 | E774 | H710 | R648 | E587 | E523 | T461 | R407 | G340 | E278 | E209 | R154 | |
| E1096 | T905 | E1031 | E1096 | T905 | E1031 | E775 | H711 | R649 | E588 | E524 | T462 | R408 | G341 | E279 | E210 | P155 | |
| E1097 | T906 | E1032 | E1097 | T906 | E1032 | E776 | H712 | R650 | E589 | E525 | T463 | S402 | G342 | K280 | Q219 | R156 | |
| E1098 | T907 | E1033 | E1098 | T907 | E1033 | E777 | H713 | R651 | E590 | E526 | T464 | L403 | G343 | L281 | G220 | E158 | |
| E1099 | T908 | E1034 | E1099 | T908 | E1034 | E778 | H714 | R652 | E591 | E527 | T465 | R405 | G344 | G282 | E221 | I159 | |
| E1100 | T909 | E1035 | E1100 | T909 | E1035 | E779 | H715 | R653 | E592 | E528 | T466 | R406 | G345 | L283 | E222 | | |
| E1101 | T910 | E1036 | E1101 | T910 | E1036 | E780 | H716 | R654 | E593 | E529 | T467 | R407 | G346 | R284 | D223 | I162 | |
| E1102 | T911 | E1037 | E1102 | T911 | E1037 | E781 | H717 | R655 | E594 | E530 | T468 | R408 | G347 | E224 | E224 | I163 | |
| E1103 | T912 | E1038 | E1103 | T912 | E1038 | E782 | H718 | R656 | E595 | E531 | T469 | R409 | G348 | S286 | S225 | P164 | |
| E1104 | T913 | E1039 | E1104 | T913 | E1039 | E783 | H719 | R657 | E596 | E532 | T470 | I410 | A349 | G287 | V226 | L165 | |
| E1105 | T914 | E1040 | E1105 | T914 | E1040 | E784 | H720 | R658 | E597 | E533 | T471 | S411 | R350 | R289 | E227 | P166 | |
| E1106 | T915 | E1041 | E1106 | T915 | E1041 | E785 | H721 | R659 | E598 | E534 | T472 | L413 | A352 | L290 | E228 | R167 | |
| E1107 | T916 | E1042 | E1107 | T916 | E1042 | E786 | H722 | R660 | E599 | E535 | T473 | L414 | A353 | L291 | E229 | R168 | |
| E1108 | T917 | E1043 | E1108 | T917 | E1043 | E787 | H723 | R661 | E600 | E536 | T474 | G415 | R354 | A291 | R230 | P170 | |
| E1109 | T918 | E1044 | E1109 | T918 | E1044 | E788 | H724 | R662 | E601 | E537 | T475 | G416 | G352 | R292 | P231 | L171 | |
| E1110 | T919 | E1045 | E1110 | T919 | E1045 | E789 | H725 | R663 | E602 | E538 | T476 | G417 | G353 | F293 | E232 | I172 | |
| E1111 | T920 | E1046 | E1111 | T920 | E1046 | E790 | H726 | R664 | E603 | E539 | T477 | G418 | R354 | E294 | E233 | K109 | |
| E1112 | T921 | E1047 | E1112 | T921 | E1047 | E791 | H727 | R665 | E604 | F540 | T478 | L418 | R355 | D295 | L234 | D173 | |
| E1113 | T922 | E1048 | E1113 | T922 | E1048 | E792 | H728 | R666 | E605 | S541 | T480 | T419 | R356 | G296 | L235 | L174 | |
| E1114 | T923 | E1049 | E1114 | T923 | E1049 | E793 | H729 | R667 | E606 | F542 | T481 | R420 | R357 | E297 | L236 | E175 | |
| E1115 | T924 | E1050 | E1115 | T924 | E1050 | E794 | H730 | R668 | E607 | E543 | T482 | E421 | L360 | E298 | R237 | V176 | |
| E1116 | T925 | E1051 | E1116 | T925 | E1051 | E795 | H731 | R669 | E608 | E544 | T483 | R422 | G361 | D300 | L238 | E177 | |
| E1117 | T926 | E1052 | E1117 | T926 | E1052 | E796 | H732 | R670 | E609 | E545 | T484 | A423 | G362 | E301 | F239 | F178 | |
| E1118 | T927 | E1053 | E1118 | T927 | E1053 | E797 | H733 | R671 | E610 | E546 | T485 | G424 | S363 | F302 | T240 | G116 | |
| E1119 | T928 | E1054 | E1119 | T928 | E1054 | E798 | H734 | R672 | E611 | E547 | T486 | F425 | S364 | F303 | L241 | G180 | |
| E1120 | T929 | E1055 | E1120 | T929 | E1055 | E799 | H735 | R673 | E612 | E548 | T487 | D426 | S365 | F304 | L242 | V181 | |
| E1121 | T930 | E1056 | E1121 | T930 | E1056 | E800 | H736 | R674 | E613 | E549 | T488 | V427 | S366 | F305 | L243 | V182 | |
| E1122 | T931 | E1057 | E1122 | T931 | E1057 | E801 | H737 | R675 | E614 | E550 | T489 | R428 | S367 | P306 | R244 | S183 | |
| E1123 | T932 | E1058 | E1123 | T932 | E1058 | E802 | H738 | R676 | E615 | E551 | T490 | R429 | G368 | L307 | G245 | M184 | |
| E1124 | T933 | E1059 | E1124 | T933 | E1059 | E803 | H739 | R677 | E616 | E552 | T491 | R430 | G369 | L308 | D246 | K185 | |
| E1125 | T934 | E1060 | E1125 | T934 | E1060 | E804 | H740 | R678 | E617 | E553 | T492 | R431 | G370 | L309 | Y309 | V186 | |
| E1126 | T935 | E1061 | E1126 | T935 | E1061 | E805 | H741 | R679 | E618 | E554 | T493 | R432 | G371 | Y310 | | | |
| E1127 | T936 | E1062 | E1127 | T936 | E1062 | E806 | H742 | R680 | E619 | E555 | T494 | R433 | G372 | Y311 | | | |
| E1128 | T937 | E1063 | E1128 | T937 | E1063 | E807 | H743 | R681 | E620 | E556 | T495 | R434 | G373 | Y312 | | | |
| E1129 | T938 | E1064 | E1129 | T938 | E1064 | E808 | H744 | R682 | E621 | E557 | T496 | R435 | G374 | Y313 | | | |
| E1130 | T939 | E1065 | E1130 | T939 | E1065 | E809 | H745 | R683 | E622 | E558 | T497 | R436 | G375 | Y314 | | | |
| E1131 | T940 | E1066 | E1131 | T940 | E1066 | E810 | H746 | R684 | E623 | E559 | T498 | R437 | G376 | Y315 | | | |
| E1132 | T941 | E1067 | E1132 | T941 | E1067 | E811 | H747 | R685 | E624 | E560 | T499 | R438 | G377 | Y316 | | | |
| E1133 | T942 | E1068 | E1133 | T942 | E1068 | E812 | H748 | R686 | E625 | E561 | T500 | R439 | G378 | Y317 | | | |
| E1134 | T943 | E1069 | E1134 | T943 | E1069 | E813 | H749 | R687 | E626 | E562 | T501 | R440 | G379 | Y318 | | | |
| E1135 | T944 | E1070 | E1135 | T944 | E1070 | E814 | H750 | R688 | E627 | E563 | T502 | R441 | G380 | Y319 | | | |
| E1136 | T945 | E1071 | E1136 | T945 | E1071 | E815 | H751 | R689 | E628 | E564 | T503 | R442 | G381 | Y320 | | | |
| E1137 | T946 | E1072 | E1137 | T946 | E1072 | E816 | H752 | R690 | E629 | E565 | T504 | R443 | G382 | Y321 | | | |
| E1138 | T947 | E1073 | E1138 | T947 | E1073 | E817 | H753 | R691 | E630 | E566 | T505 | R444 | G383 | Y322 | | | |
| E1139 | T948 | E1074 | E1139 | T948 | E1074 | E818 | H754 | R692 | E631 | E567 | T506 | R445 | G384 | Y323 | | | |
| E1140 | T949 | E1075 | E1140 | T949 | E1075 | E819 | H755 | R693 | E632 | E568 | T507 | R446 | G385 | Y324 | | | |
| E1141 | T950 | E1076 | E1141 | T950 | E1076 | E820 | H756 | R694 | E633 | E569 | T508 | R447 | G386 | Y325 | | | |
| E1142 | T951 | E1077 | E1142 | T951 | E1077 | E821 | H757 | R695 | E634 | E570 | T509 | R448 | G387 | Y326 | | | |
| E1143 | T952 | E1078 | E1143 | T952 | E1078 | E822 | H758 | R696 | E635 | E571 | T510 | R449 | G388 | Y327 | | | |
| E1144 | T953 | E1079 | E1144 | T953 | E1079 | E823 | H759 | R697 | E636 | E572 | T511 | R450 | G389 | Y328 | | | |
| E1145 | T954 | E1080 | E1145 | T954 | E1080 | E824 | H760 | R698 | E637 | E573 | T512 | R451 | G390 | Y329 | | | |
| E1146 | T955 | E1081 | E1146 | T955 | E1081 | E825 | H761 | R699 | E638 | E574 | T513 | R452 | G391 | Y330 | | | |
| E1147 | T956 | E1082 | E1147 | T956 | E1082 | E826 | H762 | R700 | E639 | E575 | T514 | R453 | G392 | Y331 | | | |
| E1148 | T957 | E1083 | E1148 | T957 | E1083 | E827 | H763 | R701 | E640 | E576 | T515 | R454 | G393 | Y332 | | | |
| E1149 | T958 | E1084 | E1149 | T958 | E1084 | E828 | | | | | | | | | | | |

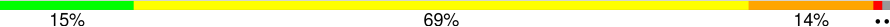
● Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M

Chain M:  17% 69% 13%



| | | | |
|-------|-------|-------|-------|
| M1000 | G1062 | Q1026 | A1045 |
| V1001 | R1063 | F1027 | A1046 |
| E1002 | M1064 | G1028 | A1047 |
| D1003 | A1065 | G1029 | M1047 |
| K1004 | A1066 | K1090 | T1048 |
| M1005 | Y1067 | E1091 | L1049 |
| H1006 | E1068 | L1097 | V1109 |
| A1007 | A1069 | D1098 | Q1050 |
| L1008 | I1070 | V1037 | E1051 |
| S1009 | K1071 | Q1032 | M1052 |
| T1010 | K1072 | G1033 | L1053 |
| K1011 | G1073 | A1094 | T1054 |
| P1012 | E1074 | L1095 | L1055 |
| G1013 | D1075 | M1035 | K1056 |
| L1014 | P1077 | L1097 | S1057 |
| I1016 | E1078 | E1036 | D1058 |
| T1017 | P1079 | V1037 | D1059 |
| Q1018 | S1080 | V1099 | I1060 |
| Q1019 | V1081 | Q1100 | E1061 |
| P1020 | P1082 | T1101 | L1041 |
| L1021 | E1083 | L1102 | D1103 |
| G1022 | S1084 | R41 | A1042 |
| G1023 | F1085 | D1103 | E1104 |
| | R1086 | E1104 | A1045 |
| | V1087 | K1105 | A1046 |
| | L1088 | M1107 | T1048 |
| | V1089 | P1108 | L1049 |
| | K1090 | V1109 | Q1050 |
| | E1091 | D1110 | E1051 |
| | L1092 | S1111 | M1052 |
| | Q1093 | F1112 | L1053 |
| | A1094 | E1113 | T1054 |
| | L1095 | G1114 | L1055 |
| | M1035 | L1115 | K1056 |
| | L1097 | A1116 | S1057 |
| | D1098 | V1117 | D1058 |
| | V1037 | K1118 | D1059 |
| | V1099 | R1119 | I1060 |
| | Q1100 | | E1061 |
| | T1101 | | |
| | L1102 | | |
| | R41 | | |
| | D1103 | | |
| | E1104 | | |
| | A1042 | | |
| | E1104 | | |
| | K1105 | | |
| | M1107 | | |
| | P1108 | | |
| | V1109 | | |
| | D1110 | | |
| | S1111 | | |
| | F1112 | | |
| | E1113 | | |
| | G1114 | | |
| | L1115 | | |
| | A1116 | | |
| | V1117 | | |
| | K1118 | | |
| | R1119 | | |

• Molecule 3: BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N

Chain D:  15% 69% 14% ..

| | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| WET | G61 | T121 | E183 | E247 | K308 | L371 | R434 | K494 | L554 | R615 | R675 | J737 | K799 |
| R2 | K62 | E122 | E184 | F248 | G309 | D372 | V435 | R495 | K555 | Q616 | M676 | A738 | K800 |
| K3 | Y63 | E123 | V185 | L249 | L310 | P373 | E436 | L496 | K556 | R617 | L677 | A739 | G801 |
| E4 | K64 | E124 | V186 | L250 | L311 | E374 | E437 | E497 | L557 | L618 | E678 | F740 | A802 |
| V5 | R65 | Q125 | K187 | F251 | M313 | E375 | D438 | V498 | L558 | L619 | R679 | D741 | G803 |
| R6 | Q66 | V126 | K188 | R252 | R314 | E376 | L439 | V499 | A559 | G620 | Q680 | G742 | L804 |
| K7 | R67 | L127 | K189 | A253 | R315 | V677 | V440 | R500 | Q560 | K621 | R681 | D743 | E805 |
| L8 | F68 | Y128 | E190 | E254 | Q316 | L378 | R441 | A501 | G561 | K622 | D682 | Q744 | F806 |
| R9 | E69 | F129 | L191 | E255 | V317 | E380 | M442 | F502 | A562 | G623 | L683 | Q745 | A807 |
| I10 | K71 | K130 | A192 | G257 | R318 | E381 | V444 | D504 | P563 | E624 | K684 | A746 | T808 |
| A11 | K72 | K131 | P193 | G258 | R319 | E382 | V445 | S505 | E564 | G625 | D685 | V747 | P809 |
| L12 | V72 | Y132 | G194 | V259 | R320 | V384 | R446 | G506 | I565 | S626 | E686 | H748 | E810 |
| E13 | C73 | E133 | V195 | E260 | V322 | R386 | V447 | R507 | I566 | G627 | V687 | V749 | E811 |
| S14 | E74 | V134 | R198 | L261 | E323 | L387 | E448 | R508 | E567 | R628 | M688 | F750 | A812 |
| P15 | C76 | L135 | L199 | K262 | A324 | E388 | S449 | P509 | R568 | S629 | D689 | L751 | L813 |
| E16 | C77 | D136 | D200 | E263 | E325 | E389 | Y450 | E510 | M569 | Q630 | A690 | S752 | A814 |
| G77 | K17 | P137 | D201 | E264 | E326 | E390 | D451 | M511 | E570 | I631 | L691 | S753 | A815 |
| T18 | V78 | K138 | P208 | L264 | E327 | P390 | D452 | M512 | E571 | G632 | E592 | F754 | H816 |
| R19 | E79 | G139 | R209 | E265 | E328 | A391 | I453 | M513 | R572 | V633 | E593 | A755 | E817 |
| S20 | V80 | A140 | L204 | E266 | G329 | S392 | D454 | L514 | M573 | Q634 | V694 | Q756 | L818 |
| E21 | T81 | I141 | Y205 | G267 | T330 | L394 | R455 | E515 | L574 | P635 | L695 | A757 | G819 |
| S22 | K82 | L142 | R206 | F269 | V331 | V395 | M456 | A516 | Q575 | Q636 | H696 | E758 | E820 |
| S83 | S83 | J143 | F207 | F269 | V332 | V396 | G457 | A517 | E576 | L637 | E697 | A759 | V821 |
| G24 | I84 | G144 | P208 | L270 | Y332 | V397 | D458 | V517 | E577 | K638 | K698 | R760 | A822 |
| E85 | V85 | V145 | R209 | V271 | L333 | K397 | E459 | P518 | V578 | L639 | V699 | I761 | L823 |
| E25 | R86 | P146 | R210 | L272 | T334 | A398 | E460 | V519 | D579 | H640 | V700 | H762 | H824 |
| V26 | R87 | V147 | V211 | R273 | L335 | R399 | I461 | L520 | A580 | Q641 | L701 | L764 | A825 |
| E27 | Y88 | E148 | R212 | R274 | F336 | V400 | E462 | P521 | L581 | C642 | L702 | S765 | P826 |
| K28 | R89 | K149 | R213 | E213 | L337 | E401 | Q463 | P522 | L582 | G643 | N703 | A766 | L827 |
| F29 | E90 | K150 | E214 | E214 | E338 | P402 | Q464 | D583 | L583 | L644 | R704 | H767 | K828 |
| N90 | N90 | R150 | G215 | E215 | E339 | F403 | L464 | L524 | M584 | P645 | A705 | N768 | V829 |
| G91 | T31 | Q151 | Y215 | E216 | K339 | E404 | L465 | R525 | G585 | K646 | V706 | L769 | A830 |
| H92 | H92 | L152 | V216 | V278 | T340 | E405 | K466 | P526 | R586 | L647 | T707 | L770 | G831 |
| I93 | I93 | L153 | K217 | V279 | E341 | D405 | E467 | M527 | R587 | M648 | L708 | S771 | E832 |
| Y34 | E94 | T154 | K218 | T282 | P342 | D406 | L468 | Q529 | P590 | A649 | H709 | F772 | T834 |
| L95 | L95 | D155 | E219 | Y282 | D344 | E407 | D469 | V530 | V591 | L650 | R710 | A773 | S835 |
| A96 | A96 | E156 | R220 | F283 | D345 | V408 | L470 | D531 | T592 | L652 | G712 | S774 | T836 |
| T36 | T36 | E157 | A221 | L284 | R346 | S410 | E471 | G532 | L593 | F653 | G713 | G775 | G837 |
| T37 | T37 | E158 | G222 | G222 | R347 | T411 | A472 | G533 | M594 | K654 | L713 | F776 | R838 |
| K38 | K38 | Y159 | L223 | L223 | Q348 | G412 | L473 | R534 | P595 | L655 | Q714 | F777 | L839 |
| P39 | P39 | E160 | R224 | G287 | P349 | D413 | E474 | G535 | S596 | F656 | A715 | L778 | K840 |
| E40 | E40 | L161 | L225 | M288 | P350 | R414 | K475 | A536 | D597 | L657 | F716 | A779 | H841 |
| R41 | R41 | R162 | P226 | T289 | M351 | V415 | E476 | T597 | E598 | L658 | Q717 | K780 | Y842 |
| D42 | D42 | Y163 | L227 | P290 | N352 | A416 | L477 | T598 | P599 | K659 | L720 | S782 | F843 |
| Q43 | Q43 | G164 | E164 | V292 | V353 | E417 | L478 | S533 | L600 | K660 | V721 | H783 | A844 |
| L44 | L44 | K165 | V230 | V292 | V354 | G418 | E479 | D539 | R601 | M661 | | D784 | N845 |
| F45 | F45 | Q166 | E231 | H294 | V355 | L421 | E480 | L540 | S602 | E662 | Q724 | I785 | P846 |
| M107 | M107 | E167 | E232 | H294 | P356 | A422 | M481 | N541 | L603 | E663 | S725 | I786 | D847 |
| E47 | E47 | T168 | E233 | G295 | E357 | D423 | K482 | D542 | T604 | G664 | L726 | L787 | E848 |
| R48 | R48 | Y169 | E234 | E236 | G358 | D424 | H483 | L543 | G665 | Q665 | Q727 | G788 | A849 |
| I49 | I49 | P170 | A235 | L297 | A359 | G425 | P484 | Y544 | L606 | L666 | L728 | | L850 |
| F50 | F50 | L171 | Y236 | V298 | R360 | G426 | S485 | R545 | L607 | L667 | H729 | Y791 | L851 |
| G51 | G51 | P172 | R237 | E299 | V361 | V427 | R486 | L546 | S608 | A667 | F730 | I792 | A852 |
| I53 | I53 | P173 | P238 | K300 | G301 | K428 | E487 | L547 | G609 | P668 | L731 | T793 | V853 |
| E54 | E54 | V175 | T241 | G301 | D365 | S429 | R488 | L548 | K610 | N669 | V732 | Q794 | A854 |
| D55 | D55 | A176 | L242 | P302 | K366 | K428 | E489 | I549 | R550 | K671 | C733 | V795 | G855 |
| V56 | V56 | D177 | A243 | P303 | L367 | D430 | A480 | N549 | N551 | G612 | E734 | T796 | G856 |
| E57 | E57 | L178 | A244 | L304 | V368 | D431 | A491 | R552 | N552 | H613 | R797 | H797 | L857 |
| C58 | C58 | L118 | E244 | L304 | V369 | Y432 | A492 | R553 | F614 | R674 | F736 | E798 | V858 |
| S119 | S119 | D181 | L245 | E306 | A369 | G433 | R493 | | | | | | |
| A120 | A120 | G182 | P246 | A307 | A370 | | | | | | | | |

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| P1048 | P1049 | P1050 | P1051 | P1052 | P1053 | P1054 | P1055 | P1056 | P1057 | P1058 | P1059 | P1060 | P1061 | P1062 | L1065 | L1066 | L1067 | L1068 | L1069 | L1070 | L1071 | L1072 | L1073 | L1074 | L1075 | L1076 | L1077 | L1078 | L1079 | L1080 | L1081 | L1082 | L1083 | L1084 | L1085 | L1086 | L1087 | L1088 | L1089 | L1090 | L1091 | L1092 | L1093 | L1094 | L1095 | L1096 | L1097 | L1098 | L1099 | D1100 | D1101 | D1102 | D1103 | D1104 | D1105 | D1106 | D1107 | D1108 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| S1049 | G1050 | E1051 | T1052 | F1053 | E1054 | V1055 | P1056 | V1057 | R1058 | S1059 | S1060 | F1061 | R1062 | L1065 | T1066 | V1067 | L1068 | E1069 | F1070 | F1071 | L1072 | S1073 | S1074 | H1075 | G1076 | A1077 | R1078 | K1079 | G1080 | L1081 | A1082 | D1083 | T1084 | A1085 | L1086 | A1087 | T1088 | A1089 | D1090 | S1091 | G1092 | L1093 | L1094 | T1095 | R1096 | K1097 | L1098 | V1099 | D1100 | V1101 | T1102 | R1103 | E1104 | L1105 | V1106 | V1107 | V1108 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| T1114 | N1115 | N1116 | I1117 | I1118 | E1119 | V1120 | P1121 | P1122 | F1123 | Q1124 | P1125 | D1126 | E1127 | L1128 | T1129 | S1130 | S1131 | L1132 | L1133 | L1134 | L1135 | K1136 | L1137 | A1138 | L1139 | I1140 | A1141 | A1142 | L1143 | L1144 | G1145 | L1146 | L1147 | V1148 | L1149 | A1150 | A1151 | E1152 | V1153 | E1154 | V1155 | L1156 | G1157 | V1158 | R1159 | L1160 | E1161 | L1162 | G1163 | Y1165 | L1166 | T1167 | S1168 | D1169 | D1170 | V1171 | H1172 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| L1173 | L1174 | K1175 | A1177 | A1178 | E1179 | A1180 | G1181 | E1182 | L1183 | Q1184 | E1185 | V1186 | P1187 | V1188 | L1189 | S1190 | P1191 | L1192 | L1193 | C1194 | Q1195 | T1196 | L1197 | Y1198 | G1199 | K1203 | C1204 | Y1205 | G1206 | T1207 | D1208 | L1209 | L1281 | L1282 | L1283 | E1284 | M1211 | A1212 | R1213 | P1214 | V1215 | S1216 | I1217 | G1218 | E1219 | A1220 | V1221 | G1222 | L1223 | V1224 | Q1227 | S1228 | L1229 | G1230 | E1231 | P1232 | G1233 | P1234 | Q1235 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| L1236 | T1237 | R1238 | G1245 | V1246 | A1249 | T1252 | T1253 | Q1254 | G1255 | P1257 | L1258 | R1259 | I1260 | E1261 | L1262 | Q1263 | E1264 | K1269 | A1270 | L1274 | L1277 | D1278 | G1279 | V1280 | L1281 | R1282 | L1283 | E1284 | M1211 | A1212 | R1213 | P1214 | V1215 | S1216 | I1217 | G1218 | E1219 | A1220 | V1221 | G1222 | L1223 | V1224 | Q1227 | S1228 | L1229 | G1230 | E1231 | P1232 | G1233 | P1234 | Q1235 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| R1310 | L1311 | L1312 | K1313 | D1314 | G1315 | L1316 | L1317 | L1318 | V1319 | Q1323 | P1324 | L1325 | R1327 | L1330 | D1331 | P1332 | H1333 | Q1334 | L1335 | L1336 | E1337 | A1338 | K1339 | G1340 | P1341 | A1342 | A1343 | L1344 | E1345 | L1346 | Y1347 | L1348 | V1349 | E1350 | E1351 | L1352 | Q1353 | K1354 | V1355 | L1356 | R1357 | P1358 | Q1359 | G1360 | V1361 | K1362 | L1363 | H1364 | L1365 | K1366 | H1367 | L1368 | S1369 | L1370 | V1371 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V1372 | R1373 | M1374 | M1375 | K1376 | L1377 | L1378 | V1379 | E1380 | L1381 | T1382 | D1383 | P1384 | S1387 | R1388 | L1389 | L1390 | E1391 | G1392 | Q1393 | V1394 | L1395 | E1396 | K1397 | M1398 | L1399 | A1400 | E1401 | A1402 | L1403 | E1404 | E1405 | L1406 | L1407 | G1408 | L1409 | E1410 | G1411 | K1412 | P1413 | P1414 | V1415 | A1416 | L1417 | K1418 | T1419 | P1420 | L1421 | M1422 | G1423 | V1424 | T1425 | K1426 | L1427 | D1428 | L1429 | S1430 | T1431 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V1434 | L1435 | S1436 | A1437 | A1438 | S1439 | F1440 | Q1441 | M1442 | T1443 | T1444 | H1445 | L1446 | L1447 | T1448 | E1449 | A1450 | A1451 | I1452 | A1453 | G1454 | K1455 | K1456 | D1457 | E1458 | L1459 | G1460 | G1461 | L1462 | K1463 | E1464 | M1465 | V1466 | L1467 | G1468 | G1469 | R1470 | L1471 | I1472 | P1473 | A1474 | G1475 | T1476 | G1477 | S1478 | D1479 | F1480 | V1481 | R1482 | F1483 | T1484 | Q1485 | V1486 | L1487 | D1488 | Q1489 | K1490 | T1491 | L1492 | K1493 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A1494 | I1495 | E1496 | E1497 | A1498 | R1499 | K1500 | E1501 | A1502 | V1503 | E1504 | A1505 | L1506 | L1507 | L1508 | L1509 | L1510 | L1511 | L1512 | L1513 | L1514 | L1515 | L1516 | L1517 | L1518 | L1519 | L1520 | L1521 | L1522 | L1523 | L1524 | L1525 | L1526 | L1527 | L1528 | L1529 | L1530 | L1531 | L1532 | L1533 | L1534 | L1535 | L1536 | L1537 | L1538 | L1539 | L1540 | L1541 | L1542 | L1543 | L1544 | L1545 | L1546 | L1547 | L1548 | L1549 | L1550 | L1551 | L1552 | L1553 | L1554 | L1555 | L1556 | L1557 | L1558 | L1559 | L1560 | L1561 | L1562 | L1563 | L1564 | L1565 | L1566 | L1567 | L1568 | L1569 | L1570 | L1571 | L1572 | L1573 | L1574 | L1575 | L1576 | L1577 | L1578 | L1579 | L1580 | L1581 | L1582 | L1583 | L1584 | L1585 | L1586 | L1587 | L1588 | L1589 | L1590 | L1591 | L1592 | L1593 | L1594 | L1595 | L1596 | L1597 | L1598 | L1599 | L1600 | L1601 | L1602 | L1603 | L1604 | L1605 | L1606 | L1607 | L1608 | L1609 | L1610 | L1611 | L1612 | L1613 | L1614 | L1615 | L1616 | L1617 | L1618 | L1619 | L1620 | L1621 | L1622 | L1623 | L1624 | L1625 | L1626 | L1627 | L1628 | L1629 | L1630 | L1631 | L1632 | L1633 | L1634 | L1635 | L1636 | L1637 | L1638 | L1639 | L1640 | L1641 | L1642 | L1643 | L1644 | L1645 | L1646 | L1647 | L1648 | L1649 | L1650 | L1651 | L1652 | L1653 | L1654 | L1655 | L1656 | L1657 | L1658 | L1659 | L1660 | L1661 | L1662 | L1663 | L1664 | L1665 | L1666 | L1667 | L1668 | L1669 | L1670 | L1671 | L1672 | L1673 | L1674 | L1675 | L1676 | L1677 | L1678 | L1679 | L1680 | L1681 | L1682 | L1683 | L1684 | L1685 | L1686 | L1687 | L1688 | L1689 | L1690 | L1691 | L1692 | L1693 | L1694 | L1695 | L1696 | L1697 | L1698 | L1699 | L1700 | L1701 | L1702 | L1703 | L1704 | L1705 | L1706 | L1707 | L1708 | L1709 | L1710 | L1711 | L1712 | L1713 | L1714 | L1715 | L1716 | L1717 | L1718 | L1719 | L1720 | L1721 | L1722 | L1723 | L1724 | L1725 | L1726 | L1727 | L1728 | L1729 | L1730 | L1731 | L1732 | L1733 | L1734 | L1735 | L1736 | L1737 | L1738 | L1739 | L1740 | L1741 | L1742 | L1743 | L1744 | L1745 | L1746 | L1747 | L1748 | L1749 | L1750 | L1751 | L1752 | L1753 | L1754 | L1755 | L1756 | L1757 | L1758 | L1759 | L1760 | L1761 | L1762 | L1763 | L1764 | L1765 | L1766 | L1767 | L1768 | L1769 | L1770 | L1771 | L1772 | L1773 | L1774 | L1775 | L1776 | L1777 | L1778 | L1779 | L1780 | L1781 | L1782 | L1783 | L1784 | L1785 | L1786 | L1787 | L1788 | L1789 | L1790 | L1791 | L1792 | L1793 | L1794 | L1795 | L1796 | L1797 | L1798 | L1799 | L1800 | L1801 | L1802 | L1803 | L1804 | L1805 | L1806 | L1807 | L1808 | L1809 | L1810 | L1811 | L1812 | L1813 | L1814 | L1815 | L1816 | L1817 | L1818 | L1819 | L1820 | L1821 | L1822 | L1823 | L1824 | L1825 | L1826 | L1827 | L1828 | L1829 | L1830 | L1831 | L1832 | L1833 | L1834 | L1835 | L1836 | L1837 | L1838 | L1839 | L1840 | L1841 | L1842 | L1843 | L1844 | L1845 | L1846 | L1847 | L1848 | L1849 | L1850 | L1851 | L1852 | L1853 | L1854 | L1855 | L1856 | L1857 | L1858 | L1859 | L1860 | L1861 | L1862 | L1863 | L1864 | L1865 | L1866 | L1867 | L1868 | L1869 | L1870 | L1871 | L1872 | L1873 | L1874 | L1875 | L1876 | L1877 | L1878 | L1879 | L1880 | L1881 | L1882 | L1883 | L1884 | L1885 | L1886 | L1887 | L1888 | L1889 | L1890 | L1891 | L1892 | L1893 | L1894 | L1895 | L1896 | L1897 | L1898 | L1899 | L1900 | L1901 | L1902 | L1903 | L1904 | L1905 | L1906 | L1907 | L1908 | L1909 | L1910 | L1911 | L1912 | L1913 | L1914 | L1915 | L1916 | L1917 | L1918 | L1919 | L1920 | L1921 | L1922 | L1923 | L1924 | L1925 | L1926 | L1927 | L1928 | L1929 | L1930 | L1931 | L1932 | L1933 | L1934 | L1935 | L1936 | L1937 | L1938 | L1939 | L1940 | L1941 | L1942 | L1943 | L1944 | L1945 | L1946 | L1947 | L1948 | L1949 | L1950 | L1951 | L1952 | L1953 | L1954 | L1955 | L1956 | L1957 | L1958 | L1959 | L1960 | L1961 | L1962 | L1963 | L1964 | L1965 | L1966 | L1967 | L1968 | L1969 | L1970 | L1971 | L1972 | L1973 | L1974 | L1975 | L1976 | L1977 | L1978 | L1979 | L1980 | L1981 | L1982 | L1983 | L1984 | L1985 | L1986 | L1987 | L1988 | L1989 | L1990 | L1991 | L1992 | L1993 | L1994 | L1995 | L1996 | L1997 | L1998 | L1999 | L2000 | L2001 | L2002 | L2003 | L2004 | L2005 | L2006 | L2007 | L2008 | L2009 | L2010 | L2011 | L2012 | L2013 | L2014 | L2015 | L2016 | L2017 | L2018 | L2019 | L2020 | L2021 | L2022 | L2023 | L2024 | L2025 | L2026 | L2027 | L2028 | L2029 | L2030 | L2031 | L2032 | L2033 | L2034 | L2035 | L2036 | L2037 | L2038 | L2039 | L2040 | L2041 | L2042 | L2043 | L2044 | L2045 | L2046 | L2047 | L2048 | L2049 | L2050 | L2051 | L2052 | L2053 | L2054 | L2055 | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | L2064 | L2065 | L2066 | L2067 | L2068 | L2069 | L2070 | L2071 | L2072 | L2073 | L2074 | L2075 | L2076 | L2077 | L2078 | L2079 | L2080 | L2081 | L2082 | L2083 | L2084 | L2085 | L2086 | L2087 | L2088 | L2089 | L2090 | L2091 | L2092 | L2093 | L2094 | L2095 | L2096 | L2097 | L2098 | L2099 | L2100 | L2101 | L2102 | L2103 | L2104 | L2105 | L2106 | L2107 | L2108 | L2109 | L2110 | L2111 | L2112 | L2113 | L2114 | L2115 | L2116 | L2117 | L2118 | L2119 | L2120 | L2121 | L2122 | L2123 | L2124 | L2125 | L2126 | L2127 | L2128 | L2129 | L2130 | L2131 | L2132 | L2133 | L2134 | L2135 | L2136 | L2137 | L2138 | L2139 | L2140 | L2141 | L2142 | L2143 | L2144 | L2145 | L2146 | L2147 | L2148 | L2149 | L2150 | L2151 | L2152 | L2153 | L2154 | L2155 | L2156 | L2157 | L2158 | L2159 | L2160 | L2161 | L2162 | L2163 | L2164 | L2165 | L2166 | L2167 | L2168 | L2169 | L2170 | L2171 | L2172 | L2173 | L2174 | L2175 | L2176 | L2177 | L2178 | L2179 | L2180 | L2181 | L2182 | L2183 | L2184 | L2185 | L2186 | L2187 | L2188 | L2189 | L2190 | L2191 | L2192 | L2193 | L2194 | L2195 | L2196 | L2197 | L2198 | L2199 | L2200 | L2201 | L2202 | L2203 | L2204 | L2205 | L2206 | L2207 | L2208 | L2209 | L2210 | L2211 | L2212 | L2213 | L2214 | L2215 | L2216 | L2217 | L2218 | L2219 | L2220 | L2221 | L2222 | L2223 | L2224 | L2225 | L2226 | L2227 | L2228 | L2229 | L2230 | L2231 | L2232 | L2233 | L2234 | L2235 | L2236 | L2237 | L2238 | L2239 | L2240 | L2241 | L2242 | L2243 | L2244 | L2245 | L2246 | L2247 | L2248 | L2249 | L2250 | L2251 | L2252 | L2253 | L2254 | L2255 | L2256 | L2257 | L2258 | L2259 | L2260 | L2261 | L2262 | L2263 | L2264 | L2265 | L2266 | L2267 | L2268 | L2269 | L2270 | L2271 | L2272 | L2273 | L2274 | L2275 | L2276 | L2277 | L2278 | L2279 | L2280 | L2281 | L2282 | L2283 | L2284 | L2285 | L2286 | L2287 | L2288 | L2289 | L2290 | L2291 | L2292 | L2293 | L2294 | L2295 | L2296 | L2297 | L2298 | L2299 | L2300 | L2301 | L2302 | L2303 | L2304 | L2305 | L2306 | L2307 | L2308 | L2309 | L2310 | L2311 | L2312 | L2313 | L2314 | L2315 | L2316 | L2317 | L2318 | L2319 | L2320 | L2321 | L2322 | L2323 | L2324 | L2325 | L2326 | L2327 | L2328 | L2329 | L2330 | L2331 | L2332 | L2333 | L2334 | L2335 | L2336 | L2337 | L2338 | L2339 | L2340 | L2341 | L2342 | L2343 | L2344 | L2345 | L2346 | L2347 | L2348 | L2349 | L2350 | L2351 | L2352 | L2353 | L2354 | L2355 | L2356 | L2357 | L2358 | L2359 | L2360 | L2361 | L2362 | L2363 | L2364 | L2365 | L2366 | L2367 | L2368 | L2369 | L2370 | L2371 | L2372 | L2373 | L2374 | L2375 | L2376 | L2377 | L2378 | L2379 | L2380 | L2381 | L2382 | L2383 | L2384 | L2385 | L |

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| G1248 | G1251 | G1253 | G1254 | G1255 | G1256 | P1257 | G1258 | G1259 | G1260 | E1261 | L1262 | F1263 | A1265 | A1266 | B1267 | P1268 | K1269 | C1270 | A1271 | A1272 | V1273 | I1274 | L1275 | E1276 | L1277 | D1278 | G1279 | V1280 | V1281 | R1282 | L1283 | G1284 | E1285 | T1286 | E1287 | E1288 | L1289 | S1291 | V1292 | F1293 | S1296 | E1297 | G1298 | F1299 | S1300 | K1301 | E1302 | Y1303 | L1304 | T1305 | L1306 | P1307 | E1308 | A1309 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Q1183 | Q1184 | V1185 | V1186 | P1187 | V1188 | B1189 | S1190 | P1191 | L1192 | T1193 | C1194 | Q1195 | E1196 | L1197 | R1198 | G1199 | V1200 | D1201 | L1202 | Y1203 | G1204 | L1205 | L1206 | L1207 | L1208 | L1209 | S1210 | L1211 | R1212 | E1213 | P1214 | V1215 | L1216 | L1217 | G1218 | E1219 | E1220 | V1221 | G1222 | L1223 | V1224 | A1225 | A1226 | Q1227 | S1228 | L1229 | G1230 | E1231 | P1232 | G1233 | T1234 | Q1235 | L1236 | T1237 | L1238 | L1239 | P1240 | G1241 | G1242 | A1243 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| P1121 | L1122 | F1123 | Q1124 | P1125 | D1126 | E1127 | L1128 | T1129 | L1130 | S1131 | L1132 | R1133 | L1134 | R1135 | L1136 | R1137 | L1138 | D1139 | Y1140 | L1141 | L1142 | L1143 | L1144 | Y1145 | G1146 | R1147 | Y1148 | L1149 | A1150 | R1151 | E1152 | V1153 | L1154 | V1155 | L1156 | G1157 | V1158 | R1159 | L1160 | E1161 | G1162 | R1163 | Y1164 | L1165 | L1166 | S1167 | L1168 | D1169 | L1170 | V1171 | H1172 | L1173 | Q1174 | L1175 | L1176 | L1177 | L1178 | E1179 | G1180 | L1181 | L1182 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| S1059 | S1060 | R1061 | R1062 | G1063 | G1064 | L1065 | T1066 | V1067 | L1068 | L1069 | Y1070 | F1071 | L1072 | S1073 | S1074 | R1075 | A1076 | L1077 | L1078 | K1079 | G1080 | L1081 | D1082 | L1083 | T1084 | L1085 | L1086 | R1087 | L1088 | S1089 | G1090 | L1091 | L1092 | Y1093 | L1094 | T1095 | R1096 | K1097 | L1098 | V1099 | D1100 | V1101 | T1102 | L1103 | E1104 | L1105 | V1106 | L1107 | R1108 | E1109 | L1110 | D1111 | Q1112 | L1113 | T1114 | Y1115 | L1116 | L1117 | L1118 | S1119 | V1120 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| T997 | E998 | T999 | T1000 | E1001 | K1002 | V1003 | T1004 | Q1005 | A1006 | V1007 | F1008 | K1009 | H1010 | F1011 | E1012 | E1013 | L1014 | Y1015 | P1016 | L1017 | N1018 | F1019 | D1020 | Y1021 | V1022 | M1023 | A1024 | L1025 | G1026 | S1027 | A1028 | R1029 | G1030 | N1031 | P1032 | R1033 | L1034 | L1035 | R1036 | Q1037 | L1038 | L1039 | G1040 | L1041 | R1042 | G1043 | Q1044 | Q1045 | Q1046 | L1047 | P1048 | S1049 | G1050 | E1051 | T1052 | F1053 | P1054 | P1055 | P1056 | V1057 | R1058 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| P1121 | L1122 | F1123 | Q1124 | P1125 | D1126 | E1127 | L1128 | T1129 | L1130 | S1131 | L1132 | R1133 | L1134 | R1135 | L1136 | R1137 | L1138 | D1139 | Y1140 | L1141 | L1142 | L1143 | L1144 | Y1145 | G1146 | R1147 | Y1148 | L1149 | A1150 | R1151 | E1152 | V1153 | L1154 | V1155 | L1156 | G1157 | V1158 | R1159 | L1160 | E1161 | G1162 | R1163 | Y1164 | L1165 | L1166 | S1167 | L1168 | D1169 | L1170 | V1171 | H1172 | L1173 | Q1174 | L1175 | L1176 | L1177 | L1178 | E1179 | G1180 | L1181 | L1182 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| T1183 | Q1184 | V1185 | V1186 | P1187 | V1188 | B1189 | S1190 | P1191 | L1192 | T1193 | C1194 | Q1195 | E1196 | L1197 | R1198 | G1199 | V1200 | D1201 | L1202 | Y1203 | G1204 | L1205 | L1206 | L1207 | L1208 | L1209 | S1210 | L1211 | R1212 | E1213 | P1214 | V1215 | L1216 | L1217 | G1218 | E1219 | E1220 | V1221 | G1222 | L1223 | V1224 | A1225 | A1226 | Q1227 | S1228 | L1229 | G1230 | E1231 | P1232 | G1233 | T1234 | Q1235 | L1236 | T1237 | L1238 | L1239 | P1240 | G1241 | G1242 | A1243 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G309 | L310 | L311 | R312 | R313 | R314 | R315 | R316 | Q317 | Q318 | L319 | R320 | R321 | R322 | R323 | R324 | R325 | R326 | R327 | R328 | R329 | R330 | R331 | R332 | R333 | R334 | R335 | R336 | R337 | R338 | R339 | R340 | R341 | R342 | R343 | R344 | R345 | R346 | R347 | R348 | R349 | R350 | R351 | R352 | R353 | R354 | R355 | R356 | R357 | R358 | R359 | R360 | R361 | R362 | R363 | R364 | R365 | R366 | R367 | R368 | R369 | R370 | R371 | R372 | R373 | R374 | R375 | R376 | R377 | R378 | R379 | R380 | R381 | R382 | R383 | R384 | R385 | R386 | R387 | R388 | R389 | R390 | R391 | R392 | R393 | R394 | R395 | R396 | R397 | R398 | R399 | R400 | R401 | R402 | R403 | R404 | R405 | R406 | R407 | R408 | R409 | R410 | R411 | R412 | R413 | R414 | R415 | R416 | R417 | R418 | R419 | R420 | R421 | R422 | R423 | R424 | R425 | R426 | R427 | R428 | R429 | R430 | R431 | R432 | R433 | R434 | R435 | R436 | R437 | R438 | R439 | R440 | R441 | R442 | R443 | R444 | R445 | R446 | R447 | R448 | R449 | R450 | R451 | R452 | R453 | R454 | R455 | R456 | R457 | R458 | R459 | R460 | R461 | R462 | R463 | R464 | R465 | R466 | R467 | R468 | R469 | R470 | R471 | R472 | R473 | R474 | R475 | R476 | R477 | R478 | R479 | R480 | R481 | R482 | R483 | R484 | R485 | R486 | R487 | R488 | R489 | R490 | R491 | R492 | R493 | R494 | R495 | R496 | R497 | R498 | R499 | R500 | R501 | R502 | R503 | R504 | R505 | R506 | R507 | R508 | R509 | R510 | R511 | R512 | R513 | R514 | R515 | R516 | R517 | R518 | R519 | R520 | R521 | R522 | R523 | R524 | R525 | R526 | R527 | R528 | R529 | R530 | R531 | R532 | R533 | R534 | R535 | R536 | R537 | R538 | R539 | R540 | R541 | R542 | R543 | R544 | R545 | R546 | R547 | R548 | R549 | R550 | R551 | R552 | R553 | R554 | R555 | R556 | R557 | R558 | R559 | R560 | R561 | R562 | R563 | R564 | R565 | R566 | R567 | R568 | R569 | R570 | R571 | R572 | R573 | R574 | R575 | R576 | R577 | R578 | R579 | R580 | R581 | R582 | R583 | R584 | R585 | R586 | R587 | R588 | R589 | R590 | R591 | R592 | R593 | R594 | R595 | R596 | R597 | R598 | R599 | R600 | R601 | R602 | R603 | R604 | R605 | R606 | R607 | R608 | R609 | R610 | R611 | R612 | R613 | R614 | R615 | R616 | R617 | R618 | R619 | R620 | R621 | R622 | R623 | R624 | R625 | R626 | R627 | R628 | R629 | R630 | R631 | R632 | R633 | R634 | R635 | R636 | R637 | R638 | R639 | R640 | R641 | R642 | R643 | R644 | R645 | R646 | R647 | R648 | R649 | R650 | R651 | R652 | R653 | R654 | R655 | R656 | R657 | R658 | R659 | R660 | R661 | R662 | R663 | R664 | R665 | R666 | R667 | R668 | R669 | R670 | R671 | R672 | R673 | R674 | R675 | R676 | R677 | R678 | R679 | R680 | R681 | R682 | R683 | R684 | R685 | R686 | R687 | R688 | R689 | R690 | R691 | R692 | R693 | R694 | R695 | R696 | R697 | R698 | R699 | R700 | R701 | R702 | R703 | R704 | R705 | R706 | R707 | R708 | R709 | R710 | R711 | R712 | R713 | R714 | R715 | R716 | R717 | R718 | R719 | R720 | R721 | R722 | R723 | R724 | R725 | R726 | R727 | R728 | R729 | R730 | R731 | R732 | R733 | R734 | R735 | R736 | R737 | R738 | R739 | R740 | R741 | R742 | R743 | R744 | R745 | R746 | R747 | R748 | R749 | R750 | R751 | R752 | R753 | R754 | R755 | R756 | R757 | R758 | R759 | R760 | R761 | R762 | R763 | R764 | R765 | R766 | R767 | R768 | R769 | R770 | R771 | R772 | R773 | R774 | R775 | R776 | R777 | R778 | R779 | R780 | R781 | R782 | R783 | R784 | R785 | R786 | R787 | R788 | R789 | R790 | R791 | R792 | R793 | R794 | R795 | R796 | R797 | R798 | R799 | R800 | R801 | R802 | R803 | R804 | R805 | R806 | R807 | R808 | R809 | R810 | R811 | R812 | R813 | R814 | R815 | R816 | R817 | R818 | R819 | R820 | R821 | R822 | R823 | R824 | R825 | R826 | R827 | R828 | R829 | R830 | R831 | R832 | R833 | R834 | R835 | R836 | R837 | R838 | R839 | R840 | R841 | R842 | R843 | R844 | R845 | R846 | R847 | R848 | R849 | R850 | R851 | R852 | R853 | R854 | R855 | R856 | R857 | R858 | R859 | R860 | R861 | R862 | R863 | R864 | R865 | R866 | R867 | R868 | R869 | R870 | R871 | R872 | R873 | R874 | R875 | R876 | R877 | R878 | R879 | R880 | R881 | R882 | R883 | R884 | R885 | R886 | R887 | R888 | R889 | R890 | R891 | R892 | R893 | R894 | R895 | R896 | R897 | R898 | R899 | R900 | R901 | R902 | R903 | R904 | R905 | R906 | R907 | R908 | R909 | R910 | R911 | R912 | R913 | R914 | R915 | R916 | R917 | R918 | R919 | R920 | R921 | R922 | R923 | R924 | R925 | R926 | R927 | R928 | R929 | R930 | R931 | R932 | R933 | R934 | R935 | R936 | R937 | R938 | R939 | R940 | R941 | R942 | R943 | R944 | R945 | R946 | R947 | R948 | R949 | R950 | R951 | R952 | R953 | R954 | R955 | R956 | R957 | R958 | R959 | R960 | R961 | R962 | R963 | R964 | R965 | R966 | R967 | R968 | R969 | R970 | R971 | R972 | R973 | R974 | R975 | R976 | R977 | R978 | R979 | R980 | R981 | R982 | R983 | R984 | R985 | R986 | R987 | R988 | R989 | R990 | R991 | R992 | R993 | R994 | R995 | R996 | R997 | R998 | R999 | R1000 | R1001 | R1002 | R1003 | R1004 | R1005 | R1006 | R1007 | R1008 | R1009 | R1010 | R1011 | R1012 | R1013 | R1014 | R1015 | R1016 | R1017 | R1018 | R1019 | R1020 | R1021 | R1022 | R1023 | R1024 | R1025 | R1026 | R1027 | R1028 | R1029 | R1030 | R1031 | R1032 | R1033 | R1034 | R1035 | R1036 | R1037 | R1038 | R1039 | R1040 | R1041 | R1042 | R1043 | R1044 | R1045 | R1046 | R1047 | R1048 | R1049 | R1050 | R1051 | R1052 | R1053 | R1054 | R1055 | R1056 | R1057 | R1058 | R1059 | R1060 | R1061 | R1062 | R1063 | R1064 | R1065 | R1066 | R1067 | R1068 | R1069 | R1070 | R1071 | R1072 | R1073 | R1074 | R1075 | R1076 | R1077 | R1078 | R1079 | R1080 | R1081 | R1082 | R1083 | R1084 | R1085 | R1086 | R1087 | R1088 | R1089 | R1090 | R1091 | R1092 | R1093 | R1094 | R1095 | R1096 | R1097 | R1098 | R1099 | R1100 | R1101 | R1102 | R1103 | R1104 | R1105 | R1106 | R1107 | R1108 | R1109 | R1110 | R1111 | R1112 | R1113 | R1114 | R1115 | R1116 | R1117 | R1118 | R1119 | R1120 | R1121 | R1122 | R1123 | R1124 | R1125 | R1126 | R1127 | R1128 | R1129 | R1130 | R1131 | R1132 | R1133 | R1134 | R1135 | R1136 | R1137 | R1138 | R1139 | R1140 | R1141 | R1142 | R1143 | R1144 | R1145 | R1146 | R1147 | R1148 | R1149 | R1150 | R1151 | R1152 | R1153 | R1154 | R1155 | R1156 | R1157 | R1158 | R1159 | R1160 | R1161 | R1162 | R1163 | R1164 | R1165 | R1166 | R1167 | R1168 | R1169 | R1170 | R1171 | R1172 | R1173 | R1174 | R1175 | R1176 | R1177 | R1178 | R1179 | R1180 | R1181 | R1182 | R1183 | R1184 | R1185 | R1186 | R1187 | R1188 | R1189 | R1190 | R1191 | R1192 | R1193 | R1194 | R1195 | R1196 | R1197 | R1198 | R1199 | R1200 | R1201 | R1202 | R1203 | R1204 | R1205 | R1206 | R1207 | R1208 | R1209 | R1210 | R1211 | R1212 | R1213 | R1214 | R1215 | R1216 | R1217 | R1218 | R1219 | R1220 | R1221 | R1222 | R1223 | R1224 | R1225 | R1226 | R1227 | R1228 | R1229 | R1230 | R1231 | R1232 | R1233 | R1234 | R1235 | R1236 | R1237 | R1238 | R1239 | R1240 | R1241 | R1242 | R1243 | R1244 | R1245 | R1246 | R1247 | R1248 | R1249 | R1250 | R1251 | R1252 | R1253 | R1254 | R1255 | R1256 | R1257 | R1258 | R1259 | R1260 | R1261 | R1262 | R1263 | R1264 | R1265 | R1266 | R1267 | R1268 | R1269 | R1270 | R1271 | R1272 | R1273 | R1274 | R1275 | R1276 | R1277 | R1278 | R1279 | R1280 | R1281 | R1282 | R1283 | R1284 | R1285 | R1286 | R1287 | R1288 | R1289 | R1290 | R1291 | R1292 | R1293 | R1294 | R1295 | R1296 | R1297 | R1298 | R1299 | R1300 | R1301 | R1302 | R1303 | R1304 | R1305 | R1306 | R1307 | R1308 | R1309 |
| Q435 | E436 | V437 | D438 | L439 | V44 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

| | |
|------|------|
| L308 | V368 |
| K309 | L369 |
| I310 | L370 |
| A311 | L371 |
| K312 | L372 |
| E313 | K373 |
| P314 | K374 |
| V315 | L375 |
| S316 | L376 |
| D377 | D378 |
| L317 | K379 |
| E318 | R379 |
| T319 | E380 |
| P320 | H381 |
| I321 | L382 |
| G322 | L383 |
| D323 | L384 |
| E324 | T385 |
| K325 | E385 |
| V326 | S386 |
| S327 | G387 |
| F328 | |
| Y329 | V392 |
| G330 | T393 |
| D331 | K394 |
| F332 | E395 |
| I333 | R396 |
| P334 | L397 |
| D335 | E398 |
| E336 | K399 |
| H337 | Q399 |
| L338 | I400 |
| P339 | E401 |
| S340 | N402 |
| P341 | K403 |
| V342 | A404 |
| D343 | L405 |
| A344 | R406 |
| K345 | K407 |
| T346 | L408 |
| Q347 | K409 |
| S348 | Y410 |
| L349 | H411 |
| L350 | E412 |
| S351 | S413 |
| E352 | N414 |
| E353 | T415 |
| L354 | R416 |
| E355 | K417 |
| K356 | L418 |
| K357 | L419 |
| L358 | D420 |
| S359 | F421 |
| K360 | L422 |
| L361 | |
| S362 | ASP |
| E363 | |
| K364 | |
| E365 | |
| A366 | |
| M367 | |

- Molecule 5: RNA polymerase pricipal sigma factor (RpoD); CHAIN F, P

Chain P:  9% 55% 18% 17%

| | | | | | | |
|-----|------|------|------|------|------|------|
| RET | LEU | G121 | E181 | I243 | R303 | E385 |
| LYS | ASP | L122 | A182 | R244 | V304 | A386 |
| LYS | LEU | D123 | A183 | Q245 | E306 | K387 |
| SER | GLU | P124 | R184 | A246 | T307 | V388 |
| LYS | GLU | D125 | Q185 | I247 | L308 | K389 |
| ARG | GLU | L126 | H186 | R248 | K309 | L370 |
| LYS | GLU | I127 | L187 | R249 | I310 | L371 |
| ASN | GLU | A128 | I188 | A250 | K372 | K372 |
| ALA | ASP | E129 | E189 | I251 | A311 | R373 |
| GLN | LEU | V130 | A190 | A252 | Q312 | G374 |
| ALA | PRO | V131 | N191 | D253 | E313 | L375 |
| GLN | PRO | L132 | L192 | G254 | P314 | L376 |
| PRO | PRO | A133 | R193 | A255 | V315 | D377 |
| ALA | K74 | K134 | L194 | R256 | S316 | G378 |
| GLN | I75 | I135 | V195 | T257 | L317 | G378 |
| GLU | S76 | L136 | V196 | I258 | E318 | E380 |
| THR | T77 | G137 | | R259 | T319 | H381 |
| GLU | S78 | S138 | K200 | I260 | P320 | K382 |
| VAL | D79 | A139 | K201 | P261 | I321 | L383 |
| LEU | P80 | R140 | Y202 | V262 | G322 | E384 |
| VAL | V81 | V141 | T203 | H263 | D323 | E385 |
| GLN | R82 | R142 | G204 | M264 | E324 | V386 |
| GLU | Q83 | H143 | R205 | V265 | K325 | G387 |
| GLU | Y84 | I144 | G206 | E266 | D326 | A388 |
| ALA | L85 | P145 | L207 | T267 | S327 | F389 |
| GLU | H86 | G146 | S208 | I268 | F328 | |
| GLU | E87 | L147 | F209 | R269 | Y329 | V392 |
| GLU | I88 | K148 | L210 | K270 | G330 | T393 |
| PRO | G89 | E149 | D211 | L271 | D331 | R394 |
| GLU | Q90 | L150 | L212 | S272 | F332 | E395 |
| PHE | V91 | L151 | T213 | K273 | I333 | R396 |
| PRO | P92 | D152 | Q214 | T274 | P334 | L397 |
| GLU | L93 | E153 | E215 | A275 | D335 | R398 |
| GLY | L94 | K154 | G216 | R276 | E336 | Q399 |
| GLY | T95 | T155 | N217 | Q277 | P339 | E401 |
| ASP | L96 | V156 | Q218 | L278 | I402 | N402 |
| PRO | E97 | E157 | G219 | Q279 | K403 | L405 |
| PRO | E98 | E158 | L220 | E280 | A404 | R406 |
| ASP | E99 | I159 | I221 | E281 | L405 | K407 |
| LEU | V100 | D160 | R222 | L282 | A344 | L408 |
| GLU | E101 | Q161 | A223 | G283 | T345 | K409 |
| ASP | L102 | K162 | V224 | R284 | K407 | Y410 |
| PRO | A103 | L163 | E225 | E285 | Q347 | L408 |
| ASP | R104 | K164 | K226 | P286 | S348 | K409 |
| LEU | K105 | S165 | F227 | T287 | L349 | Y410 |
| THR | V106 | L166 | E228 | Y288 | H411 | R412 |
| GLU | E107 | P167 | K230 | E289 | S351 | E412 |
| ASP | G108 | K168 | R231 | E290 | E352 | S413 |
| ASP | M110 | H170 | R232 | I291 | E353 | R414 |
| LEU | E111 | K171 | F233 | A292 | L354 | T415 |
| LEU | A112 | R172 | K234 | E293 | E355 | R416 |
| ASP | I113 | Y173 | F235 | A294 | K356 | K417 |
| LEU | K114 | L174 | S236 | M295 | A357 | L418 |
| PRO | K115 | H175 | T237 | G296 | R419 | L419 |
| GLU | L116 | I176 | Y238 | P297 | S359 | D420 |
| GLU | S117 | A177 | A239 | G298 | K360 | F421 |
| GLY | E118 | R178 | T240 | W299 | L361 | L422 |
| GLY | I119 | E179 | W241 | D300 | E362 | ASP |
| GLY | T120 | E179 | W242 | A301 | E363 | |
| | | G180 | | K302 | R364 | |

4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 32 | Depositor |
| Cell constants a, b, c, α , β , γ | 235.09 Å 235.09 Å 250.88 Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 50.00 – 3.00 46.80 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 96.3 (50.00-3.00) 96.0 (46.80-3.00) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.52 (at 3.01 Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.235 , 0.289 0.221 , 0.274 | Depositor DCC |
| R_{free} test set | 2351 reflections (0.79%) | DCC |
| Wilson B-factor (Å ²) | 83.8 | Xtriage |
| Anisotropy | 0.053 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | (Not available) , (Not available) | EDS |
| Estimated twinning fraction | 0.499 for -h,-k,l 0.047 for h,-h-k,-l 0.047 for -k,-h,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Outliers | 0 of 299146 reflections | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 56149 | wwPDB-VP |
| Average B, all atoms (Å ²) | 81.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, ZN, MPD, NE6, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.43 | 0/1848 | 0.73 | 0/2512 |
| 1 | B | 0.39 | 0/1936 | 0.68 | 0/2633 |
| 1 | K | 0.43 | 0/1848 | 0.72 | 1/2512 (0.0%) |
| 1 | L | 0.41 | 0/1936 | 0.70 | 0/2633 |
| 2 | C | 0.43 | 0/8997 | 0.73 | 8/12164 (0.1%) |
| 2 | M | 0.43 | 0/8997 | 0.73 | 3/12164 (0.0%) |
| 3 | D | 0.44 | 0/12073 | 0.77 | 11/16324 (0.1%) |
| 3 | N | 0.46 | 2/12073 (0.0%) | 0.76 | 9/16324 (0.1%) |
| 4 | E | 0.40 | 0/783 | 0.69 | 0/1054 |
| 4 | O | 0.41 | 0/783 | 0.65 | 0/1054 |
| 5 | F | 0.40 | 0/2874 | 0.72 | 1/3866 (0.0%) |
| 5 | P | 0.40 | 0/2874 | 0.69 | 1/3866 (0.0%) |
| All | All | 0.43 | 2/57022 (0.0%) | 0.74 | 34/77106 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | N | 0 | 1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | N | 58 | CYS | CB-SG | -5.87 | 1.72 | 1.81 |
| 3 | N | 60 | CYS | CB-SG | -5.42 | 1.73 | 1.81 |

The worst 5 of 34 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3 | D | 831 | GLY | N-CA-C | -12.95 | 80.74 | 113.10 |
| 3 | N | 831 | GLY | N-CA-C | -11.03 | 85.51 | 113.10 |
| 2 | C | 177 | GLU | N-CA-C | -8.93 | 86.88 | 111.00 |
| 5 | F | 313 | GLU | N-CA-C | 8.15 | 133.01 | 111.00 |
| 2 | M | 58 | ASP | N-CA-C | -8.08 | 89.18 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 3 | N | 1117 | TYR | Sidechain |

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 | A | 1816 | 0 | 1871 | 279 | 0 |
| 1 | B | 1902 | 0 | 1951 | 321 | 0 |
| 1 | K | 1816 | 0 | 1871 | 296 | 0 |
| 1 | L | 1902 | 0 | 1951 | 318 | 0 |
| 2 | C | 8829 | 0 | 8933 | 1694 | 0 |
| 2 | M | 8829 | 0 | 8933 | 1598 | 0 |
| 3 | D | 11864 | 0 | 12094 | 2489 | 0 |
| 3 | N | 11864 | 0 | 12094 | 2441 | 0 |
| 4 | E | 769 | 0 | 775 | 163 | 0 |
| 4 | O | 769 | 0 | 775 | 123 | 0 |
| 5 | F | 2829 | 0 | 2914 | 587 | 0 |
| 5 | P | 2829 | 0 | 2914 | 671 | 0 |
| 6 | A | 5 | 0 | 0 | 0 | 0 |
| 6 | D | 5 | 0 | 0 | 1 | 0 |
| 7 | B | 1 | 0 | 0 | 0 | 0 |
| 7 | D | 1 | 0 | 0 | 0 | 0 |
| 7 | N | 1 | 0 | 0 | 0 | 0 |
| 8 | D | 2 | 0 | 0 | 0 | 0 |
| 8 | N | 2 | 0 | 0 | 0 | 0 |
| 9 | D | 30 | 0 | 30 | 8 | 0 |
| 9 | N | 30 | 0 | 30 | 7 | 0 |
| 10 | C | 16 | 0 | 26 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10 | M | 8 | 0 | 13 | 0 | 0 |
| 11 | A | 1 | 0 | 0 | 1 | 0 |
| 11 | B | 1 | 0 | 0 | 1 | 0 |
| 11 | C | 7 | 0 | 0 | 2 | 0 |
| 11 | D | 10 | 0 | 0 | 0 | 0 |
| 11 | F | 1 | 0 | 0 | 1 | 0 |
| 11 | M | 5 | 0 | 0 | 1 | 0 |
| 11 | N | 4 | 0 | 0 | 0 | 0 |
| 11 | O | 1 | 0 | 0 | 0 | 0 |
| All | All | 56149 | 0 | 57175 | 10419 | 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 92.

The worst 5 of 10419 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:M:283:ILE:HG22 | 2:M:284:ARG:H | 1.03 | 1.17 |
| 3:D:416:ALA:HB2 | 3:D:432:TYR:HA | 1.19 | 1.17 |
| 3:D:1489:GLN:HA | 3:D:1492:LEU:HG | 1.23 | 1.17 |
| 3:N:272:LEU:HD12 | 3:N:280:ALA:HB3 | 1.23 | 1.16 |
| 3:N:322:VAL:HA | 3:N:335:LEU:HG | 1.20 | 1.16 |

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 | 229/315 (73%) | 160 (70%) | 54 (24%) | 15 (7%) | 1 8 |
| 1 | B | 241/315 (76%) | 159 (66%) | 64 (27%) | 18 (8%) | 1 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-----------|-------------|----|
| 1 | K | 229/315 (73%) | 168 (73%) | 50 (22%) | 11 (5%) | 3 | 17 |
| 1 | L | 241/315 (76%) | 171 (71%) | 55 (23%) | 15 (6%) | 2 | 10 |
| 2 | C | 1117/1119 (100%) | 774 (69%) | 251 (22%) | 92 (8%) | 1 | 5 |
| 2 | M | 1117/1119 (100%) | 767 (69%) | 246 (22%) | 104 (9%) | 1 | 4 |
| 3 | D | 1502/1524 (99%) | 931 (62%) | 422 (28%) | 149 (10%) | 1 | 3 |
| 3 | N | 1502/1524 (99%) | 907 (60%) | 445 (30%) | 150 (10%) | 1 | 3 |
| 4 | E | 93/99 (94%) | 54 (58%) | 25 (27%) | 14 (15%) | 0 | 1 |
| 4 | O | 93/99 (94%) | 56 (60%) | 27 (29%) | 10 (11%) | 0 | 2 |
| 5 | F | 347/423 (82%) | 167 (48%) | 130 (38%) | 50 (14%) | 0 | 1 |
| 5 | P | 347/423 (82%) | 171 (49%) | 117 (34%) | 59 (17%) | 0 | 1 |
| All | All | 7058/7590 (93%) | 4485 (64%) | 1886 (27%) | 687 (10%) | 1 | 3 |

5 of 687 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 59 | GLU |
| 1 | A | 112 | ARG |
| 1 | A | 155 | LYS |
| 1 | B | 75 | VAL |
| 1 | B | 118 | ALA |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 202/273 (74%) | 192 (95%) | 10 (5%) | 30 | 70 |
| 1 | B | 210/273 (77%) | 193 (92%) | 17 (8%) | 15 | 47 |
| 1 | K | 202/273 (74%) | 190 (94%) | 12 (6%) | 24 | 63 |
| 1 | L | 210/273 (77%) | 196 (93%) | 14 (7%) | 20 | 57 |
| 2 | C | 941/941 (100%) | 863 (92%) | 78 (8%) | 14 | 46 |
| 2 | M | 941/941 (100%) | 859 (91%) | 82 (9%) | 13 | 43 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 3 | D | 1264/1279 (99%) | 1152 (91%) | 112 (9%) | 12 | 42 |
| 3 | N | 1264/1279 (99%) | 1141 (90%) | 123 (10%) | 10 | 37 |
| 4 | E | 83/87 (95%) | 76 (92%) | 7 (8%) | 14 | 45 |
| 4 | O | 83/87 (95%) | 74 (89%) | 9 (11%) | 8 | 30 |
| 5 | F | 304/371 (82%) | 274 (90%) | 30 (10%) | 10 | 35 |
| 5 | P | 304/371 (82%) | 266 (88%) | 38 (12%) | 6 | 24 |
| All | All | 6008/6448 (93%) | 5476 (91%) | 532 (9%) | 12 | 42 |

5 of 532 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | F | 335 | ASP |
| 2 | M | 184 | MET |
| 4 | O | 86 | GLN |
| 5 | F | 398 | ARG |
| 1 | L | 68 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 1489 | GLN |
| 1 | K | 81 | ASN |
| 5 | P | 170 | HIS |
| 4 | E | 86 | GLN |
| 5 | F | 263 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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 | $\# Z > 2$ |
| 6 | PO4 | A | 316 | - | 4,4,4 | 1.06 | 0 | 6,6,6 | 0.27 | 0 |
| 10 | MPD | C | 1120 | - | 6,7,7 | 2.12 | 1 (16%) | 7,10,10 | 0.89 | 0 |
| 10 | MPD | C | 1121 | - | 6,7,7 | 2.15 | 1 (16%) | 7,10,10 | 0.88 | 0 |
| 6 | PO4 | D | 1528 | - | 4,4,4 | 1.11 | 0 | 6,6,6 | 0.27 | 0 |
| 9 | NE6 | D | 1529 | - | 26,30,30 | 2.64 | 5 (19%) | 22,39,39 | 1.96 | 5 (22%) |
| 10 | MPD | M | 1120 | - | 6,7,7 | 2.04 | 1 (16%) | 7,10,10 | 0.88 | 0 |
| 9 | NE6 | N | 1528 | - | 26,30,30 | 2.55 | 4 (15%) | 22,39,39 | 2.00 | 5 (22%) |

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 |
|-----|------|-------|------|------|----------|------------|---------|
| 6 | PO4 | A | 316 | - | - | 0/0/0/0 | 0/0/0/0 |
| 10 | MPD | C | 1120 | - | - | 0/5/5/5 | 0/0/0/0 |
| 10 | MPD | C | 1121 | - | - | 0/5/5/5 | 0/0/0/0 |
| 6 | PO4 | D | 1528 | - | - | 0/0/0/0 | 0/0/0/0 |
| 9 | NE6 | D | 1529 | - | 1/1/9/13 | 0/24/46/46 | 0/0/1/1 |
| 10 | MPD | M | 1120 | - | - | 0/5/5/5 | 0/0/0/0 |
| 9 | NE6 | N | 1528 | - | 1/1/9/13 | 0/24/46/46 | 0/0/1/1 |

The worst 5 of 12 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | C | 1121 | MPD | O2-C2 | -5.04 | 1.30 | 1.44 |
| 10 | C | 1120 | MPD | O2-C2 | -5.01 | 1.30 | 1.44 |
| 10 | M | 1120 | MPD | O2-C2 | -4.74 | 1.31 | 1.44 |
| 9 | D | 1529 | NE6 | O14-C13 | 2.10 | 1.38 | 1.33 |
| 9 | N | 1528 | NE6 | C15-C16 | 2.23 | 1.52 | 1.48 |

The worst 5 of 10 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9 | D | 1529 | NE6 | O4-C4-C5 | -4.05 | 114.87 | 121.62 |
| 9 | N | 1528 | NE6 | O4-C4-C5 | -4.04 | 114.89 | 121.62 |
| 9 | N | 1528 | NE6 | C9-C10-C11 | -2.01 | 111.19 | 114.53 |
| 9 | D | 1529 | NE6 | C21-C20-C19 | 2.01 | 126.22 | 122.61 |
| 9 | N | 1528 | NE6 | C2-C3-C15 | 2.21 | 119.26 | 111.11 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 9 | N | 1528 | NE6 | C3 |
| 9 | D | 1529 | NE6 | C3 |

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6 | D | 1528 | PO4 | 1 | 0 |
| 9 | D | 1529 | NE6 | 8 | 0 |
| 9 | N | 1528 | NE6 | 7 | 0 |

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, 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 | 231/315 (73%) | -0.65 | 0 100 100 | 43, 72, 100, 115 | 0 |
| 1 | B | 243/315 (77%) | -0.81 | 0 100 100 | 51, 93, 113, 117 | 0 |
| 1 | K | 231/315 (73%) | -0.67 | 0 100 100 | 45, 73, 105, 117 | 0 |
| 1 | L | 243/315 (77%) | -0.80 | 0 100 100 | 56, 89, 112, 117 | 0 |
| 2 | C | 1119/1119 (100%) | -0.72 | 0 100 100 | 36, 77, 115, 117 | 0 |
| 2 | M | 1119/1119 (100%) | -0.71 | 0 100 100 | 31, 79, 115, 117 | 0 |
| 3 | D | 1504/1524 (98%) | -0.69 | 1 (0%) 95 90 | 35, 78, 117, 117 | 0 |
| 3 | N | 1504/1524 (98%) | -0.67 | 4 (0%) 94 84 | 34, 75, 113, 117 | 0 |
| 4 | E | 95/99 (95%) | -0.81 | 0 100 100 | 51, 88, 113, 117 | 0 |
| 4 | O | 95/99 (95%) | -0.77 | 0 100 100 | 52, 85, 109, 116 | 0 |
| 5 | F | 349/423 (82%) | -0.85 | 0 100 100 | 52, 84, 110, 117 | 0 |
| 5 | P | 349/423 (82%) | -0.80 | 0 100 100 | 51, 85, 110, 117 | 0 |
| All | All | 7082/7590 (93%) | -0.71 | 5 (0%) 95 90 | 31, 79, 115, 117 | 0 |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | N | 243 | ALA | 4.2 |
| 3 | N | 242 | LEU | 3.3 |
| 3 | N | 328 | GLY | 3.1 |
| 3 | D | 329 | GLU | 2.2 |
| 3 | N | 223 | LEU | 2.0 |

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 9 | NE6 | N | 1528 | 30/30 | 0.94 | 0.29 | 3.45 | 72,84,90,91 | 0 |
| 8 | ZN | N | 1525 | 1/1 | 0.99 | 0.19 | 2.79 | 50,50,50,50 | 0 |
| 8 | ZN | D | 1525 | 1/1 | 0.96 | 0.17 | 2.42 | 91,91,91,91 | 0 |
| 8 | ZN | D | 1526 | 1/1 | 1.00 | 0.18 | 2.25 | 77,77,77,77 | 0 |
| 7 | MG | B | 701 | 1/1 | 0.97 | 0.20 | 1.38 | 55,55,55,55 | 0 |
| 9 | NE6 | D | 1529 | 30/30 | 0.96 | 0.22 | 1.28 | 52,70,81,85 | 0 |
| 8 | ZN | N | 1526 | 1/1 | 1.00 | 0.18 | 0.87 | 55,55,55,55 | 0 |
| 6 | PO4 | A | 316 | 5/5 | 0.96 | 0.18 | 0.57 | 71,73,77,77 | 0 |
| 10 | MPD | C | 1120 | 8/8 | 0.97 | 0.17 | 0.57 | 51,56,57,57 | 0 |
| 10 | MPD | M | 1120 | 8/8 | 0.92 | 0.17 | 0.09 | 71,79,84,85 | 0 |
| 6 | PO4 | D | 1528 | 5/5 | 0.96 | 0.14 | -0.61 | 86,86,86,89 | 0 |
| 7 | MG | D | 1527 | 1/1 | 0.96 | 0.07 | - | 79,79,79,79 | 0 |
| 7 | MG | N | 1527 | 1/1 | 0.97 | 0.04 | - | 56,56,56,56 | 0 |
| 10 | MPD | C | 1121 | 8/8 | 0.96 | 0.15 | - | 70,72,73,73 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.