



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 07:33 am GMT

PDB ID : 4BOG
EMDB ID : EMD-2376
Title : The structure and super-organization of acetylcholine receptor-rapsyn complexes
Authors : Zuber, B.; Unwin, N.
Deposited on : 2013-05-20
Resolution : 50.00 Å(reported)
Based on initial model : 2BG9

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

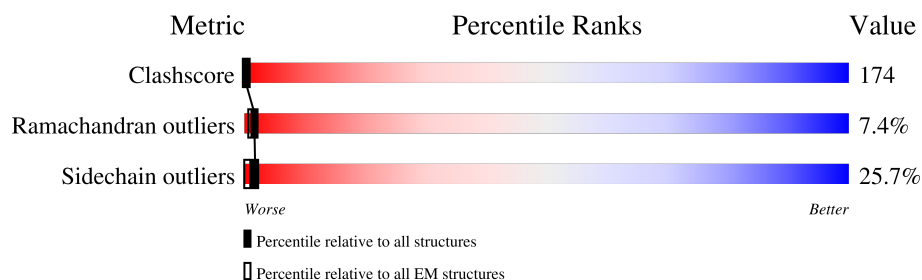
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 50.00 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.







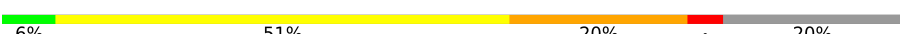
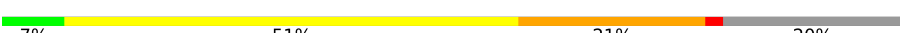
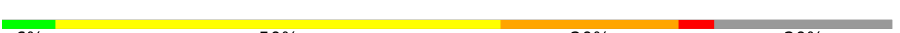







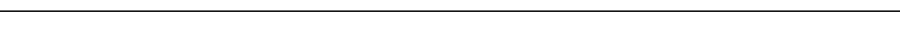
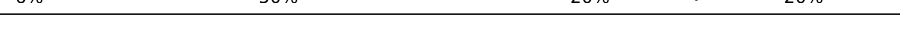





| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 0 | 493 | 5% 49% 19% . 25% |
| 1 | B | 493 | 5% 50% 19% . 25% |
| 1 | G | 493 | 5% 50% 19% . 25% |
| 1 | L | 493 | 5% 50% 19% . 25% |
| 1 | Q | 493 | 5% 49% 19% . 25% |
| 1 | V | 493 | 5% 49% 19% . 25% |
| 2 | 1 | 522 | 7% 44% 19% . 29% |
| 2 | C | 522 | 7% 43% 19% . 29% |
| 2 | H | 522 | 7% 43% 19% . 29% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | M | 522 |  |
| 2 | R | 522 |  |
| 2 | W | 522 |  |
| 3 | 2 | 461 |  |
| 3 | A | 461 |  |
| 3 | D | 461 |  |
| 3 | F | 461 |  |
| 3 | I | 461 |  |
| 3 | K | 461 |  |
| 3 | N | 461 |  |
| 3 | P | 461 |  |
| 3 | S | 461 |  |
| 3 | U | 461 |  |
| 3 | X | 461 |  |
| 3 | Z | 461 |  |
| 4 | 3 | 505 |  |
| 4 | E | 505 |  |
| 4 | J | 505 |  |
| 4 | O | 505 |  |
| 4 | T | 505 |  |
| 4 | Y | 505 |  |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 89544 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Acetylcholine receptor beta subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | 0 | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2972 | 1938 | 465 | 554 | 15 | | |
| 1 | B | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2972 | 1938 | 465 | 554 | 15 | | |
| 1 | G | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2972 | 1938 | 465 | 554 | 15 | | |
| 1 | L | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2972 | 1938 | 465 | 554 | 15 | | |
| 1 | Q | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2972 | 1938 | 465 | 554 | 15 | | |
| 1 | V | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2972 | 1938 | 465 | 554 | 15 | | |

- Molecule 2 is a protein called Acetylcholine receptor delta subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | 1 | 370 | Total | C | N | O | S | 0 | 1 |
| | | | 2983 | 1944 | 489 | 536 | 14 | | |
| 2 | C | 370 | Total | C | N | O | S | 0 | 1 |
| | | | 2983 | 1944 | 489 | 536 | 14 | | |
| 2 | H | 370 | Total | C | N | O | S | 0 | 1 |
| | | | 2983 | 1944 | 489 | 536 | 14 | | |
| 2 | M | 370 | Total | C | N | O | S | 0 | 1 |
| | | | 2983 | 1944 | 489 | 536 | 14 | | |
| 2 | R | 370 | Total | C | N | O | S | 0 | 1 |
| | | | 2983 | 1944 | 489 | 536 | 14 | | |
| 2 | W | 370 | Total | C | N | O | S | 0 | 1 |
| | | | 2983 | 1944 | 489 | 536 | 14 | | |

- Molecule 3 is a protein called Acetylcholine receptor subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | 2 | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2991 | 1954 | 478 | 540 | 19 | | |

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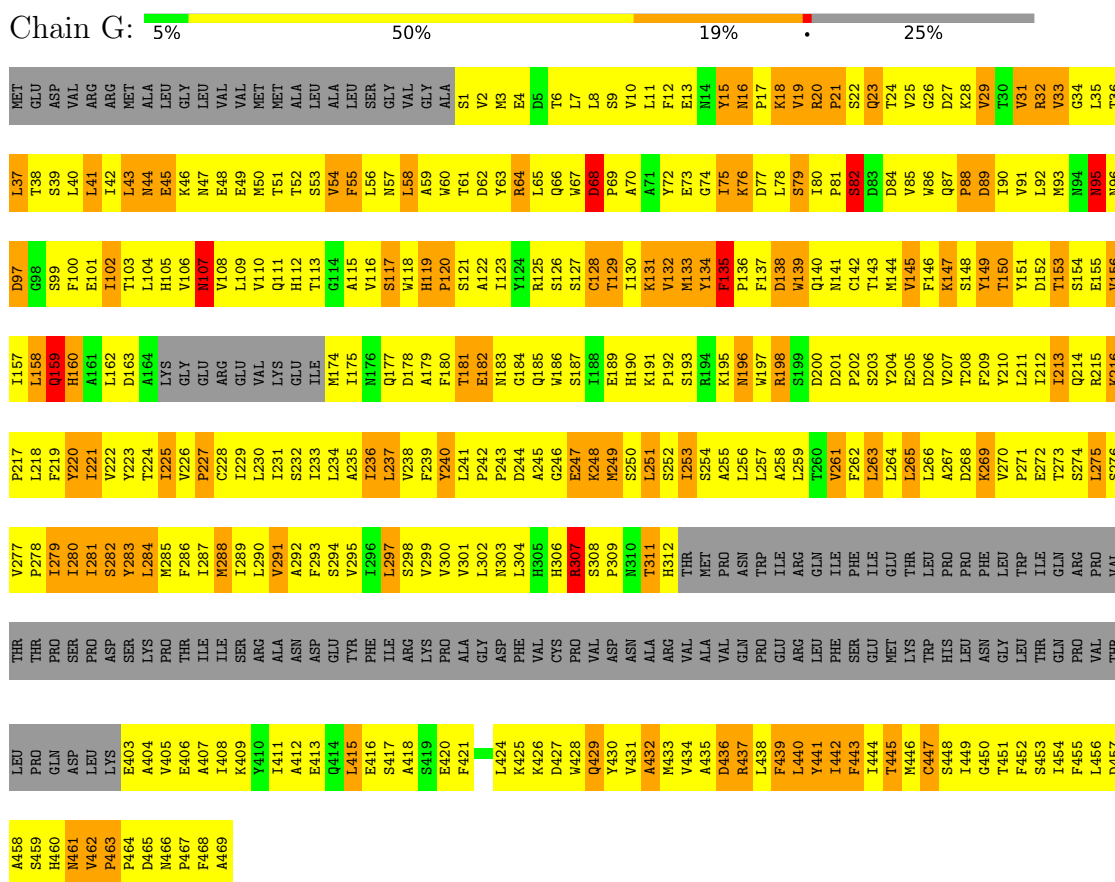
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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 3 | A | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | D | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | F | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | I | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | K | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | N | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | P | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | S | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | U | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | X | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |
| 3 | Z | 370 | Total 2991 | C 1954 | N 478 | O 540 | S 19 | 0 | 0 |

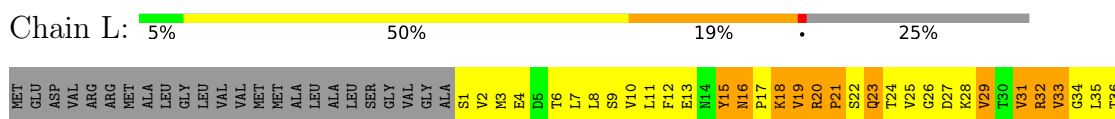
- Molecule 4 is a protein called Acetylcholine receptor gamma subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 4 | 3 | 371 | Total 2987 | C 1948 | N 478 | O 551 | S 10 | 0 | 1 |
| 4 | E | 371 | Total 2987 | C 1948 | N 478 | O 551 | S 10 | 0 | 1 |
| 4 | J | 371 | Total 2987 | C 1948 | N 478 | O 551 | S 10 | 0 | 1 |
| 4 | O | 371 | Total 2987 | C 1948 | N 478 | O 551 | S 10 | 0 | 1 |
| 4 | T | 371 | Total 2987 | C 1948 | N 478 | O 551 | S 10 | 0 | 1 |
| 4 | Y | 371 | Total 2987 | C 1948 | N 478 | O 551 | S 10 | 0 | 1 |

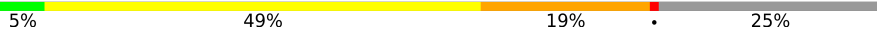
- Molecule 1: Acetylcholine receptor beta subunit



- Molecule 1: Acetylcholine receptor beta subunit






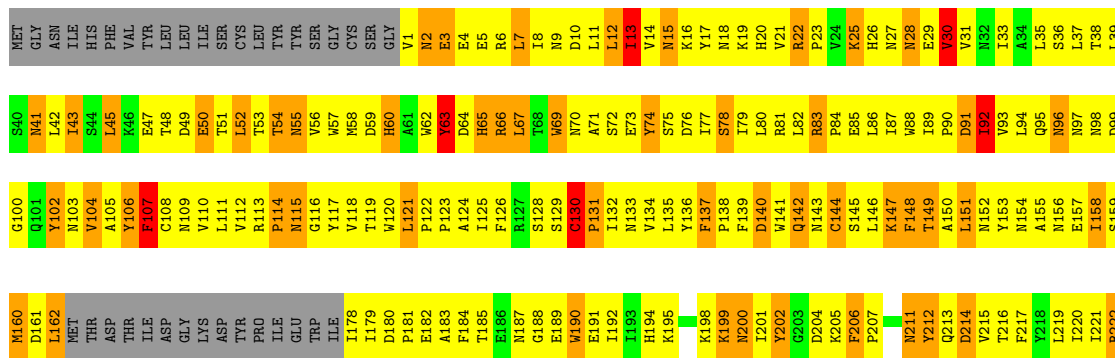
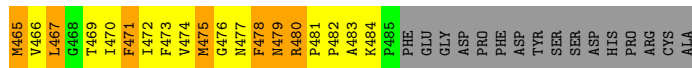
Chain V:  5% 49% 19% 25%

| | | | | | | | | |
|-----|-----|------|------|------|------|-----|------|------|
| MET | L37 | D97 | I157 | P217 | V277 | THR | LEU | A458 |
| GLU | T38 | G98 | L158 | L218 | P278 | THR | PRO | S459 |
| ASP | S39 | S99 | Q159 | F219 | I279 | PRO | GLN | N460 |
| VAL | L40 | F100 | Q159 | Y220 | I280 | SER | ASP | N461 |
| ARG | L41 | E101 | A161 | I221 | I281 | PRO | LEU | N462 |
| ARG | L42 | I102 | L162 | V222 | S282 | ASP | LYS | P463 |
| MET | L43 | T103 | D163 | Y223 | Y283 | SER | E403 | P464 |
| ALA | N44 | T104 | A164 | T224 | L284 | LYS | A404 | D465 |
| LEU | E45 | H105 | LYS | I225 | V405 | PRO | V405 | N466 |
| GLY | K46 | N106 | GLY | V226 | F286 | THR | E406 | P467 |
| LEU | N47 | N107 | GLU | F227 | I287 | ILE | A407 | F468 |
| VAL | E48 | V108 | ARG | C228 | M288 | ILE | I408 | A469 |
| VAL | E49 | L109 | GLU | I229 | I289 | SER | K409 | |
| MET | N50 | V110 | VAL | L230 | L290 | ARG | F410 | |
| MET | T51 | Q111 | LYS | I231 | V291 | ALA | I411 | |
| ALA | T52 | Q112 | GLY | S232 | V292 | ASN | A412 | |
| LEU | S53 | T113 | ILE | I233 | F293 | ASP | E413 | |
| ALA | V54 | G114 | M174 | L234 | S294 | GLU | G414 | |
| LEU | F55 | A115 | I175 | A235 | V295 | TYR | L415 | |
| SER | L56 | V116 | N176 | I236 | I296 | PHE | E416 | |
| GLY | N57 | W118 | Q177 | I237 | I297 | ILE | S417 | |
| VAL | L58 | H119 | D178 | V238 | S298 | ARG | A418 | |
| GLY | A59 | H119 | A179 | F239 | V299 | LYS | S419 | |
| ALA | N60 | F120 | F180 | Y240 | V300 | PRO | E420 | |
| ALA | T61 | S121 | T181 | L241 | V301 | ALA | F421 | |
| V2 | D62 | A122 | E182 | P242 | L302 | GLY | L424 | |
| M3 | Y63 | I123 | N183 | P243 | N303 | ASP | K425 | |
| E4 | R64 | Y124 | G184 | D244 | L304 | PHE | K426 | |
| D6 | L65 | R125 | Q185 | A245 | H305 | VAL | K427 | |
| T6 | O66 | S126 | W186 | G246 | H306 | CYS | W428 | |
| L7 | N67 | S127 | S187 | E247 | R307 | PRO | Q429 | |
| L8 | N68 | C128 | I188 | K248 | S308 | VAL | F430 | |
| S9 | F69 | T129 | E189 | K249 | P309 | ASP | V431 | |
| V10 | N70 | I130 | H190 | S250 | N310 | ASN | A432 | |
| L11 | A71 | L131 | K191 | L251 | T311 | ALA | M433 | |
| F12 | Y72 | M132 | P192 | S252 | H312 | ARG | V434 | |
| E13 | E73 | M133 | S193 | I253 | THR | VAL | A435 | |
| N14 | G74 | Y134 | R194 | S254 | MET | ALA | D436 | |
| Y15 | I75 | F135 | K195 | A255 | PRO | VAL | R437 | |
| N16 | K76 | P136 | N196 | L256 | ASN | GLN | L438 | |
| P17 | D77 | F137 | W197 | L257 | TRP | PRO | F439 | |
| K18 | L78 | D138 | R198 | A258 | ILE | ARG | L440 | |
| V19 | S79 | W139 | S199 | L259 | ARG | LEU | Y441 | |
| R20 | I80 | Q140 | D200 | T260 | GLN | GLN | I442 | |
| P21 | F81 | N141 | D201 | V261 | ILE | PHE | F443 | |
| S22 | S82 | C142 | P202 | F262 | PHE | SER | T444 | |
| Q23 | D83 | T143 | S203 | L263 | ILE | GLU | M445 | |
| T24 | N84 | M144 | Y204 | L264 | GLU | MET | C447 | |
| V25 | Y85 | Y145 | E205 | L265 | THR | LYS | S448 | |
| G26 | N86 | F146 | D206 | L266 | TRP | LEU | I449 | |
| D27 | Q87 | K147 | V207 | A267 | HIS | HIS | G450 | |
| K28 | P88 | T148 | T208 | D268 | LEU | PRO | T451 | |
| V29 | D89 | Y149 | F209 | K269 | ASN | ASN | F452 | |
| T30 | I90 | T150 | Y210 | V270 | GLY | LEU | S453 | |
| V31 | V91 | Y151 | L211 | P271 | TRP | THR | I454 | |
| R32 | I92 | D152 | T212 | E272 | ILE | GLN | F455 | |
| V33 | N93 | T153 | T213 | T273 | GLN | PRO | L456 | |
| G34 | N94 | E154 | Q214 | S274 | ARG | VAL | D457 | |
| L35 | N95 | E155 | R215 | L275 | PRO | THR | | |
| T36 | N96 | V156 | K216 | S276 | VAL | | | |

• Molecule 2: Acetylcholine receptor delta subunit

Chain 1:  7% 44% 19% 29%

| | | | | | | |
|-----|------|------|------|------|------|-----|
| MET | S40 | G100 | M160 | R223 | V285 | GLU |
| GLY | N41 | Q101 | D161 | K224 | P286 | ILE |
| ASN | L42 | Y102 | L162 | P225 | L287 | GLU |
| ILE | I43 | N103 | MET | L226 | I288 | GLN |
| HIS | S44 | V104 | THR | F227 | G289 | PRO |
| PHE | L45 | A105 | ASP | Y228 | K290 | ASP |
| VAL | K46 | Y106 | THR | Y229 | Y291 | TRP |
| TYR | E47 | F107 | ILE | I230 | L292 | GLN |
| LEU | T48 | C108 | ASP | N231 | M293 | ASN |
| LEU | D49 | N109 | GLY | F232 | F294 | ASP |
| LEU | E50 | V110 | LYS | I233 | I295 | LEU |
| SER | T51 | L111 | ASP | T234 | M296 | LYS |
| CYS | L52 | V112 | TYR | P235 | S297 | LEU |
| LEU | T53 | R113 | PRO | | L298 | ARG |
| GLY | T54 | P114 | ILE | L238 | V299 | ARG |
| TYR | N55 | N115 | GLU | I239 | T300 | ARG |
| SER | V56 | G116 | TRP | G240 | G301 | SER |
| GLY | W57 | Y117 | ILE | F241 | V302 | SER |
| CYS | M58 | V118 | GLY | L242 | V303 | VAL |
| SER | D59 | T119 | | A243 | V304 | GLY |
| GLY | H60 | W120 | I178 | A244 | N305 | TYR |
| V1 | A61 | L121 | D180 | A245 | G306 | ILE |
| N2 | W62 | P122 | P181 | A246 | G307 | ILE |
| E3 | Y63 | F123 | E182 | F247 | I308 | SER |
| E4 | D64 | A124 | F184 | Y248 | V309 | LYS |
| E5 | H65 | I125 | T185 | L249 | L310 | ALA |
| R6 | R66 | F126 | E186 | P250 | N311 | GLN |
| L7 | L67 | R127 | N187 | A251 | F312 | GLU |
| I8 | T68 | S128 | G188 | P252 | H313 | TYR |
| N9 | W69 | S129 | E189 | S253 | F314 | PHE |
| D10 | N70 | C130 | W190 | | R315 | ASN |
| L11 | A71 | P131 | E191 | K256 | T316 | ILE |
| L12 | S72 | I132 | I192 | M257 | P317 | LYS |
| I13 | E73 | N133 | H193 | S258 | S318 | SER |
| V14 | Y74 | V134 | H194 | T259 | T319 | ARG |
| N15 | S75 | L135 | K195 | A260 | H320 | GLN |
| K16 | D76 | Y136 | | I261 | VAL | LEU |
| Y17 | I77 | F137 | K198 | C262 | LEU | MET |
| N18 | S78 | P138 | K199 | V263 | SER | PHE |
| K19 | I79 | F139 | N200 | L264 | THR | GLU |
| H20 | L80 | D140 | I201 | L265 | ARG | LYS |
| V21 | R81 | W141 | Y202 | A266 | VAL | GLN |
| R22 | L82 | Q142 | G203 | Q267 | SER | LYS |
| P23 | R83 | N143 | D204 | A268 | GLN | GLY |
| V24 | P84 | C144 | K205 | V269 | ILE | ARG |
| K25 | E85 | S145 | F206 | F270 | PHE | ARG |
| H26 | L86 | L146 | P207 | L271 | GLY | GLY |
| N27 | I87 | K147 | F148 | L272 | LEU | VAL |
| N28 | W88 | T149 | I89 | L273 | LEU | VAL |
| E29 | P90 | T149 | Y212 | T274 | PRO | ARG |
| V30 | D91 | A150 | Q213 | S275 | ARG | ARG |
| V31 | L151 | L151 | Q214 | S276 | VAL | VAL |
| N32 | I92 | N152 | D215 | L277 | THR | THR |
| I33 | V93 | Y153 | T216 | L278 | PRO | PRO |
| A34 | L94 | N154 | L94 | P279 | ARG | ARG |
| L35 | Q95 | A155 | Y218 | E280 | ILE | ILE |
| S36 | N96 | N156 | L219 | T281 | MET | GLY |
| L37 | N97 | E157 | I220 | A282 | SER | PHE |
| T38 | N98 | I158 | I221 | L283 | ARG | GLY |
| L39 | D99 | S159 | R222 | A284 | ASN | ASN |



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| M465 | V466 | L467 | G468 | T469 | I470 | F471 | I472 | F473 | M474 | M475 | G476 | N477 | F478 | N479 | R480 | P481 | P482 | A483 | K484 | P485 | PHE | GLU | GLY | ASP | PRO | PHE | ASP | TYR | SER | SER | ASP | HIS | PRO | ARG | ARG | CYS | ALA | ASN | ASN | GLU | ILE | GLU | GLN | PRO | ASP | ALA | ALA | SER | GLN | ASN | ASP | LEU | HIS | ASP | GLN | LEU | LEU | ARG | ILE | SER | SER | SER | VAL | GLY | TYR | ILE | TYR | ASN | GLN | GLN | GLU | ALA | LYS | LYS | LEU | LEU | ASP | TRP | ASP | PRO | GLN | LEU | Y291 | K290 | G289 | L288 | P286 | V285 | R223 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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• Molecule 2: Acetylcholine receptor delta subunit

Chain M: 7% 43% 19% 29%

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| M465 | V466 | L467 | G468 | T469 | I470 | F471 | I472 | F473 | M474 | M475 | G476 | N477 | F478 | N479 | R480 | P481 | P482 | A483 | K484 | PHE | GLU | GLY | ASP | PRO | PHE | ASP | TYR | SER | SER | ASP | HIS | PRO | PHE | E441 | V442 | G443 | N444 | W445 | W446 | N447 | L448 | V449 | G450 | T451 | I452 | I453 | D454 | R455 | L456 | S457 | M458 | F459 | I460 | I461 | T462 | P463 | V464 | | | | | | | | |
| GLU | ILE | GLU | GLN | PRO | ASP | TRP | GLN | ASN | ASP | LEU | LYS | LEU | ARG | ARG | SER | SER | VAL | GLY | TYR | ILE | G307 | LYS | ALA | GLN | GLU | TYR | PHE | ASN | ILE | LYS | SER | ARG | ARG | GLU | LEU | MET | PHE | GLU | LYS | ARG | VAL | GLN | LYS | ARG | VAL | PRO | ARG | ILE | THR | PRO | ARG | HIS | MET | SER | GLY | ASN | | | | | | | | | |
| V285 | P286 | L287 | G288 | G289 | K290 | Y291 | L292 | M293 | F294 | I295 | M296 | S297 | L298 | V299 | T300 | G301 | V302 | V303 | Y304 | N305 | C306 | G307 | I308 | V309 | L310 | N311 | F312 | H313 | E314 | R315 | T316 | F317 | S318 | T319 | H320 | VAL | LEU | MET | PHE | GLU | THR | LYS | ARG | VAL | GLN | LYS | ILE | PHE | LEU | GLU | LYS | VAL | PRO | ARG | ILE | THR | PRO | ARG | HIS | MET | SER | GLY | PHE | VAL | ASP |
| R223 | K224 | P225 | L226 | F227 | Y228 | V229 | I230 | N231 | F232 | I233 | T234 | P235 | L238 | I239 | S240 | F241 | V242 | A243 | A244 | L245 | A246 | F247 | Y248 | L249 | P250 | A251 | E252 | S253 | K256 | M257 | S258 | T259 | A260 | I261 | C262 | V263 | L264 | A266 | Q267 | A268 | V269 | F270 | L271 | L272 | L273 | T274 | S275 | Q276 | R277 | L278 | P279 | E280 | T281 | A282 | L283 | A284 | | | | | | | | | |
| M160 | D161 | L162 | MET | THR | ASP | THR | ILE | ASP | GLY | LYS | ASP | TYR | PRO | ILE | GLU | TRP | ILE | I178 | I179 | D180 | P181 | E182 | A183 | F184 | T185 | E186 | G188 | E189 | W190 | E191 | I192 | I193 | H194 | K195 | K198 | K199 | N200 | T201 | Y202 | G203 | D204 | K205 | F206 | P207 | N211 | Y212 | Q213 | D214 | V215 | T216 | F217 | Y218 | L219 | I220 | T221 | R222 | | | | | | | | | |
| G100 | Q101 | Y102 | MET | THR | ASP | THR | ILE | ASP | GLY | LYS | ASP | TYR | PRO | ILE | GLU | TRP | ILE | I178 | I179 | D180 | P181 | E182 | A183 | F184 | T185 | E186 | G188 | E189 | W190 | E191 | I192 | I193 | H194 | K195 | K198 | K199 | N200 | T201 | Y202 | G203 | D204 | K205 | F206 | P207 | N211 | Y212 | Q213 | D214 | V215 | T216 | F217 | Y218 | L219 | I220 | T221 | R222 | | | | | | | | | |
| S40 | N41 | L42 | I43 | S44 | A45 | K46 | E47 | T48 | D49 | E50 | T51 | L52 | T53 | T54 | N55 | V56 | M58 | D59 | H60 | A61 | W62 | Y63 | D64 | H65 | R66 | L67 | T68 | W69 | N70 | A71 | S72 | E73 | Y74 | S75 | D76 | I77 | S78 | T79 | L80 | R81 | V82 | R83 | P84 | E85 | L86 | I87 | W88 | I89 | P90 | D91 | I92 | V93 | L94 | Q95 | N96 | N97 | N98 | D99 | | | | | | | |
| MET | GLY | ASN | ILE | HIS | PHE | VAL | TYR | LEU | LEU | ILE | ILE | CYS | LEU | TYR | TYR | SER | GLY | CYS | SER | GLY | V1 | N2 | E3 | E4 | E5 | R6 | L7 | I8 | N9 | D10 | L11 | L12 | I13 | V14 | M15 | K16 | Y17 | N18 | K19 | H20 | V21 | R22 | P23 | V24 | E25 | H26 | N27 | N28 | E29 | V30 | V31 | N32 | I33 | A34 | L35 | S36 | L37 | N38 | T39 | | | | | | |

• Molecule 2: Acetylcholine receptor delta subunit

Chain R: 7% 43% 19% 29%

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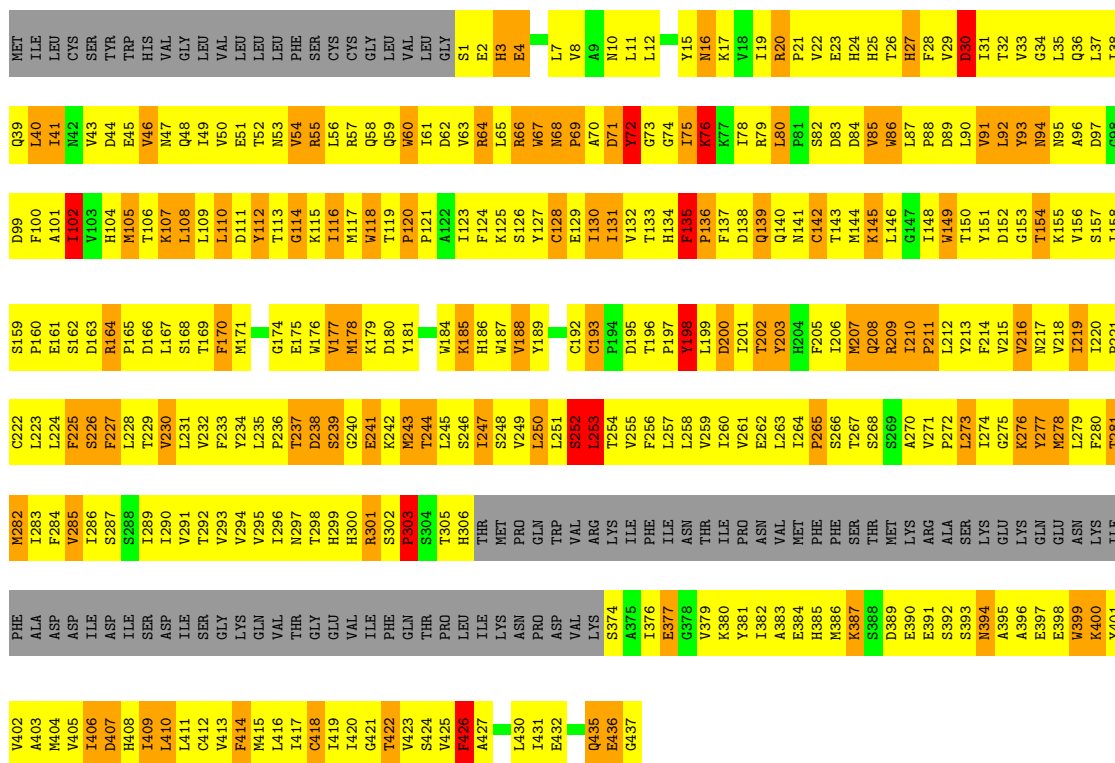
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| | G100 | Q101 | Y102 | N103 | V104 | A105 | Y106 | F107 | C108 | N109 | V110 | L111 | L112 | R113 | P114 | N115 | G116 | Y117 | V118 | T119 | W120 | P121 | E122 | P123 | A124 | I125 | F126 | R127 | S128 | S129 | G130 | P131 | I132 | N133 | V134 | L135 | Y136 | F137 | P138 | F139 | D140 | W141 | Q142 | N143 | C144 | S145 | L146 | K147 | F148 | T149 | A150 | N152 | Y153 | N154 | A155 | N156 | E157 | I158 | S159 | | | | | | | | | | |
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• Molecule 2: Acetylcholine receptor delta subunit

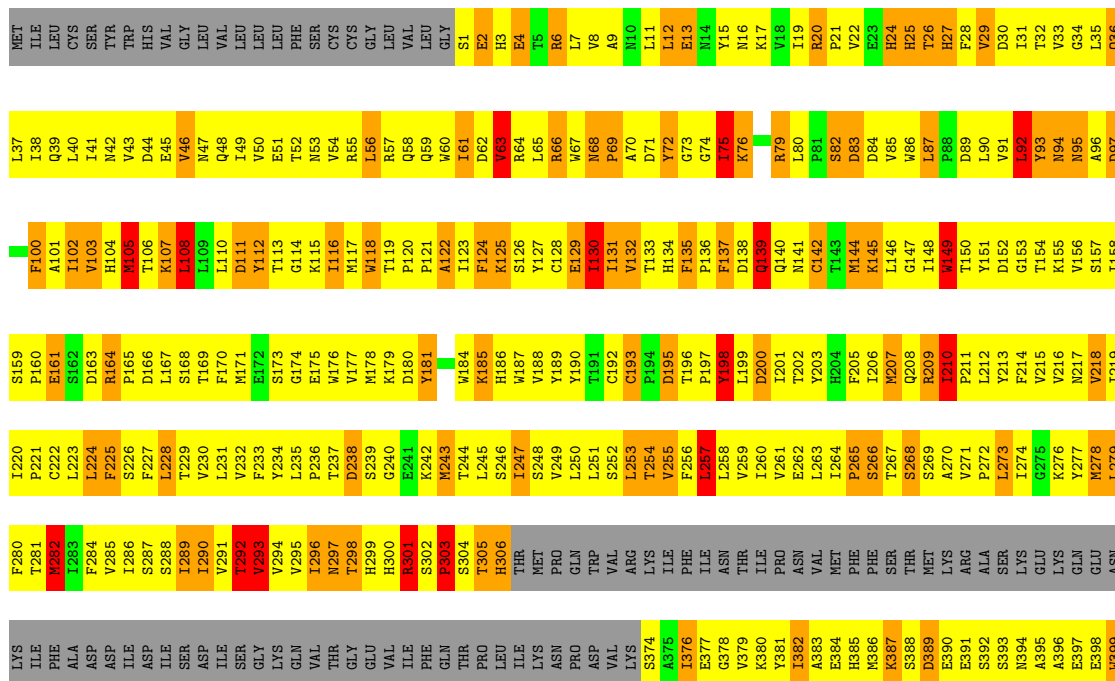
Chain W: 7% 43% 20% • 29%

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| MET | GLY | ASN | ILE | HIS | PHE | VAL | TYR | LEU | TYR | T53 | T54 | N55 | V56 | W57 | M58 | D59 | H60 | GLY | V1 | N2 | E3 | E4 | E5 | H6 | L7 | T8 | N9 | D10 | A71 | S72 | E73 | I13 | V14 | H15 | M16 | K16 | I17 | N18 | F19 | K19 | H20 | V21 | R22 | P23 | V24 | E25 | H26 | N27 | W28 | E29 | P30 | D31 | N32 | V33 | A34 | O35 | N36 | N37 | N38 | D39 | | | | | | | | | | | |
| S40 | M41 | L42 | MET | I43 | S44 | L45 | K46 | E47 | T48 | D49 | E50 | T51 | L52 | T53 | T54 | N55 | V56 | W57 | M58 | D59 | H60 | GLY | A61 | N62 | E63 | D64 | H65 | L66 | T68 | W69 | G70 | S72 | E73 | I13 | V14 | H15 | M16 | K16 | I17 | N18 | F19 | K19 | H20 | V21 | R22 | P23 | V24 | E25 | H26 | N27 | W28 | E29 | P30 | D31 | N32 | V33 | A34 | O35 | N36 | N37 | N38 | D39 | | | | | | | | | |
| G100 | Q101 | Y102 | N103 | V104 | A105 | Y106 | F107 | C108 | N109 | V110 | L111 | V112 | R113 | P114 | N115 | G116 | Y117 | V118 | T119 | W120 | P121 | E122 | P123 | A124 | I125 | F126 | R127 | S128 | S129 | G130 | P131 | I132 | N133 | V134 | L135 | Y136 | F137 | P138 | F139 | D140 | W141 | Y202 | G203 | D204 | K205 | F206 | P207 | N211 | Y212 | Q213 | D214 | V215 | T216 | P217 | Y218 | L219 | I220 | R222 | | | | | | | | | | | | | |
| M160 | D161 | L162 | MET | THR | ASP | THR | ILE | ASP | GLY | LYS | ASP | TYR | PRO | ILE | GLU | TRP | ILE | I178 | I179 | D180 | P181 | E182 | A183 | F184 | T185 | E186 | N187 | G188 | E189 | W190 | E191 | I192 | I193 | H194 | K195 | K198 | K199 | N200 | I201 | Y202 | G203 | D204 | K205 | F206 | P207 | N211 | Y212 | Q213 | D214 | V215 | T216 | P217 | Y218 | L219 | I220 | R222 | | | | | | | | | | | | | | | |
| R223 | K224 | P225 | L226 | F227 | Y228 | V229 | I230 | N231 | F232 | I233 | T234 | P235 | L238 | I239 | G301 | V302 | F303 | L242 | A243 | A244 | L245 | A246 | F247 | Y248 | L249 | P250 | A251 | E252 | S253 | K256 | M257 | S258 | T259 | A260 | I261 | C262 | V263 | L264 | L265 | A266 | Q267 | A268 | V269 | F270 | L271 | L272 | L273 | T274 | S275 | Q276 | L277 | HIS | LEU | GLY | VAL | PRO | ARG | ILE | PRO | ARG | THR | LEU | ARG | HIS | GLY | VAL | LEU | ASP | | | |
| V285 | P286 | L287 | T288 | K289 | Y291 | L292 | M293 | P294 | L295 | M296 | S297 | L298 | V299 | T300 | G301 | V302 | F303 | V304 | N305 | C306 | G307 | L308 | V309 | L310 | N311 | F312 | H313 | F314 | R315 | T316 | P317 | S318 | S319 | VAL | LEU | MET | THR | ARG | GLN | VAL | GLN | GLY | ARG | ILE | A268 | V269 | F270 | L271 | L272 | L273 | T274 | S275 | Q276 | L277 | HIS | LEU | GLY | VAL | PRO | ARG | ILE | PRO | ARG | THR | LEU | ARG | HIS | GLY | VAL | LEU | ASP |
| GLU | ILE | GLN | PRO | ASP | TRP | GLN | ASN | ASP | GLN | LEU | LYS | ASP | ARG | ARG | SER | SER | VAL | GLY | TYR | ILE | SER | LYS | ALA | GLN | GLU | TYR | TYR | PHE | ASN | ILE | LYS | SER | ARG | GLU | LEU | MET | PHE | GLU | LYS | GLN | VAL | GLY | LEU | VAL | ARG | PRO | VAL | THR | PRO | ARG | ILE | GLY | PHE | GLY | VAL | ASN | | | | | | | | | | | | | | | |
| ASN | ASN | GLU | ASN | ILE | ALA | ALA | SER | ASP | GLN | LEU | HIS | ASP | GLU | ILE | LYS | S421 | G422 | I423 | D424 | S425 | T426 | N427 | Y428 | I429 | V430 | K431 | Q432 | I433 | K434 | E435 | K436 | M437 | PRO | ARG | D440 | E441 | E442 | V443 | G444 | M445 | W446 | N447 | L448 | G450 | Q451 | T452 | I453 | D454 | R455 | L456 | S457 | M458 | A459 | I460 | T461 | T462 | P463 | V464 | | | | | | | | | | | | | |
| M465 | V466 | L467 | G468 | T469 | I470 | F471 | I472 | F473 | V474 | M475 | G476 | N477 | F478 | M479 | R480 | P481 | P482 | A483 | K484 | P485 | PHE | GLU | GLY | ASP | PHE | ASP | TYR | TYR | SER | SER | ASP | HIS | PRO | ARG | CYS | ALA | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

• Molecule 3: Acetylcholine receptor subunit alpha



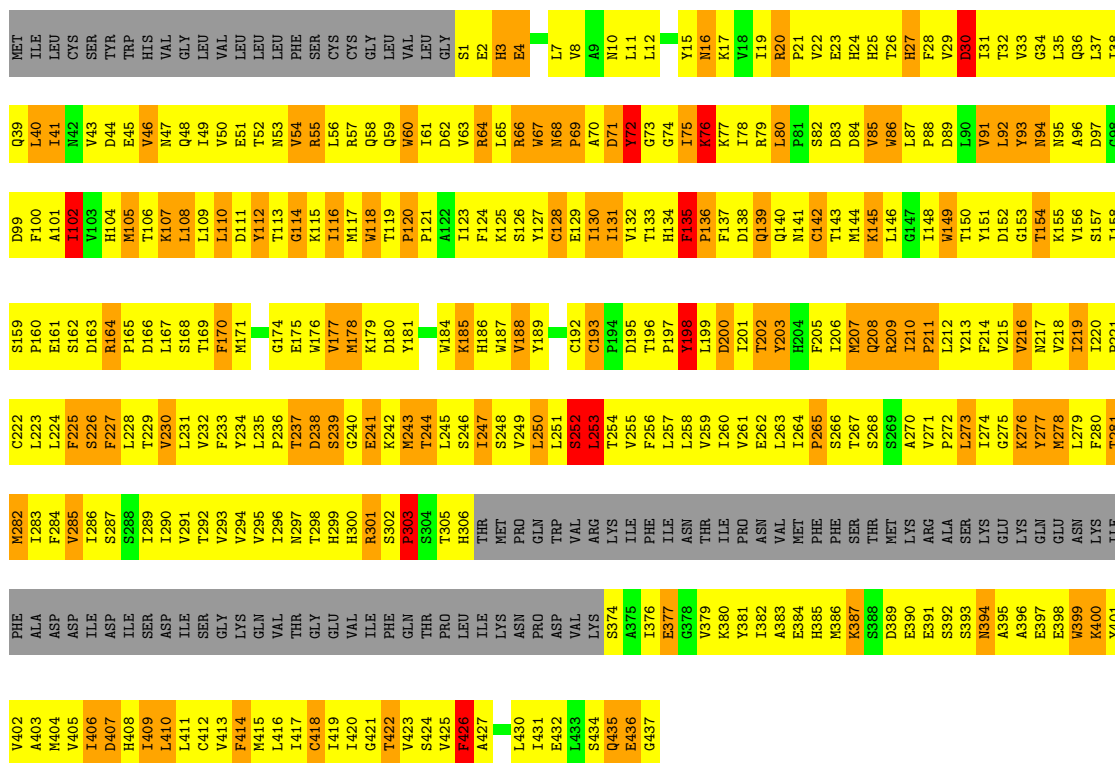
Chain A: 6% 51% 20% 1% 20%





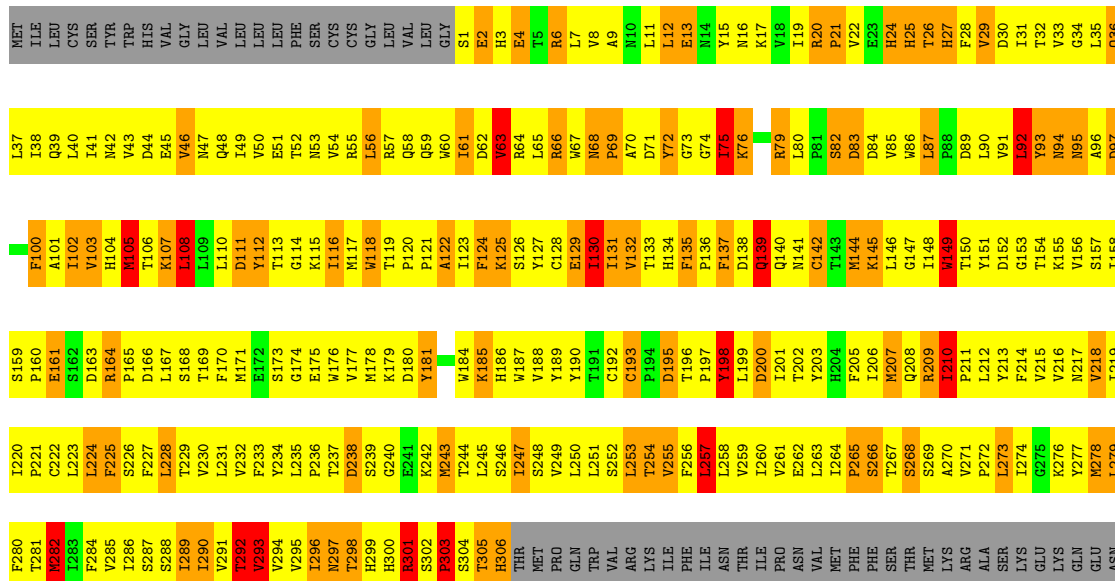
• Molecule 3: Acetylcholine receptor subunit alpha

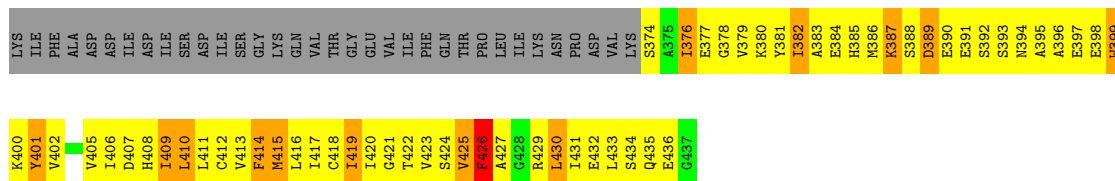
Chain D: 7% 51% 21% 20%



• Molecule 3: Acetylcholine receptor subunit alpha

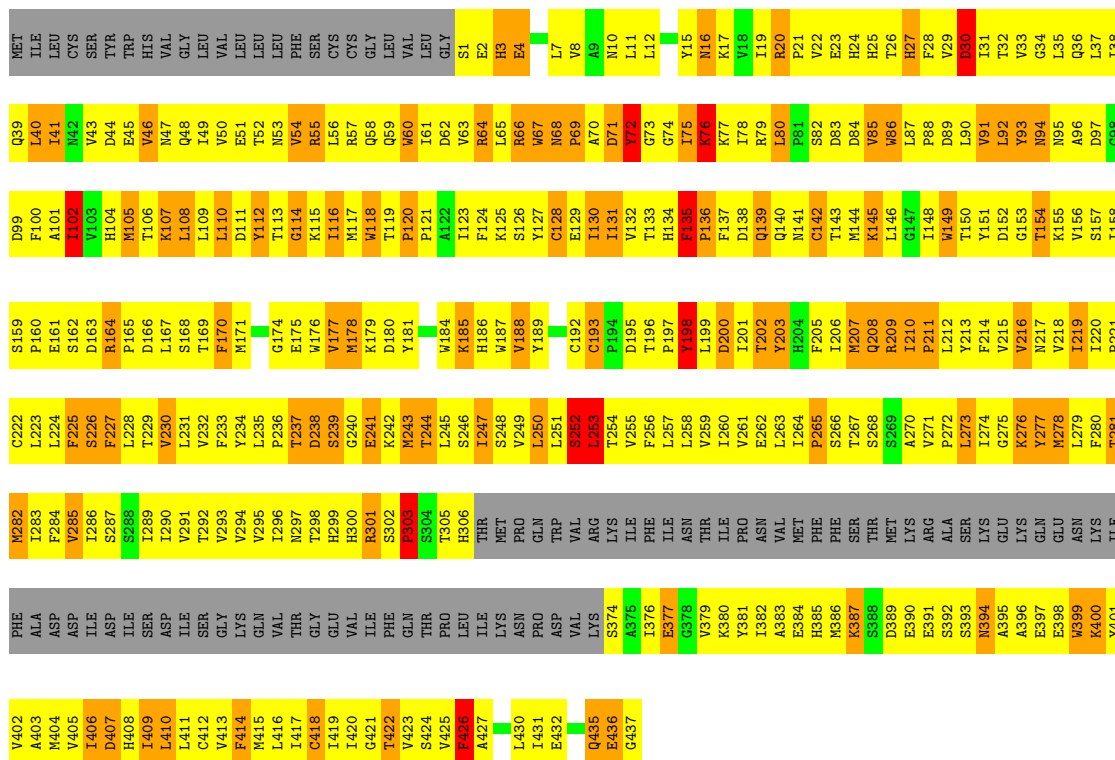
Chain F: 6% 50% 20% 20%





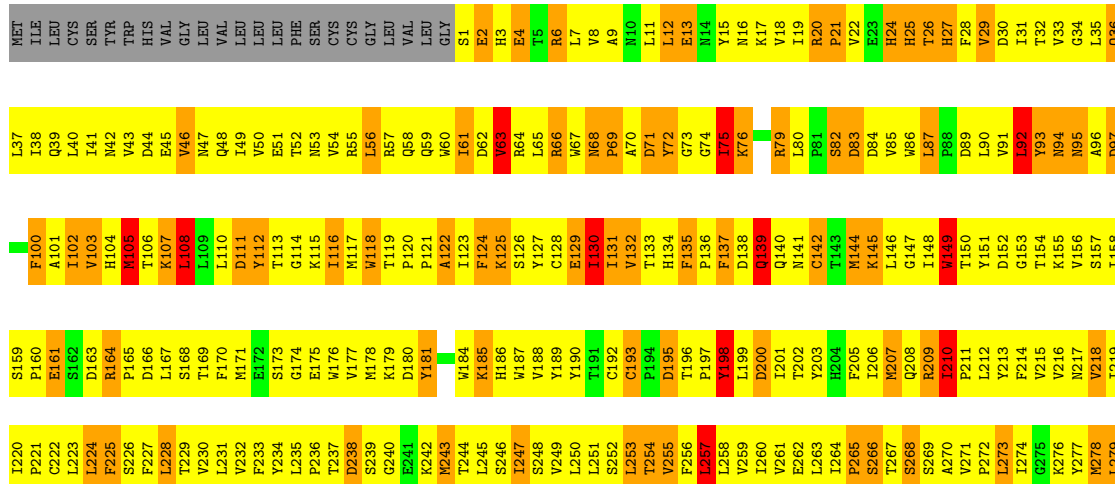
• Molecule 3: Acetylcholine receptor subunit alpha

Chain I: 7% 51% 21% 20%



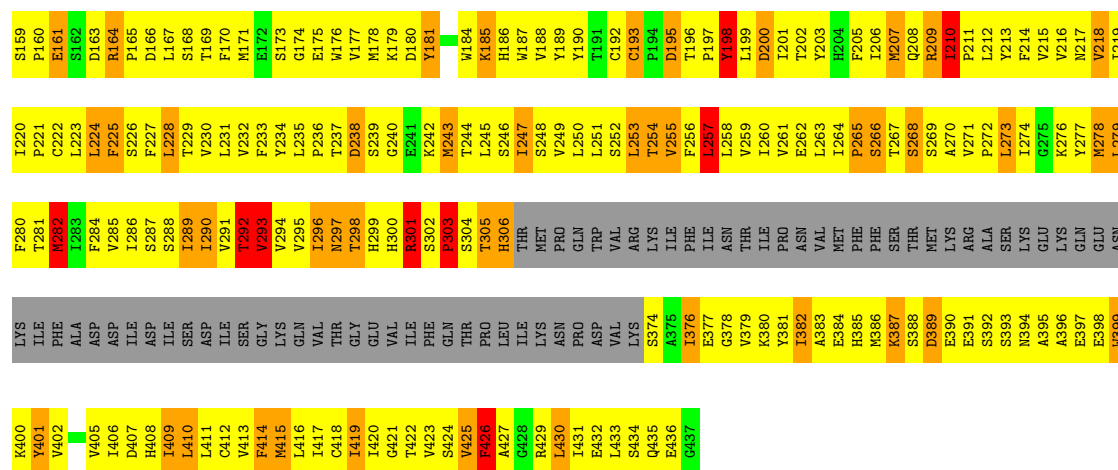
• Molecule 3: Acetylcholine receptor subunit alpha

Chain K: 6% 50% 20% 20%



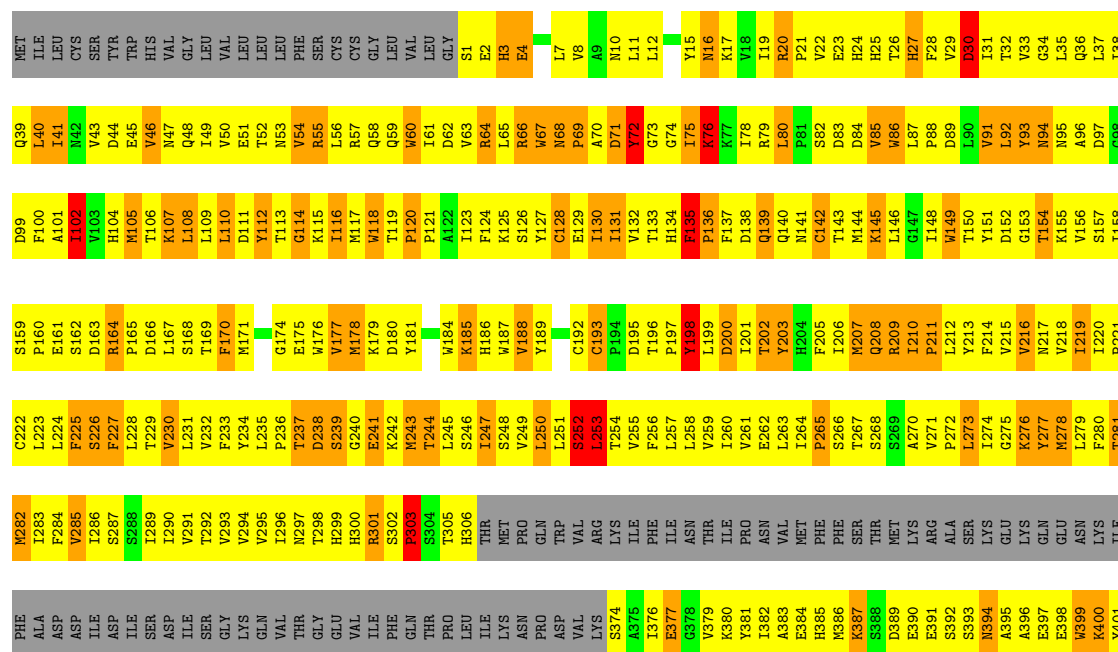






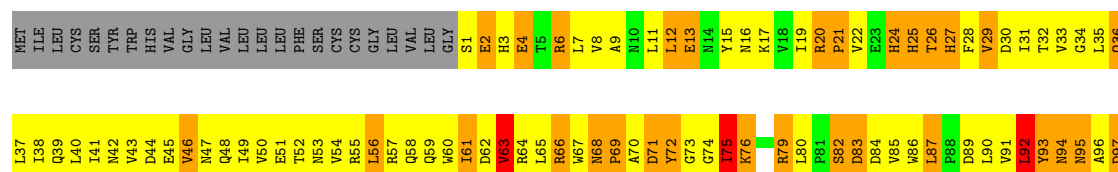
• Molecule 3: Acetylcholine receptor subunit alpha

Chain X: 7% 51% 21% 20%

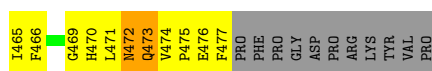


• Molecule 3: Acetylcholine receptor subunit alpha

Chain Z: 6% 50% 20% 20%

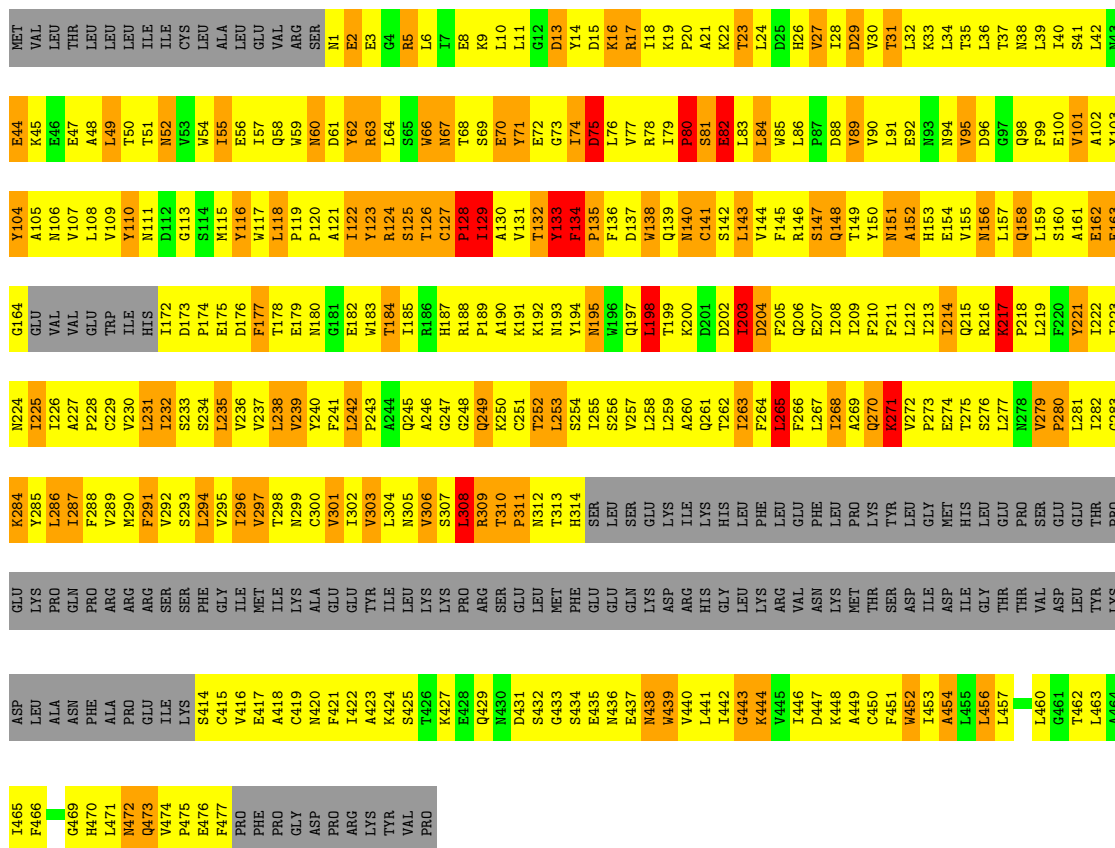


- Molecule 4: Acetylcholine receptor gamma subunit



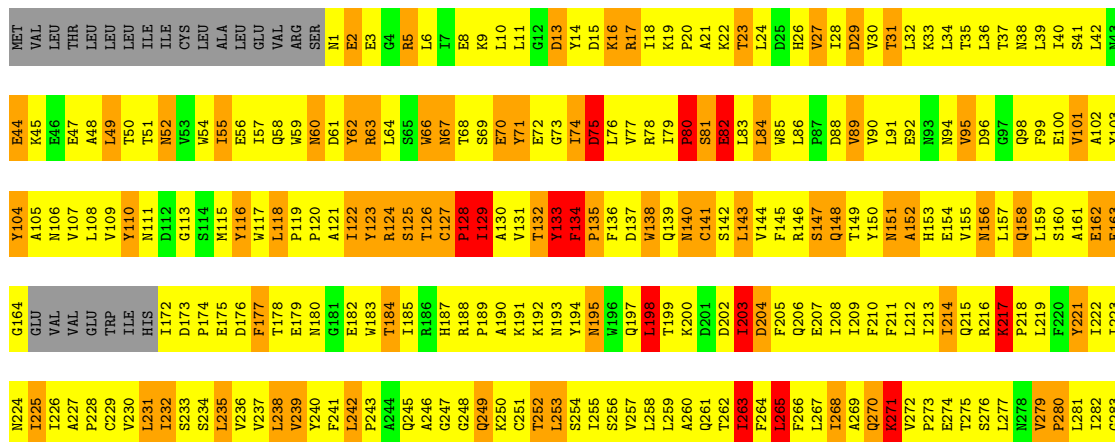
• Molecule 4: Acetylcholine receptor gamma subunit

Chain O: 6% 46% 18% 27%



• Molecule 4: Acetylcholine receptor gamma subunit

Chain T: 6% 46% 18% 27%



- Molecule 4: Acetylcholine receptor gamma subunit



| | | | | | | | | |
|------|------|------|------|------|------|------|------|-----|
| I465 | ASP | GLU | K284 | N224 | G164 | Y104 | E44 | MET |
| F466 | LEU | PRO | Y285 | I225 | GLU | N105 | K45 | VAL |
| G469 | ALA | PRO | I286 | I226 | VAL | N106 | E46 | LEU |
| | ASN | PRO | I287 | A227 | VAL | L107 | E47 | THR |
| | H470 | PRO | F288 | P228 | GLU | L108 | A48 | LEU |
| L471 | ALA | ARG | V289 | C229 | THR | V109 | L49 | LEU |
| M472 | PRO | ARG | K290 | V230 | ILE | Y110 | T50 | LEU |
| Q473 | GLU | ARG | F291 | L231 | HIS | N111 | T51 | ILE |
| V474 | ILE | SER | V292 | I232 | I172 | D112 | N52 | ILE |
| P475 | LYS | SER | S293 | S233 | D173 | G113 | N53 | CYS |
| E476 | S414 | PHE | L294 | S234 | P174 | S114 | N54 | LEU |
| F477 | C415 | GLY | V295 | L235 | E175 | M115 | T55 | ALA |
| PRO | V416 | ILE | I286 | V236 | D176 | Y116 | E56 | LEU |
| PHE | A417 | MET | V297 | V237 | F177 | W117 | T57 | GLU |
| PRO | E418 | ILE | T298 | L238 | T178 | L118 | S58 | VAL |
| GLY | C419 | LYS | N299 | V239 | E179 | P119 | N59 | ARG |
| ASP | M420 | ALA | C300 | Y240 | M180 | P120 | N60 | SER |
| PRO | F421 | GLU | V301 | F241 | G181 | A121 | D61 | N1 |
| ARG | I422 | GLU | I302 | L242 | E182 | I122 | T62 | E2 |
| LYS | A423 | TYR | V303 | P243 | H183 | Y123 | R63 | E3 |
| TYR | K424 | ILE | L304 | A244 | T184 | R124 | L64 | G4 |
| VAL | S425 | LEU | N305 | Q245 | I185 | S125 | S85 | R5 |
| PRO | T426 | LYS | V306 | A246 | R186 | T126 | N66 | L6 |
| | K427 | LYS | S307 | G247 | H187 | C127 | N67 | L7 |
| | E428 | PRO | L308 | G248 | R188 | F128 | T68 | E8 |
| Q429 | ARG | R309 | Q249 | Q249 | A189 | I129 | S69 | K9 |
| M430 | SER | T310 | K250 | A190 | A130 | E70 | L10 | L10 |
| D431 | GLU | GLU | P311 | C251 | K191 | V131 | Y71 | L11 |
| S432 | S432 | MET | N312 | T252 | K192 | T132 | E72 | G12 |
| G433 | G433 | MET | T313 | L253 | N193 | Y133 | G73 | D13 |
| PHE | S434 | PHE | H314 | S264 | K194 | F134 | I74 | GLU |
| E435 | SER | SER | L315 | T265 | N195 | P135 | D75 | D15 |
| M436 | LEU | LEU | S256 | S256 | W196 | F136 | L76 | K16 |
| E437 | GLM | GLM | V257 | V257 | Q197 | T137 | V77 | R17 |
| M438 | LYS | LYS | GLJ | L258 | L198 | W138 | R78 | L18 |
| M439 | ASP | ASP | LYS | L259 | T199 | Q139 | I79 | K19 |
| V440 | ARG | ARG | ILE | A260 | K200 | N140 | P80 | F20 |
| L441 | L441 | HIS | LYS | Q261 | D201 | C141 | S81 | A21 |
| I442 | GLY | GLY | HIS | T262 | D202 | S142 | E82 | K22 |
| G443 | LEU | LEU | LEU | L263 | K203 | L143 | L83 | T23 |
| K444 | PHE | PHE | T264 | F264 | D204 | V144 | L84 | L24 |
| V445 | ARG | ARG | LEU | L265 | F205 | F145 | N85 | T25 |
| I446 | VAL | VAL | GLU | F266 | Q206 | F146 | L86 | H26 |
| D447 | ASN | PHE | PHE | L267 | E207 | S147 | P87 | V27 |
| K448 | LEU | LEU | PRO | L268 | K208 | L148 | D88 | L28 |
| A449 | MET | ARG | PRO | A269 | I209 | T149 | R89 | D29 |
| C450 | THR | LYS | THR | Q270 | F210 | Y150 | N90 | V30 |
| F451 | SER | TYR | TYR | K271 | F211 | N151 | L91 | T31 |
| M452 | ASP | ASP | LEU | V272 | L212 | A152 | E92 | L32 |
| I453 | ILE | GLY | GLY | P273 | I213 | H153 | N93 | K33 |
| A454 | ASP | ASP | MET | E274 | I214 | E154 | N94 | L34 |
| L455 | ILE | HIS | HIS | Q215 | Q215 | N155 | N95 | T35 |
| L456 | GLY | GLY | LEU | T276 | R216 | N156 | D96 | L36 |
| L457 | THR | THR | GLU | L277 | K217 | L157 | G97 | T37 |
| PRO | | THR | PRO | K278 | P218 | Q158 | Q98 | N38 |
| | | VAL | SER | L219 | F159 | P99 | F99 | L39 |
| | L460 | ASP | GLU | P280 | F220 | S160 | E100 | L40 |
| G461 | GLU | GLU | L281 | Y221 | A161 | V101 | S41 | L41 |
| T462 | THR | THR | THR | L282 | I222 | E162 | A102 | L42 |
| L463 | VAL | VAL | PRO | C283 | F463 | K103 | L403 | L43 |

4 Experimental information

| Property | Value | Source |
|--------------------------------------|--------------------------------|-----------|
| EM reconstruction method | TOMOGRAPHY | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of tilted images used | 3564 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | Not provided | |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | 3000 | Depositor |
| Maximum defocus (nm) | 6000 | Depositor |
| Magnification | 80213 | Depositor |
| Image detector | GATAN ULTRASCAN 4000 (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 | O | 0.76 | 2/3048 (0.1%) | 0.99 | 4/4162 (0.1%) |
| 1 | B | 0.76 | 2/3048 (0.1%) | 0.99 | 4/4162 (0.1%) |
| 1 | G | 0.76 | 2/3048 (0.1%) | 0.99 | 4/4162 (0.1%) |
| 1 | L | 0.76 | 2/3048 (0.1%) | 0.99 | 4/4162 (0.1%) |
| 1 | Q | 0.76 | 2/3048 (0.1%) | 0.99 | 4/4162 (0.1%) |
| 1 | V | 0.76 | 2/3048 (0.1%) | 0.99 | 4/4162 (0.1%) |
| 2 | 1 | 0.74 | 2/3059 (0.1%) | 1.03 | 9/4175 (0.2%) |
| 2 | C | 0.74 | 2/3059 (0.1%) | 1.03 | 9/4175 (0.2%) |
| 2 | H | 0.74 | 2/3059 (0.1%) | 1.03 | 8/4175 (0.2%) |
| 2 | M | 0.74 | 2/3059 (0.1%) | 1.03 | 9/4175 (0.2%) |
| 2 | R | 0.74 | 2/3059 (0.1%) | 1.03 | 9/4175 (0.2%) |
| 2 | W | 0.75 | 2/3059 (0.1%) | 1.03 | 8/4175 (0.2%) |
| 3 | 2 | 0.74 | 2/3069 (0.1%) | 1.01 | 6/4186 (0.1%) |
| 3 | A | 0.72 | 3/3069 (0.1%) | 1.03 | 10/4186 (0.2%) |
| 3 | D | 0.74 | 2/3069 (0.1%) | 1.01 | 6/4186 (0.1%) |
| 3 | F | 0.72 | 3/3069 (0.1%) | 1.03 | 10/4186 (0.2%) |
| 3 | I | 0.74 | 2/3069 (0.1%) | 1.01 | 6/4186 (0.1%) |
| 3 | K | 0.72 | 3/3069 (0.1%) | 1.03 | 10/4186 (0.2%) |
| 3 | N | 0.74 | 2/3069 (0.1%) | 1.01 | 6/4186 (0.1%) |
| 3 | P | 0.72 | 3/3069 (0.1%) | 1.03 | 10/4186 (0.2%) |
| 3 | S | 0.74 | 2/3069 (0.1%) | 1.01 | 6/4186 (0.1%) |
| 3 | U | 0.72 | 3/3069 (0.1%) | 1.03 | 10/4186 (0.2%) |
| 3 | X | 0.74 | 2/3069 (0.1%) | 1.01 | 6/4186 (0.1%) |
| 3 | Z | 0.72 | 3/3069 (0.1%) | 1.03 | 10/4186 (0.2%) |
| 4 | 3 | 0.73 | 6/3057 (0.2%) | 1.01 | 9/4174 (0.2%) |
| 4 | E | 0.73 | 6/3057 (0.2%) | 1.01 | 9/4174 (0.2%) |
| 4 | J | 0.73 | 6/3057 (0.2%) | 1.01 | 9/4174 (0.2%) |
| 4 | O | 0.73 | 6/3057 (0.2%) | 1.01 | 9/4174 (0.2%) |
| 4 | T | 0.73 | 6/3057 (0.2%) | 1.01 | 9/4174 (0.2%) |
| 4 | Y | 0.73 | 6/3057 (0.2%) | 1.01 | 9/4174 (0.2%) |
| All | All | 0.74 | 90/91812 (0.1%) | 1.01 | 226/125298 (0.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | 1 | 0 | 2 |
| 2 | C | 0 | 2 |
| 2 | H | 0 | 2 |
| 2 | M | 0 | 2 |
| 2 | R | 0 | 2 |
| 2 | W | 0 | 2 |
| 3 | 2 | 0 | 2 |
| 3 | D | 0 | 2 |
| 3 | I | 0 | 2 |
| 3 | N | 0 | 2 |
| 3 | S | 0 | 2 |
| 3 | X | 0 | 2 |
| All | All | 0 | 24 |

The worst 5 of 90 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | B | 129 | THR | C-N | -8.43 | 1.14 | 1.34 |
| 1 | L | 129 | THR | C-N | -8.42 | 1.14 | 1.34 |
| 1 | V | 129 | THR | C-N | -8.42 | 1.14 | 1.34 |
| 1 | 0 | 129 | THR | C-N | -8.41 | 1.14 | 1.34 |
| 1 | G | 129 | THR | C-N | -8.40 | 1.14 | 1.34 |

The worst 5 of 226 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | M | 266 | ALA | N-CA-CB | 10.41 | 124.67 | 110.10 |
| 2 | C | 266 | ALA | N-CA-CB | 10.40 | 124.66 | 110.10 |
| 2 | 1 | 266 | ALA | N-CA-CB | 10.39 | 124.64 | 110.10 |
| 2 | H | 266 | ALA | N-CA-CB | 10.39 | 124.64 | 110.10 |
| 2 | R | 266 | ALA | N-CA-CB | 10.39 | 124.64 | 110.10 |

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | 1 | 63 | TYR | Sidechain |
| 2 | 1 | 74 | TYR | Sidechain |
| 3 | 2 | 277 | TYR | Sidechain |
| 3 | 2 | 72 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | C | 63 | 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 | 0 | 2972 | 0 | 2952 | 1088 | 0 |
| 1 | B | 2972 | 0 | 2952 | 1083 | 0 |
| 1 | G | 2972 | 0 | 2953 | 1088 | 0 |
| 1 | L | 2972 | 0 | 2953 | 1094 | 0 |
| 1 | Q | 2972 | 0 | 2952 | 1084 | 0 |
| 1 | V | 2972 | 0 | 2952 | 1069 | 0 |
| 2 | 1 | 2983 | 0 | 2987 | 1163 | 0 |
| 2 | C | 2983 | 0 | 2987 | 1152 | 0 |
| 2 | H | 2983 | 0 | 2987 | 1166 | 0 |
| 2 | M | 2983 | 0 | 2987 | 1156 | 0 |
| 2 | R | 2983 | 0 | 2987 | 1158 | 0 |
| 2 | W | 2983 | 0 | 2987 | 1150 | 0 |
| 3 | 2 | 2991 | 0 | 3006 | 1054 | 0 |
| 3 | A | 2991 | 0 | 3005 | 1077 | 0 |
| 3 | D | 2991 | 0 | 3006 | 1060 | 0 |
| 3 | F | 2991 | 0 | 3005 | 1085 | 0 |
| 3 | I | 2991 | 0 | 3006 | 1056 | 0 |
| 3 | K | 2991 | 0 | 3005 | 1077 | 0 |
| 3 | N | 2991 | 0 | 3006 | 1066 | 0 |
| 3 | P | 2991 | 0 | 3005 | 1069 | 0 |
| 3 | S | 2991 | 0 | 3006 | 1052 | 0 |
| 3 | U | 2991 | 0 | 3005 | 1069 | 0 |
| 3 | X | 2991 | 0 | 3006 | 1067 | 0 |
| 3 | Z | 2991 | 0 | 3005 | 1075 | 0 |
| 4 | 3 | 2987 | 0 | 2994 | 1084 | 0 |
| 4 | E | 2987 | 0 | 2994 | 1088 | 0 |
| 4 | J | 2987 | 0 | 2994 | 1093 | 0 |
| 4 | O | 2987 | 0 | 2994 | 1098 | 0 |
| 4 | T | 2987 | 0 | 2994 | 1090 | 0 |
| 4 | Y | 2987 | 0 | 2994 | 1091 | 0 |
| All | All | 89544 | 0 | 89666 | 31224 | 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 174.

The worst 5 of 31224 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) |
|-----------------|------------------|--------------------------|-------------------|
| 4:Y:183:TRP:CB | 4:Y:216:ARG:HG2 | 1.33 | 1.59 |
| 4:3:183:TRP:CB | 4:3:216:ARG:HG2 | 1.33 | 1.56 |
| 4:E:183:TRP:CB | 4:E:216:ARG:HG2 | 1.33 | 1.55 |
| 4:J:183:TRP:CB | 4:J:216:ARG:HG2 | 1.33 | 1.53 |
| 1:G:134:TYR:CE1 | 1:G:213:ILE:HG13 | 1.44 | 1.52 |

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 PDB entries followed by that with respect to all EM entries.

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 | 0 | 364/493 (74%) | 274 (75%) | 58 (16%) | 32 (9%) | 0 | 9 |
| 1 | B | 364/493 (74%) | 274 (75%) | 58 (16%) | 32 (9%) | 0 | 9 |
| 1 | G | 364/493 (74%) | 273 (75%) | 59 (16%) | 32 (9%) | 0 | 9 |
| 1 | L | 364/493 (74%) | 273 (75%) | 59 (16%) | 32 (9%) | 0 | 9 |
| 1 | Q | 364/493 (74%) | 274 (75%) | 58 (16%) | 32 (9%) | 0 | 9 |
| 1 | V | 364/493 (74%) | 274 (75%) | 58 (16%) | 32 (9%) | 0 | 9 |
| 2 | 1 | 364/522 (70%) | 289 (79%) | 57 (16%) | 18 (5%) | 2 | 16 |
| 2 | C | 364/522 (70%) | 289 (79%) | 57 (16%) | 18 (5%) | 2 | 16 |
| 2 | H | 364/522 (70%) | 288 (79%) | 58 (16%) | 18 (5%) | 2 | 16 |
| 2 | M | 364/522 (70%) | 288 (79%) | 58 (16%) | 18 (5%) | 2 | 16 |
| 2 | R | 364/522 (70%) | 288 (79%) | 58 (16%) | 18 (5%) | 2 | 16 |
| 2 | W | 364/522 (70%) | 289 (79%) | 57 (16%) | 18 (5%) | 2 | 16 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|----|
| 3 | 2 | 366/461 (79%) | 294 (80%) | 41 (11%) | 31 (8%) | 0 | 9 |
| 3 | A | 366/461 (79%) | 288 (79%) | 50 (14%) | 28 (8%) | 1 | 10 |
| 3 | D | 366/461 (79%) | 294 (80%) | 41 (11%) | 31 (8%) | 0 | 9 |
| 3 | F | 366/461 (79%) | 288 (79%) | 50 (14%) | 28 (8%) | 1 | 10 |
| 3 | I | 366/461 (79%) | 294 (80%) | 41 (11%) | 31 (8%) | 0 | 9 |
| 3 | K | 366/461 (79%) | 289 (79%) | 48 (13%) | 29 (8%) | 1 | 10 |
| 3 | N | 366/461 (79%) | 293 (80%) | 42 (12%) | 31 (8%) | 0 | 9 |
| 3 | P | 366/461 (79%) | 289 (79%) | 49 (13%) | 28 (8%) | 1 | 10 |
| 3 | S | 366/461 (79%) | 294 (80%) | 41 (11%) | 31 (8%) | 0 | 9 |
| 3 | U | 366/461 (79%) | 288 (79%) | 50 (14%) | 28 (8%) | 1 | 10 |
| 3 | X | 366/461 (79%) | 294 (80%) | 41 (11%) | 31 (8%) | 0 | 9 |
| 3 | Z | 366/461 (79%) | 289 (79%) | 48 (13%) | 29 (8%) | 1 | 10 |
| 4 | 3 | 365/505 (72%) | 281 (77%) | 58 (16%) | 26 (7%) | 1 | 11 |
| 4 | E | 365/505 (72%) | 281 (77%) | 58 (16%) | 26 (7%) | 1 | 11 |
| 4 | J | 365/505 (72%) | 281 (77%) | 58 (16%) | 26 (7%) | 1 | 11 |
| 4 | O | 365/505 (72%) | 281 (77%) | 58 (16%) | 26 (7%) | 1 | 11 |
| 4 | T | 365/505 (72%) | 281 (77%) | 58 (16%) | 26 (7%) | 1 | 11 |
| 4 | Y | 365/505 (72%) | 281 (77%) | 58 (16%) | 26 (7%) | 1 | 11 |
| All | All | 10950/14652 (75%) | 8553 (78%) | 1585 (14%) | 812 (7%) | 2 | 10 |

5 of 812 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 2 | VAL |
| 1 | 0 | 68 | ASP |
| 1 | 0 | 82 | SER |
| 1 | 0 | 95 | ASN |
| 1 | 0 | 131 | LYS |

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 PDB entries followed by that with respect to all EM entries.

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 | 0 | 340/449 (76%) | 262 (77%) | 78 (23%) | 0 | 4 |
| 1 | B | 340/449 (76%) | 262 (77%) | 78 (23%) | 0 | 4 |
| 1 | G | 340/449 (76%) | 263 (77%) | 77 (23%) | 1 | 5 |
| 1 | L | 340/449 (76%) | 262 (77%) | 78 (23%) | 0 | 4 |
| 1 | Q | 340/449 (76%) | 262 (77%) | 78 (23%) | 0 | 4 |
| 1 | V | 340/449 (76%) | 262 (77%) | 78 (23%) | 0 | 4 |
| 2 | 1 | 335/475 (70%) | 244 (73%) | 91 (27%) | 0 | 3 |
| 2 | C | 335/475 (70%) | 243 (72%) | 92 (28%) | 0 | 2 |
| 2 | H | 335/475 (70%) | 244 (73%) | 91 (27%) | 0 | 3 |
| 2 | M | 335/475 (70%) | 244 (73%) | 91 (27%) | 0 | 3 |
| 2 | R | 335/475 (70%) | 243 (72%) | 92 (28%) | 0 | 2 |
| 2 | W | 335/475 (70%) | 243 (72%) | 92 (28%) | 0 | 2 |
| 3 | 2 | 343/427 (80%) | 258 (75%) | 85 (25%) | 0 | 3 |
| 3 | A | 343/427 (80%) | 248 (72%) | 95 (28%) | 0 | 2 |
| 3 | D | 343/427 (80%) | 258 (75%) | 85 (25%) | 0 | 3 |
| 3 | F | 343/427 (80%) | 248 (72%) | 95 (28%) | 0 | 2 |
| 3 | I | 343/427 (80%) | 258 (75%) | 85 (25%) | 0 | 3 |
| 3 | K | 343/427 (80%) | 248 (72%) | 95 (28%) | 0 | 2 |
| 3 | N | 343/427 (80%) | 258 (75%) | 85 (25%) | 0 | 3 |
| 3 | P | 343/427 (80%) | 248 (72%) | 95 (28%) | 0 | 2 |
| 3 | S | 343/427 (80%) | 258 (75%) | 85 (25%) | 0 | 3 |
| 3 | U | 343/427 (80%) | 248 (72%) | 95 (28%) | 0 | 2 |
| 3 | X | 343/427 (80%) | 258 (75%) | 85 (25%) | 0 | 3 |
| 3 | Z | 343/427 (80%) | 248 (72%) | 95 (28%) | 0 | 2 |
| 4 | 3 | 337/463 (73%) | 249 (74%) | 88 (26%) | 0 | 3 |
| 4 | E | 337/463 (73%) | 249 (74%) | 88 (26%) | 0 | 3 |
| 4 | J | 337/463 (73%) | 250 (74%) | 87 (26%) | 0 | 3 |
| 4 | O | 337/463 (73%) | 249 (74%) | 88 (26%) | 0 | 3 |
| 4 | T | 337/463 (73%) | 249 (74%) | 88 (26%) | 0 | 3 |
| 4 | Y | 337/463 (73%) | 249 (74%) | 88 (26%) | 0 | 3 |
| All | All | 10188/13446 (76%) | 7565 (74%) | 2623 (26%) | 2 | 3 |

5 of 2623 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | R | 114 | PRO |
| 2 | W | 121 | LEU |
| 2 | R | 455 | ARG |
| 2 | R | 106 | TYR |
| 4 | T | 308 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 379 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | O | 93 | ASN |
| 3 | S | 134 | HIS |
| 4 | O | 158 | GLN |
| 1 | Q | 460 | HIS |
| 4 | T | 153 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | 0 | 1 |
| 1 | B | 1 |
| 1 | G | 1 |
| 1 | L | 1 |
| 1 | Q | 1 |
| 1 | V | 1 |

The worst 5 of 6 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 0 | 129:THR | C | 130:ILE | N | 1.14 |
| 1 | B | 129:THR | C | 130:ILE | N | 1.14 |
| 1 | G | 129:THR | C | 130:ILE | N | 1.14 |
| 1 | L | 129:THR | C | 130:ILE | N | 1.14 |
| 1 | Q | 129:THR | C | 130:ILE | N | 1.14 |

6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-2376. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis

This section contains the results of statistical analysis of the tomogram.

7.1 Map-value distribution

This section was not generated.

8 Map-model fit

This section was not generated.