



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 12:07 PM EST

PDB ID : 1O1C
EMDB ID : EMD-1001
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM TOMOGRAMS OF INSECT FLIGHT MUSCLE
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.
Deposited on : 2002-11-18
Resolution : 70.00 Å (reported)
Based on initial models : 2MYS, 1ATN

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

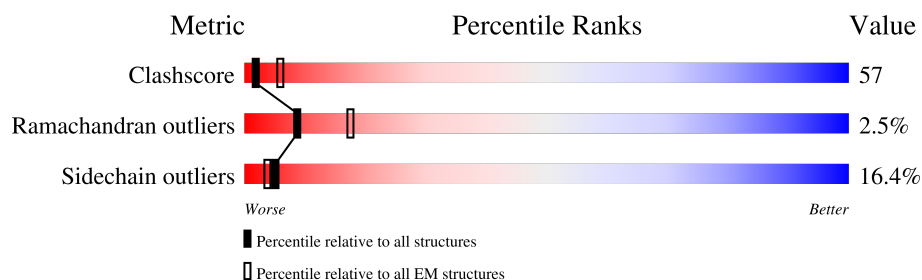
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 70.00 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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 840 | <div> <div>100%</div> <div>25% 50% 20% .</div> </div> |
| 1 | D | 840 | <div> <div>100%</div> <div>26% 51% 19% .</div> </div> |
| 1 | G | 840 | <div> <div>100%</div> <div>25% 51% 21% .</div> </div> |
| 1 | J | 840 | <div> <div>100%</div> <div>25% 50% 20% .</div> </div> |
| 1 | P | 840 | <div> <div>100%</div> <div>25% 51% 20% .</div> </div> |
| 2 | B | 145 | <div> <div>100%</div> <div>66% 26% 6% .</div> </div> |
| 2 | E | 145 | <div> <div>100%</div> <div>64% 27% 6% .</div> </div> |
| 2 | H | 145 | <div> <div>100%</div> <div>62% 29% 6% .</div> </div> |

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| Mol | Chain | Length | Quality of chain | | |
|-----|-------|--------|------------------|-----|-----------|
| 2 | K | 145 | 97% | 64% | 26% 6% . |
| 2 | Q | 145 | 100% | 66% | 26% 6% . |
| 3 | C | 147 | 100% | 60% | 37% . |
| 3 | F | 147 | 84% | 61% | 37% . |
| 3 | I | 147 | 100% | 61% | 37% . |
| 3 | L | 147 | 100% | 61% | 37% . |
| 3 | R | 147 | 100% | 61% | 37% . |
| 4 | 0 | 375 | 99% | 57% | 31% 9% .. |
| 4 | 1 | 375 | 98% | 61% | 31% 6% .. |
| 4 | 2 | 375 | 99% | 61% | 30% 6% .. |
| 4 | 3 | 375 | 99% | 62% | 29% 6% .. |
| 4 | 4 | 375 | 99% | 63% | 29% 6% .. |
| 4 | 5 | 375 | 99% | 64% | 28% 6% .. |
| 4 | 7 | 375 | 99% | 64% | 27% 6% .. |
| 4 | 8 | 375 | 99% | 59% | 31% 8% .. |
| 4 | 9 | 375 | 99% | 58% | 31% 8% .. |
| 4 | V | 375 | 99% | 56% | 33% 9% .. |
| 4 | W | 375 | 99% | 56% | 33% 9% .. |
| 4 | X | 375 | 93% | 61% | 30% 7% .. |
| 4 | Y | 375 | 99% | 62% | 29% 7% .. |
| 4 | Z | 375 | 99% | 62% | 30% 6% .. |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | MLY | A | 505 | - | - | X | - |
| 1 | MLY | A | 553 | - | - | X | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | MLY | A | 764 | - | - | X | - |
| 1 | MLY | A | 782 | - | - | X | - |
| 1 | MLY | A | 837 | - | - | X | - |
| 1 | MLY | A | 839 | - | - | X | - |
| 1 | MLY | D | 553 | - | - | X | - |
| 1 | MLY | D | 764 | - | - | X | - |
| 1 | MLY | D | 782 | - | - | X | - |
| 1 | MLY | G | 505 | - | - | X | - |
| 1 | MLY | G | 553 | - | - | X | - |
| 1 | MLY | G | 764 | - | - | X | - |
| 1 | MLY | G | 84 | - | - | X | - |
| 1 | MLY | J | 505 | - | - | X | - |
| 1 | MLY | J | 553 | - | - | X | - |
| 1 | MLY | J | 839 | - | - | X | - |
| 1 | MLY | J | 84 | - | - | X | - |
| 1 | MLY | P | 505 | - | - | X | - |
| 1 | MLY | P | 839 | - | - | X | - |
| 1 | MLY | P | 84 | - | - | X | - |

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 85919 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 SKELETAL MUSCLE MYOSIN II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | D | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | G | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | J | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | P | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | B | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | E | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | H | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | K | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | Q | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | C | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | F | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | I | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | L | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | R | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |

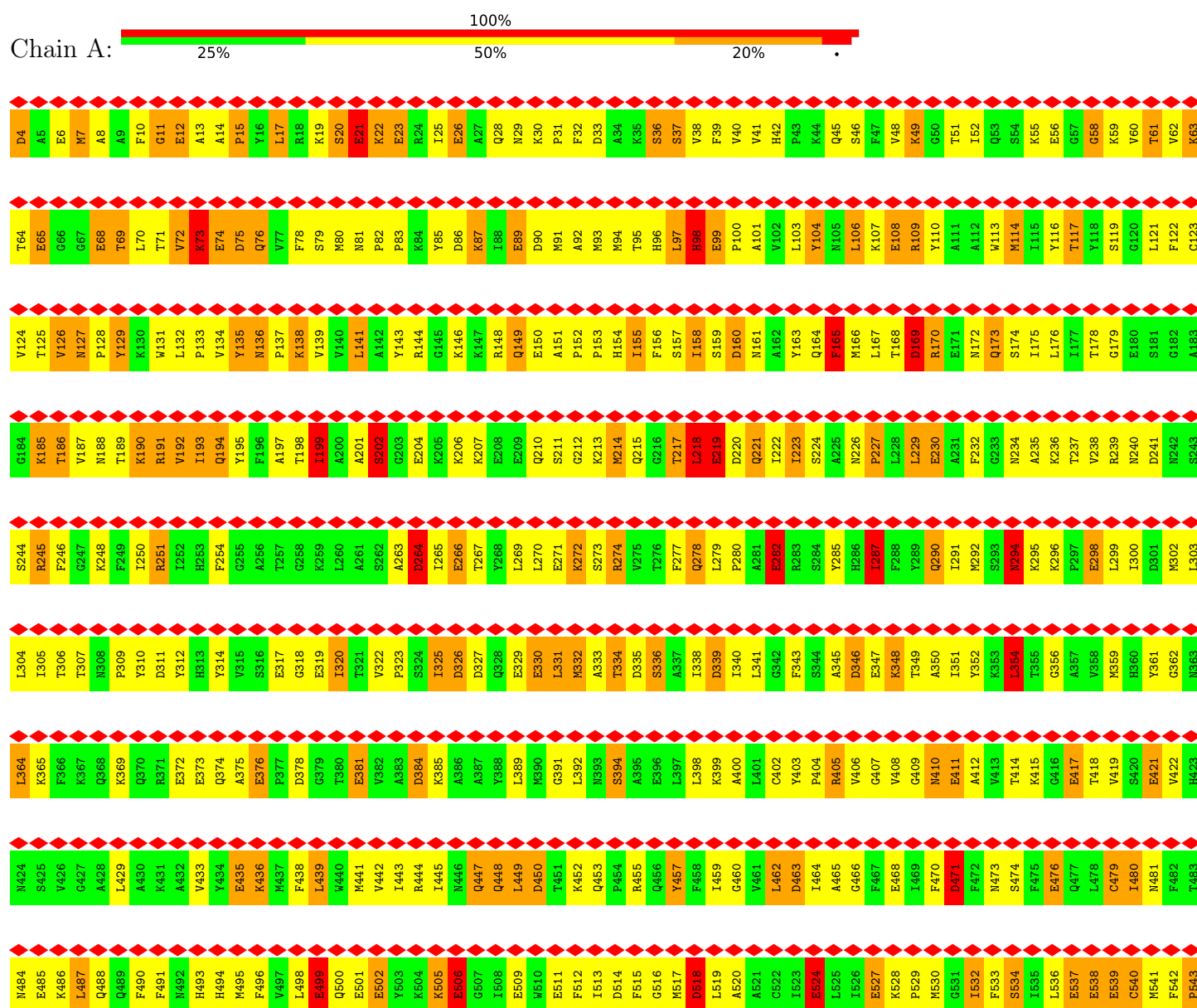
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

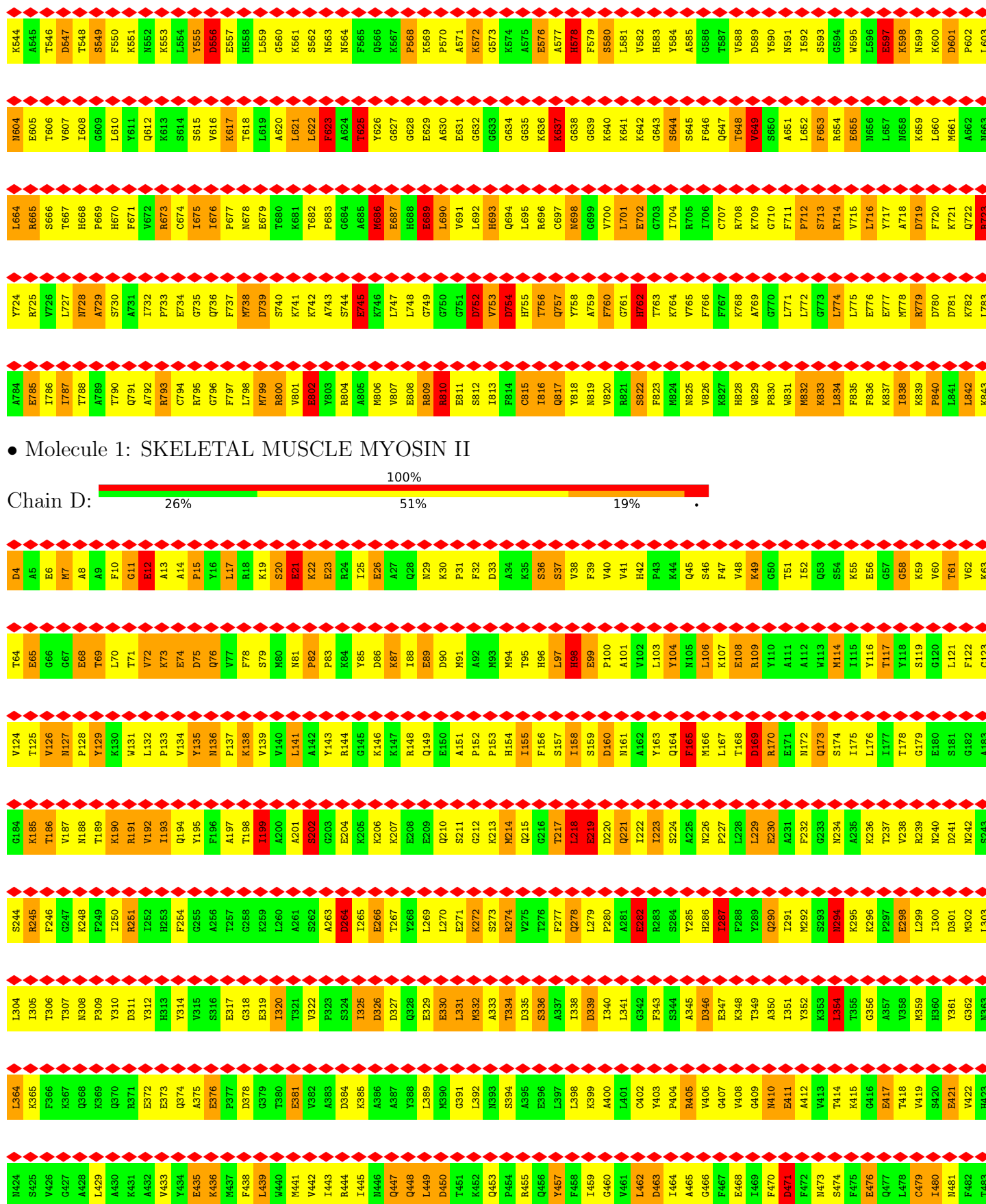
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | 0 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 1 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 2 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 3 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 4 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 5 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 7 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 8 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 9 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | V | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | W | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | X | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | Y | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | Z | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |

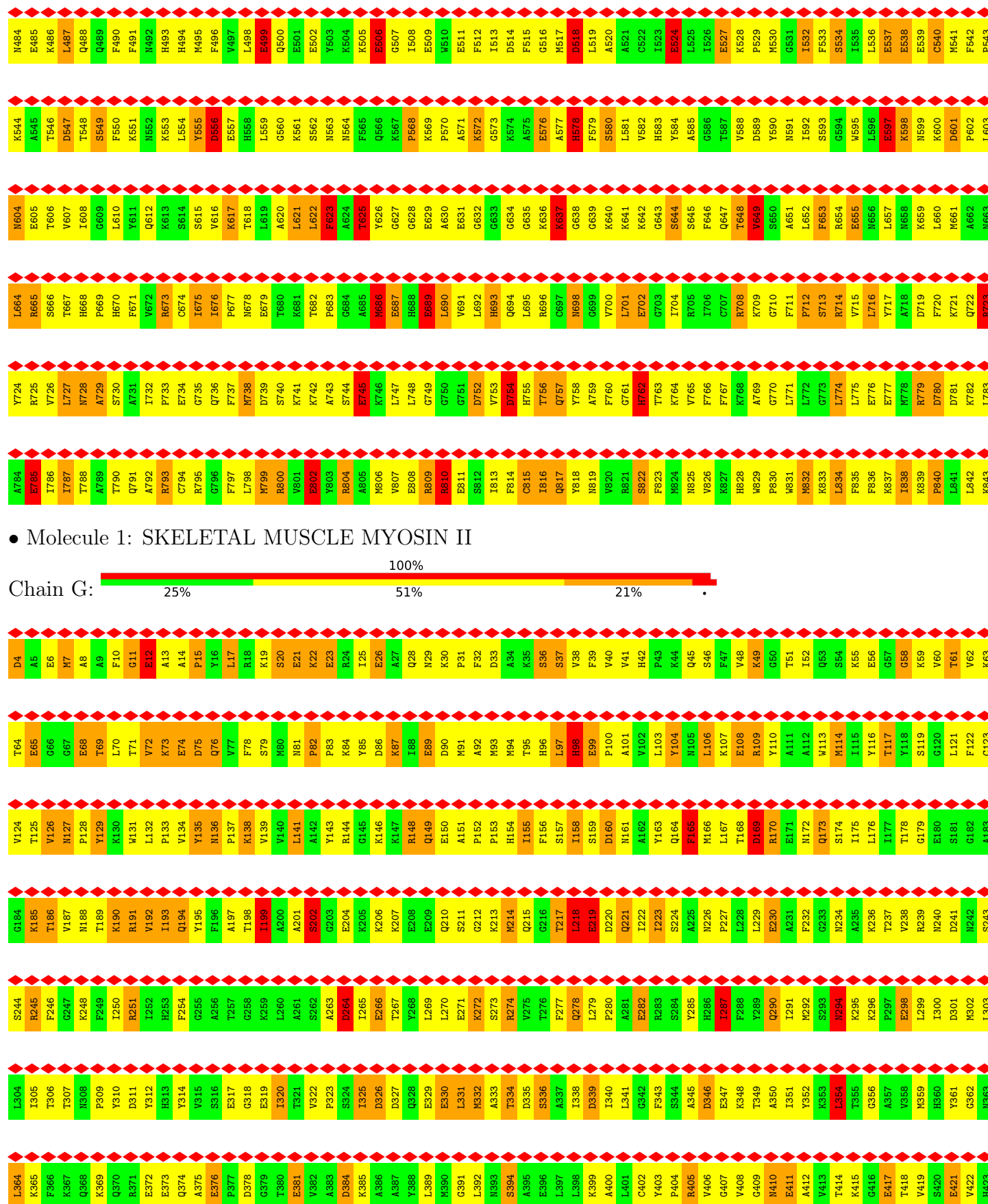
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: SKELETAL MUSCLE MYOSIN II







| | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| N424 | N484 | K544 | N604 | L664 | Y724 | A784 | N424 | N484 | K544 | N604 | L664 | Y724 | A784 |
| S425 | E485 | A545 | E505 | R665 | R725 | E785 | S425 | E485 | A545 | E505 | R665 | R725 | E785 |
| V426 | K486 | T546 | T606 | S666 | V726 | I786 | V426 | K486 | T546 | T606 | S666 | V726 | I786 |
| G427 | L487 | D547 | V607 | T667 | L727 | T787 | G427 | L487 | D547 | V607 | T667 | L727 | T787 |
| A428 | Q488 | S548 | G608 | P668 | M728 | T788 | A428 | Q488 | S548 | G608 | P668 | M728 | T788 |
| L429 | Q489 | S549 | G609 | P669 | A729 | A789 | L429 | Q489 | S549 | G609 | P669 | A729 | A789 |
| A430 | F490 | F550 | L610 | H670 | S730 | T790 | A430 | F490 | F550 | L610 | H670 | S730 | T790 |
| K431 | F491 | K551 | Y611 | F671 | A731 | Q791 | K431 | F491 | K551 | Y611 | F671 | A731 | Q791 |
| A432 | N492 | N552 | Q612 | R672 | I732 | A792 | A432 | N492 | N552 | Q612 | R672 | I732 | A792 |
| V433 | H493 | K553 | K613 | R673 | T733 | R793 | V433 | H493 | K553 | K613 | R673 | T733 | R793 |
| Y434 | H494 | L554 | S614 | C674 | E734 | C794 | Y434 | H494 | L554 | S614 | C674 | E734 | C794 |
| E435 | M495 | Y555 | S615 | I675 | G735 | R795 | E435 | M495 | Y555 | S615 | I675 | G735 | R795 |
| K436 | F496 | D556 | V616 | I676 | Q736 | G796 | K436 | F496 | D556 | V616 | I676 | Q736 | G796 |
| M437 | V497 | V557 | K617 | P677 | F737 | F797 | M437 | V497 | V557 | K617 | P677 | F737 | F797 |
| F438 | L498 | H558 | T618 | N678 | M738 | L798 | F438 | L498 | H558 | T618 | N678 | M738 | L798 |
| L439 | E499 | L559 | L619 | E679 | D739 | M799 | L439 | E499 | L559 | L619 | E679 | D739 | M799 |
| Y440 | Q500 | G560 | A620 | T680 | S740 | R800 | Y440 | Q500 | G560 | A620 | T680 | S740 | R800 |
| M441 | E501 | K561 | L621 | K681 | K741 | V601 | M441 | E501 | K561 | L621 | K681 | K741 | V601 |
| V442 | E502 | S562 | L622 | T682 | K742 | E502 | V442 | E502 | S562 | L622 | T682 | K742 | E502 |
| I443 | Y503 | N563 | F623 | P683 | A743 | R603 | I443 | Y503 | N563 | F623 | P683 | A743 | R603 |
| R444 | K504 | N564 | A624 | G684 | S744 | R604 | R444 | K504 | N564 | A624 | G684 | S744 | R604 |
| I445 | K505 | F565 | T625 | A685 | E745 | A805 | I445 | K505 | F565 | T625 | A685 | E745 | A805 |
| N446 | E506 | Q566 | Y626 | R686 | K746 | M606 | N446 | E506 | Q566 | Y626 | R686 | K746 | M606 |
| Q447 | G507 | K567 | G627 | H687 | L747 | V607 | Q447 | G507 | K567 | G627 | H687 | L747 | V607 |
| Q448 | I508 | P568 | G628 | H688 | L748 | E508 | Q448 | I508 | P568 | G628 | H688 | L748 | E508 |
| L449 | E509 | K569 | E629 | E689 | G749 | R609 | L449 | E509 | K569 | E629 | E689 | G749 | R609 |
| D450 | W510 | P570 | A630 | L690 | G750 | R610 | D450 | W510 | P570 | A630 | L690 | G750 | R610 |
| T451 | E511 | A571 | E631 | V691 | G751 | E611 | T451 | E511 | A571 | E631 | V691 | G751 | E611 |
| K452 | F512 | K572 | G632 | L692 | D752 | S612 | K452 | F512 | K572 | G632 | L692 | D752 | S612 |
| Q453 | I513 | G573 | G633 | H693 | V753 | I613 | Q453 | I513 | G573 | G633 | H693 | V753 | I613 |
| P454 | D514 | K574 | G634 | Q694 | D754 | F614 | P454 | D514 | K574 | G634 | Q694 | D754 | F614 |
| R455 | F515 | A575 | G635 | L695 | H755 | C615 | R455 | F515 | A575 | G635 | L695 | H755 | C615 |
| Q456 | G516 | E576 | K636 | R696 | T756 | I616 | Q456 | G516 | E576 | K636 | R696 | T756 | I616 |
| Y457 | M517 | A577 | K637 | C697 | Q757 | R617 | Y457 | M517 | A577 | K637 | C697 | Q757 | R617 |
| F458 | D518 | H578 | G638 | N698 | Y758 | Y618 | F458 | D518 | H578 | G638 | N698 | Y758 | Y618 |
| I459 | L519 | F579 | G639 | G699 | A759 | N619 | I459 | L519 | F579 | G639 | G699 | A759 | N619 |
| G460 | A520 | S580 | K640 | V700 | F760 | W620 | G460 | A520 | S580 | K640 | V700 | F760 | W620 |
| V461 | E521 | L581 | K641 | L701 | G761 | R621 | V461 | E521 | L581 | K641 | L701 | G761 | R621 |
| L462 | C522 | V582 | K642 | E702 | H762 | S622 | L462 | C522 | V582 | K642 | E702 | H762 | S622 |
| D463 | I523 | H583 | G643 | G703 | T763 | F623 | D463 | I523 | H583 | G643 | G703 | T763 | F623 |
| I464 | E524 | Y584 | S644 | I704 | K764 | M624 | I464 | E524 | Y584 | S644 | I704 | K764 | M624 |
| A465 | L525 | A585 | S645 | R705 | V765 | N625 | A465 | L525 | A585 | S645 | R705 | V765 | N625 |
| G466 | I526 | G586 | F646 | I706 | F766 | V626 | G466 | I526 | G586 | F646 | I706 | F766 | V626 |
| F467 | E527 | T587 | Q647 | C707 | F767 | K627 | F467 | E527 | T587 | Q647 | C707 | F767 | K627 |
| E468 | K528 | V588 | T648 | R708 | K768 | H628 | E468 | K528 | V588 | T648 | R708 | K768 | H628 |
| I469 | P529 | D589 | V649 | K709 | A769 | W629 | I469 | P529 | D589 | V649 | K709 | A769 | W629 |
| F470 | M530 | Y590 | S550 | G710 | G770 | P630 | F470 | M530 | Y590 | S550 | G710 | G770 | P630 |
| D471 | G531 | N591 | A651 | F711 | L771 | W631 | D471 | G531 | N591 | A651 | F711 | L771 | W631 |
| F472 | I532 | L592 | L652 | P712 | L772 | M632 | F472 | I532 | L592 | L652 | P712 | L772 | M632 |
| N473 | F533 | S593 | F653 | S713 | G773 | K633 | N473 | F533 | S593 | F653 | S713 | G773 | K633 |
| S474 | S534 | G594 | R654 | R714 | L774 | L634 | S474 | S534 | G594 | R654 | R714 | L774 | L634 |
| F475 | I535 | W595 | E655 | V715 | L775 | P635 | F475 | I535 | W595 | E655 | V715 | L775 | P635 |
| A476 | L536 | L596 | M556 | L716 | E776 | F636 | A476 | L536 | L596 | M556 | L716 | E776 | F636 |
| Q477 | E537 | R597 | L657 | L717 | F777 | K637 | Q477 | E537 | R597 | L657 | L717 | F777 | K637 |
| L478 | E538 | K598 | M558 | A718 | M778 | T638 | L478 | E538 | K598 | M558 | A718 | M778 | T638 |
| C479 | E539 | N599 | K659 | D719 | R779 | K639 | C479 | E539 | N599 | K659 | D719 | R779 | K639 |
| I480 | C540 | K600 | L660 | F720 | D780 | P640 | I480 | C540 | K600 | L660 | F720 | D780 | P640 |
| N481 | M541 | D601 | M661 | K721 | D781 | L641 | N481 | M541 | D601 | M661 | K721 | D781 | L641 |
| F482 | F542 | P602 | A662 | Q722 | K782 | L642 | F482 | F542 | P602 | A662 | Q722 | K782 | L642 |
| T483 | P543 | L603 | N663 | R723 | L783 | K643 | T483 | P543 | L603 | N663 | R723 | L783 | K643 |

● Molecule 1: SKELETAL MUSCLE MYOSIN II



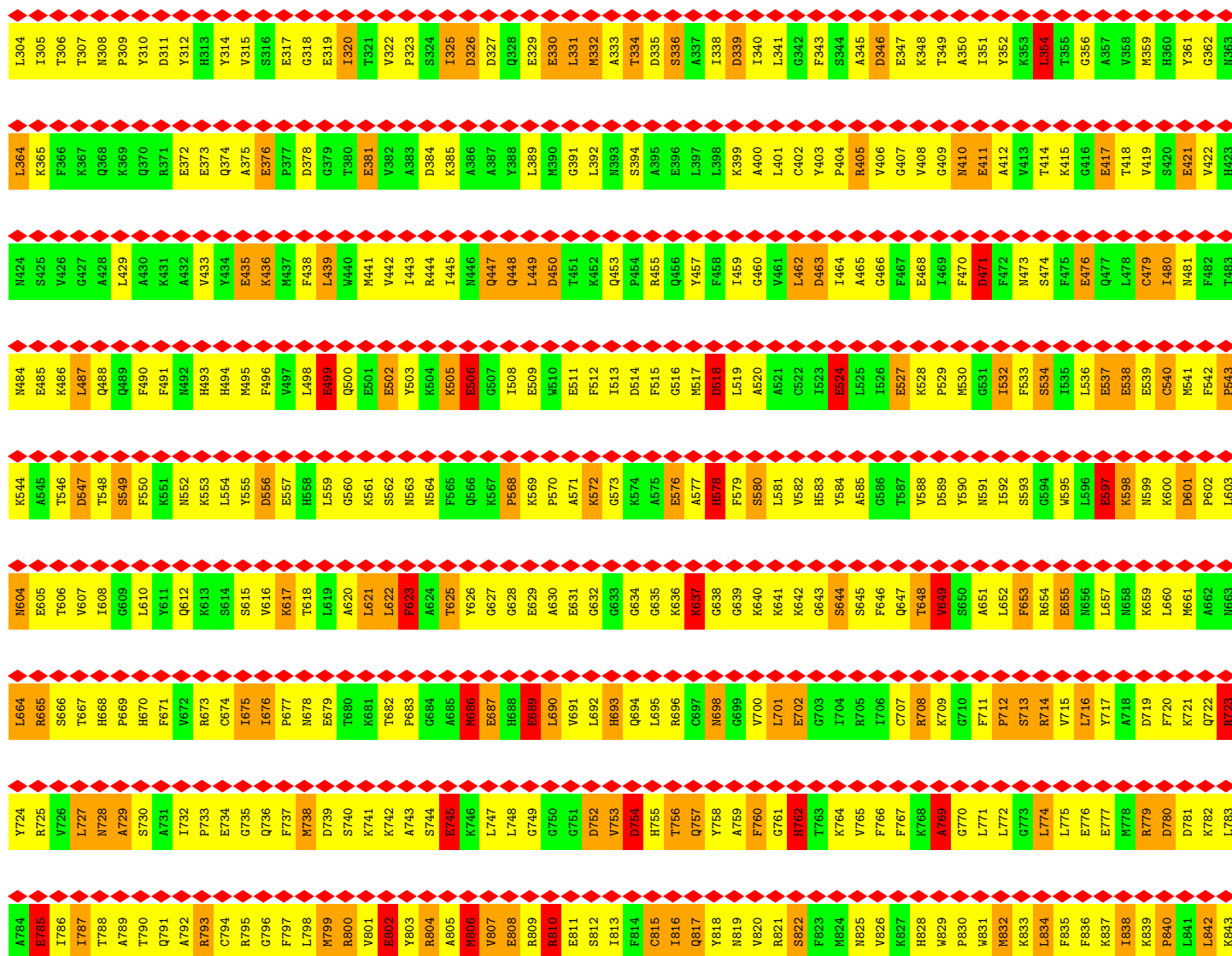
| | | | | | |
|-----|------|------|------|------|------|
| D4 | T64 | V124 | G184 | S244 | L304 |
| A5 | E65 | T125 | K185 | R245 | I305 |
| E6 | G66 | V126 | T186 | F246 | T306 |
| M7 | G67 | M127 | V187 | G247 | T307 |
| A8 | E68 | M128 | N188 | K248 | N308 |
| A9 | T69 | Y129 | T189 | F249 | P309 |
| F10 | L70 | K130 | K190 | L250 | Y310 |
| G11 | T71 | W131 | R191 | R251 | D311 |
| E12 | V72 | L132 | V192 | L252 | Y312 |
| A13 | K73 | P133 | I193 | H253 | H313 |
| A14 | E74 | V134 | Q194 | F254 | Y314 |
| P15 | D75 | Y135 | Y195 | G255 | V315 |
| Y16 | Q76 | M136 | F196 | G256 | S316 |
| L17 | V77 | P137 | A197 | T257 | E317 |
| R18 | F78 | K138 | T198 | G258 | G318 |
| K19 | S79 | V139 | I199 | K259 | E319 |
| S20 | M80 | Y140 | A200 | L260 | I320 |
| E21 | N81 | L141 | A201 | A261 | T321 |
| K22 | P82 | A142 | S202 | S262 | V322 |
| R23 | K83 | Y143 | G203 | A263 | P323 |
| G24 | K84 | G145 | E204 | D264 | S324 |
| I25 | Y85 | G146 | K206 | L265 | I325 |
| E26 | D86 | K146 | K206 | E266 | D326 |
| A27 | K87 | L147 | K207 | T267 | D327 |
| Q28 | T88 | R148 | E208 | T268 | Q328 |
| N29 | E89 | Q149 | E209 | L269 | E329 |
| K30 | D90 | E150 | Q210 | L270 | E330 |
| P31 | M91 | A151 | S211 | E271 | L331 |
| F32 | A92 | P152 | G212 | K272 | K332 |
| D33 | M93 | P153 | K213 | S273 | A333 |
| A34 | M94 | H154 | M214 | R274 | T334 |
| K35 | T95 | I155 | Q215 | V275 | D335 |
| S36 | H96 | F156 | G216 | T276 | S336 |
| S37 | L97 | S157 | T217 | F277 | A337 |
| V38 | H98 | I158 | L218 | Q278 | I338 |
| F39 | E99 | S159 | E219 | L279 | D339 |
| V40 | P100 | D160 | D220 | P280 | I340 |
| V41 | A101 | M161 | Q221 | A281 | L341 |
| H42 | Y102 | A162 | I222 | E282 | G342 |
| P43 | L103 | Y163 | I223 | R283 | F343 |
| K44 | Y104 | Q164 | S224 | S284 | S344 |
| Q45 | N105 | F165 | A225 | Y285 | A345 |
| S46 | L106 | M166 | N226 | H286 | D346 |
| F47 | K107 | L167 | P227 | T287 | E347 |
| V48 | E108 | T168 | L228 | F288 | K348 |
| K49 | R109 | D169 | L229 | Y289 | T349 |
| G50 | Y110 | R170 | E230 | Q290 | A350 |
| T51 | A111 | E171 | A231 | I291 | I351 |
| I52 | A112 | M172 | G232 | M292 | Y352 |
| Q53 | V113 | Q173 | F233 | K293 | K353 |
| S54 | M114 | S174 | N234 | D294 | L354 |
| K55 | I115 | T175 | A235 | K295 | T355 |
| E56 | Y116 | L176 | K236 | K296 | G356 |
| G57 | T117 | I177 | T237 | P297 | A357 |
| G58 | Y118 | T178 | V238 | E298 | V358 |
| K59 | S119 | G179 | R239 | L299 | K359 |
| V60 | G120 | E180 | N240 | T300 | H360 |
| T61 | L121 | S181 | D241 | Y361 | N361 |
| V62 | F122 | G182 | N242 | K362 | G362 |
| K63 | C123 | A183 | S243 | L303 | N363 |

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A784 | E785 | I786 | T787 | T788 | A789 | T790 | Q791 | A792 | R793 | C794 | R795 | G796 | F797 | L798 | M799 | V800 | E802 | Y803 | R804 | A805 | M806 | V807 | E808 | R809 | E810 | E811 | S812 | L813 | F814 | C815 | L816 | Q817 | Y818 | N819 | V820 | R821 | S822 | F823 | M824 | N825 | V826 | K827 | H828 | V829 | P830 | M831 | N832 | K833 | L834 | F835 | P836 | K837 | T838 | K839 | P840 | L841 | L842 | K843 | | |
| Y724 | R725 | V726 | L727 | H728 | A729 | S730 | A731 | I732 | P733 | E734 | G735 | Q736 | F737 | M738 | D739 | S740 | K741 | K742 | A743 | S744 | E745 | K746 | L747 | L748 | G749 | G750 | G751 | D752 | V753 | D754 | H755 | T756 | Q757 | Y758 | A759 | F760 | G761 | R762 | T763 | K764 | V765 | F766 | F767 | K768 | A769 | G770 | L771 | L772 | G773 | L774 | L775 | E776 | E777 | M778 | R779 | D780 | D781 | K782 | L783 | |
| L664 | R665 | S666 | T667 | H668 | P669 | H670 | F671 | V672 | K673 | C674 | I675 | I676 | P677 | N678 | E679 | T680 | K681 | T682 | G683 | G684 | A685 | M686 | G687 | H688 | E689 | L690 | V691 | L692 | H693 | Q694 | L695 | R696 | G697 | N698 | G699 | V700 | L701 | E702 | G703 | I704 | R705 | F706 | G707 | K708 | K709 | G710 | F711 | P712 | S713 | R714 | V715 | L716 | Y717 | A718 | D719 | F720 | D781 | K721 | Q722 | R723 |
| N604 | E605 | T606 | V607 | I608 | G609 | L610 | Y611 | Q612 | K613 | S614 | S615 | V616 | K617 | T618 | L619 | A620 | L621 | L622 | F623 | A624 | T625 | Y626 | G627 | G628 | E629 | A630 | E631 | G632 | G633 | G634 | G635 | K636 | K637 | G638 | G639 | K640 | K641 | K642 | G643 | S644 | S645 | F646 | Q647 | T648 | V649 | S650 | A651 | L652 | F653 | R654 | E655 | M656 | L657 | M658 | K659 | L660 | M661 | A662 | N663 | |
| K544 | A545 | T546 | D547 | S548 | F549 | F550 | K551 | N552 | K553 | L554 | D555 | D556 | E557 | H558 | L559 | G560 | S561 | S562 | Y563 | N564 | F565 | Q566 | K567 | P568 | K569 | P570 | A571 | K572 | G573 | D574 | A575 | E576 | A577 | H578 | F579 | S580 | L581 | V582 | H583 | Y584 | A585 | G586 | T587 | V588 | D589 | Y590 | N591 | I592 | F593 | S593 | G594 | A595 | L596 | E597 | K598 | E599 | K600 | D601 | P602 | L603 |
| N484 | E485 | K486 | L487 | Q488 | Q489 | F490 | F491 | N492 | H493 | H494 | M495 | F496 | D497 | L498 | E499 | Q500 | E501 | E502 | Y503 | K504 | K505 | E506 | G507 | I508 | E509 | W510 | E511 | F512 | I513 | D514 | F515 | G516 | N517 | D518 | L519 | A520 | A521 | C522 | I523 | E524 | L525 | I526 | E527 | K528 | P529 | M530 | G531 | I532 | F533 | S534 | I535 | L536 | E537 | E538 | E539 | C540 | M541 | F542 | P543 | |
| N424 | S425 | V426 | G427 | A428 | L429 | A430 | K431 | A432 | V433 | Y434 | E435 | K436 | M437 | F438 | L439 | M440 | V442 | I443 | R444 | I445 | M446 | Q447 | Q448 | L449 | D450 | T451 | K452 | Q453 | P454 | R455 | Q456 | Y457 | F458 | I459 | G460 | V461 | L462 | D463 | I464 | A465 | G466 | F467 | E468 | I469 | F470 | D471 | F472 | N473 | S474 | F475 | E476 | Q477 | L478 | C479 | I480 | M481 | F482 | T483 | | |
| L364 | K365 | F366 | K367 | Q368 | K369 | Q370 | R371 | E372 | E373 | Q374 | A375 | E376 | P377 | D378 | G379 | T380 | E381 | V382 | A383 | D384 | K385 | A386 | A387 | L388 | L389 | M390 | G391 | L392 | N393 | S394 | A395 | E396 | L397 | L398 | K399 | A400 | L401 | C402 | Y403 | P404 | R405 | V406 | G407 | V408 | G409 | N410 | E411 | A412 | V413 | T414 | K415 | G416 | E417 | T418 | V419 | S420 | E421 | F422 | H423 | |

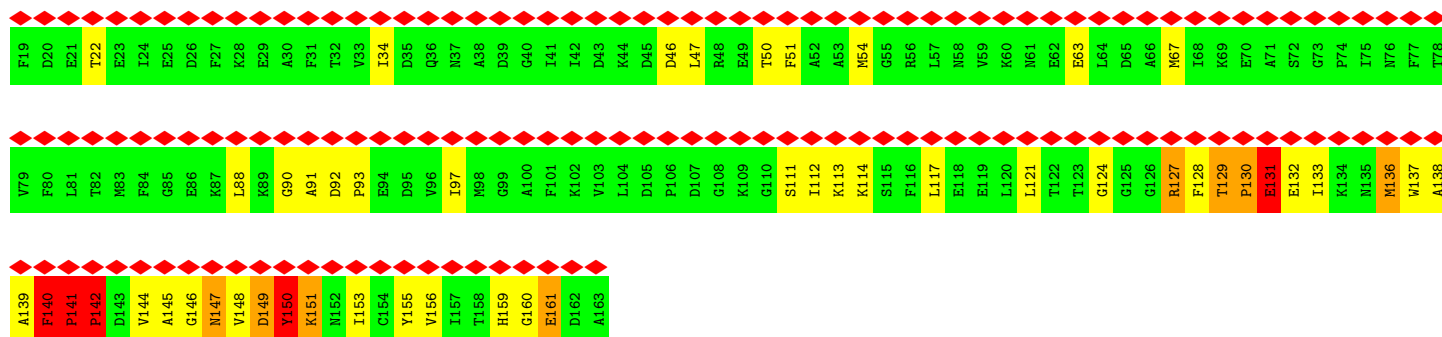
• Molecule 1: SKELETAL MUSCLE MYOSIN II



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D4 | A5 | E6 | M7 | A8 | A9 | F10 | G11 | E12 | A13 | A14 | P15 | Y16 | L17 | R18 | K19 | S20 | E21 | K22 | E23 | R24 | T25 | E26 | Q27 | N28 | K29 | P30 | F31 | F32 | D33 | A34 | K35 | S36 | S37 | V38 | F39 | V40 | V41 | H42 | P43 | K44 | Q45 | S46 | F47 | V48 | G49 | T50 | I51 | I52 | Q53 | S54 | K55 | E56 | G57 | G58 | K59 | V60 | T61 | V62 | K63 | |
| T64 | E65 | G66 | G67 | E68 | T69 | L70 | T71 | V72 | K73 | E74 | D75 | Q76 | V77 | F78 | S79 | M80 | P81 | P82 | P83 | K84 | G85 | D86 | K87 | T88 | E89 | D90 | N91 | A92 | P93 | N94 | T95 | H96 | L97 | H98 | E99 | P100 | A101 | V102 | L103 | Y104 | N105 | L106 | E107 | K107 | E108 | R109 | Y110 | A111 | A112 | M113 | M114 | I115 | Y116 | T117 | Y118 | S119 | G120 | L121 | F122 | C123 |
| V124 | T125 | V126 | N127 | P128 | Y129 | K130 | V131 | L132 | P133 | V134 | Y135 | N136 | P137 | K138 | V139 | Y140 | L141 | A142 | Y143 | G144 | L145 | K146 | K147 | R148 | Q149 | E150 | A151 | P152 | P153 | H154 | I155 | F156 | S157 | I158 | S159 | D160 | N161 | A162 | L163 | Q164 | F165 | M166 | L167 | T168 | D169 | R170 | E171 | M172 | Q173 | S174 | I175 | L176 | T177 | T178 | G179 | E180 | S181 | G182 | A183 | |
| G184 | K185 | T186 | V187 | N188 | T189 | K190 | R191 | V192 | I193 | Q194 | Y195 | F196 | A197 | T198 | N199 | A200 | A201 | S202 | G203 | E204 | K205 | K206 | K207 | E208 | E209 | Q210 | S211 | G212 | K213 | M214 | Q215 | G216 | T217 | L218 | E219 | D220 | Q221 | I222 | I223 | S224 | A225 | N226 | P227 | L228 | L229 | E230 | A231 | F232 | Q233 | N234 | A235 | K236 | T237 | V238 | R239 | I240 | D241 | N242 | S243 | |
| S244 | R245 | F246 | G247 | K248 | F249 | L250 | R251 | L252 | H253 | F254 | G255 | A256 | T257 | G258 | K259 | L260 | A261 | S262 | A263 | D264 | L265 | E266 | T267 | Y268 | L269 | L270 | E271 | K272 | S273 | R274 | V275 | T276 | Q277 | Q278 | L279 | P280 | A281 | E282 | R283 | S284 | Y285 | H286 | F287 | F288 | Y289 | Q290 | I291 | M292 | K293 | N294 | K295 | K296 | T297 | E298 | L299 | I300 | D301 | M302 | L303 | |

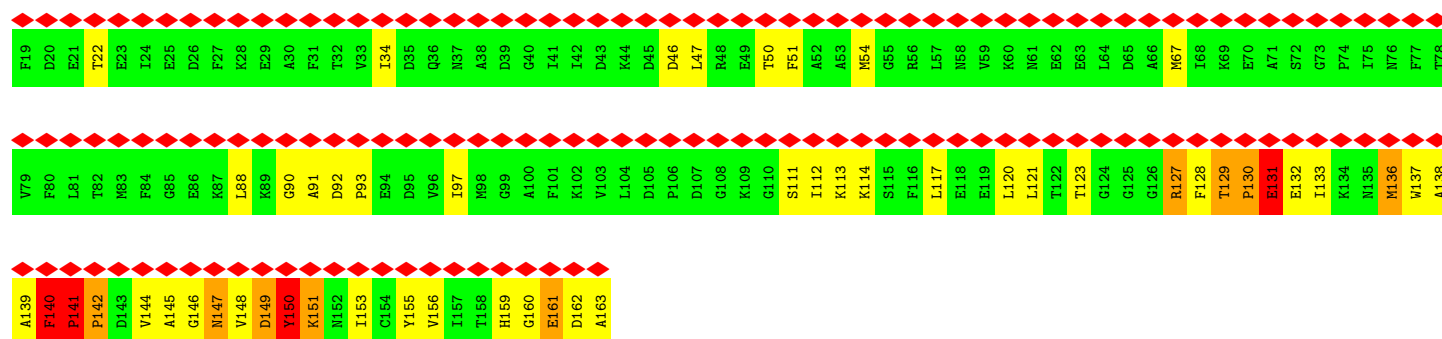


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

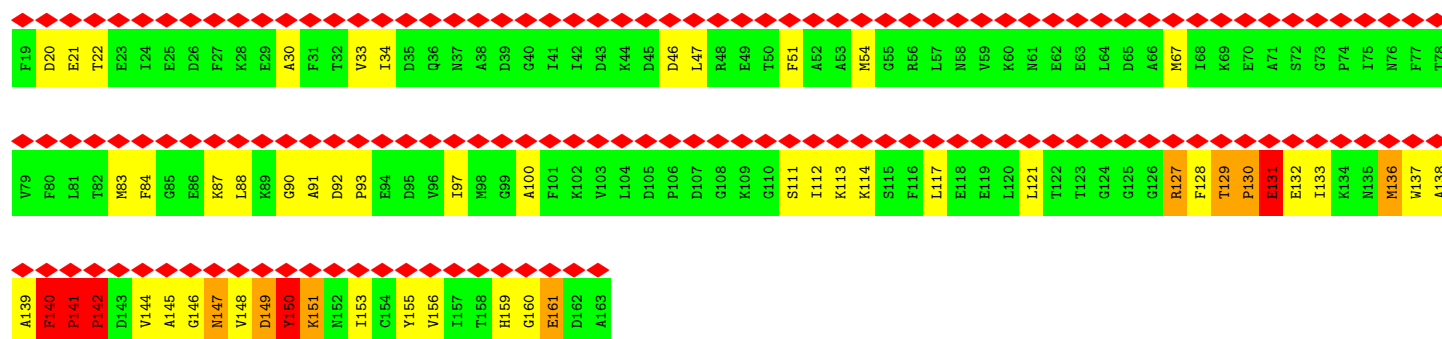


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

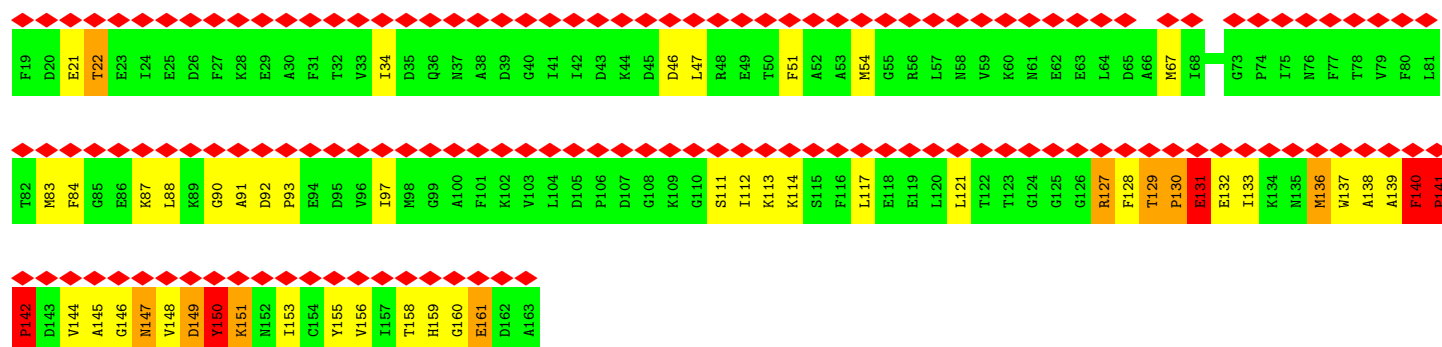




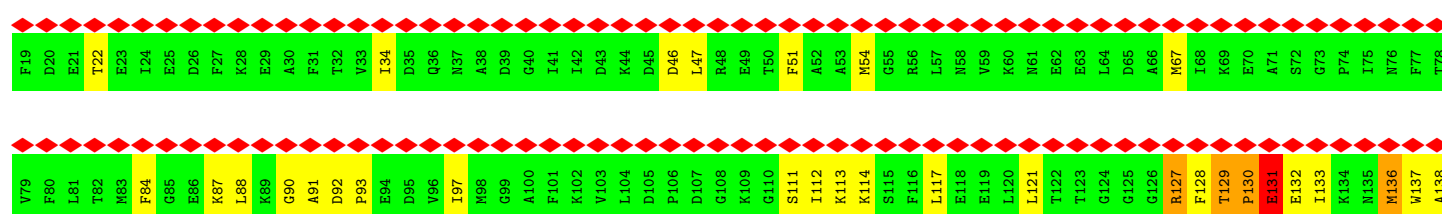
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

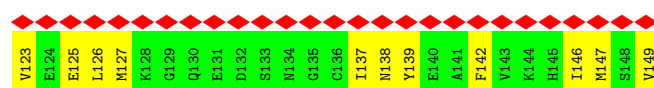


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

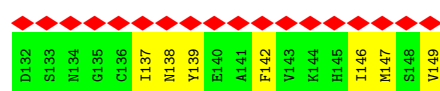
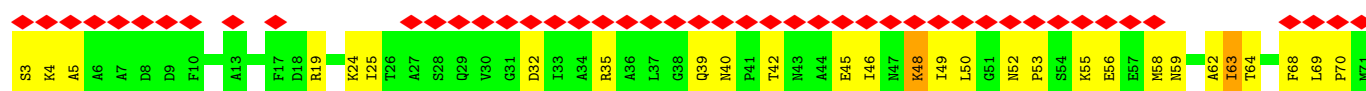
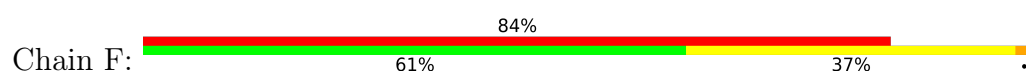




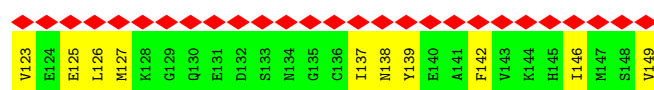
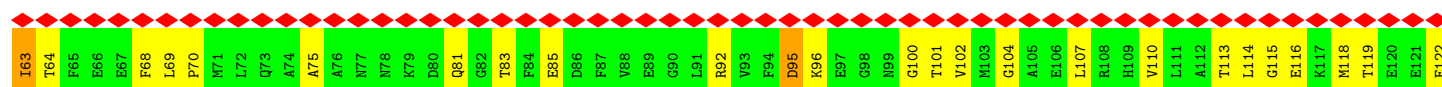
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

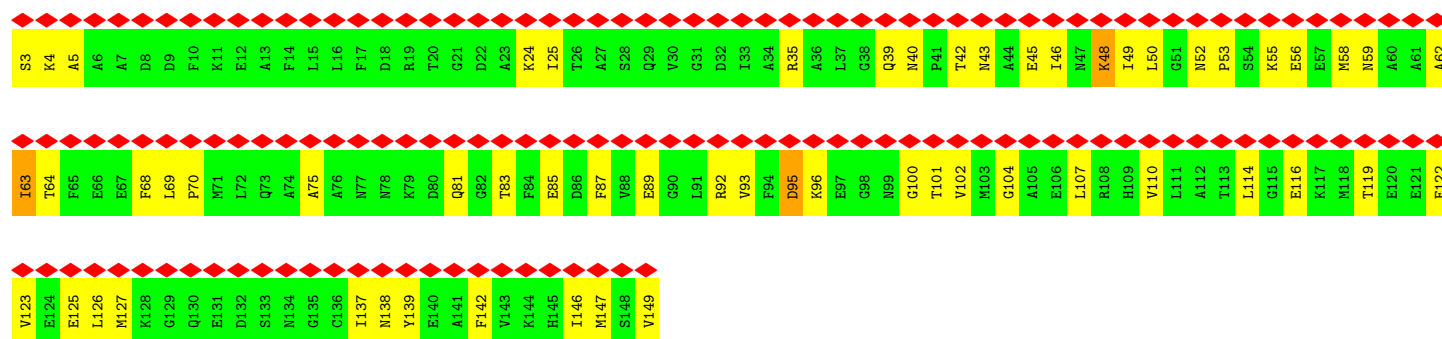


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

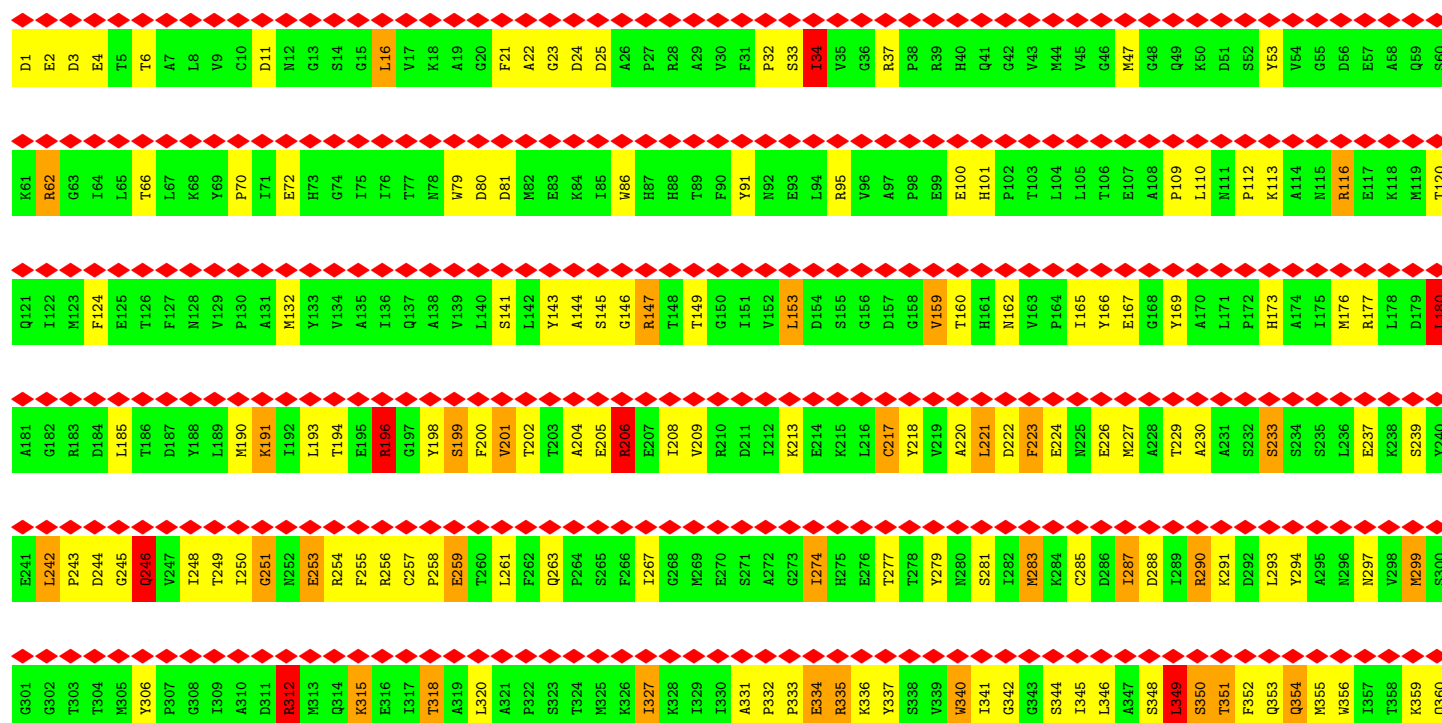


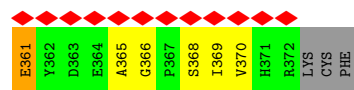


● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

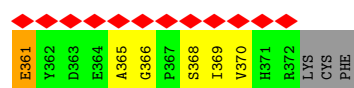
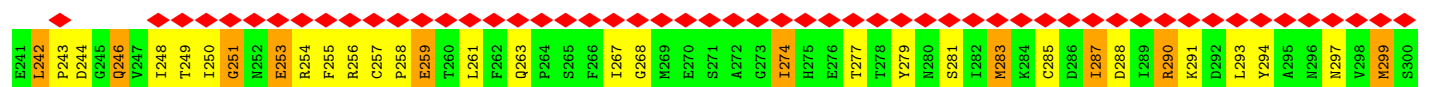
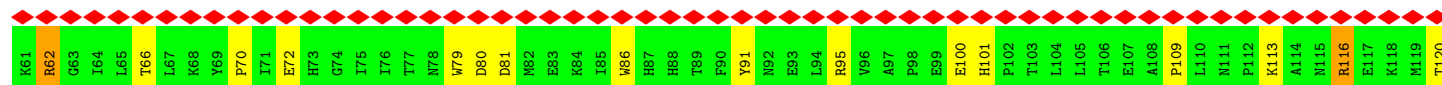
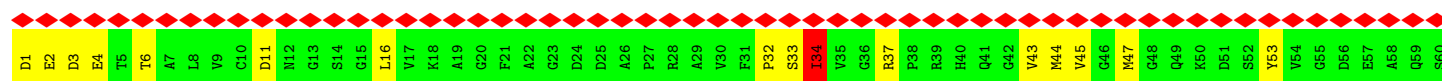


● Molecule 4: SKELETAL MUSCLE ACTIN

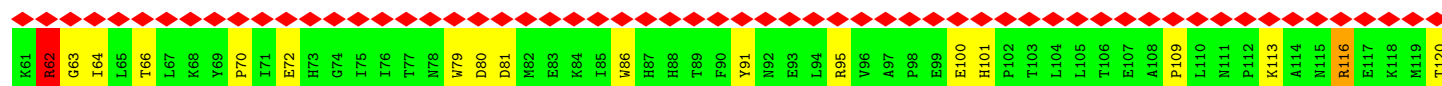
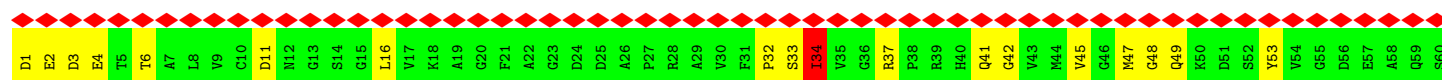




• Molecule 4: SKELETAL MUSCLE ACTIN

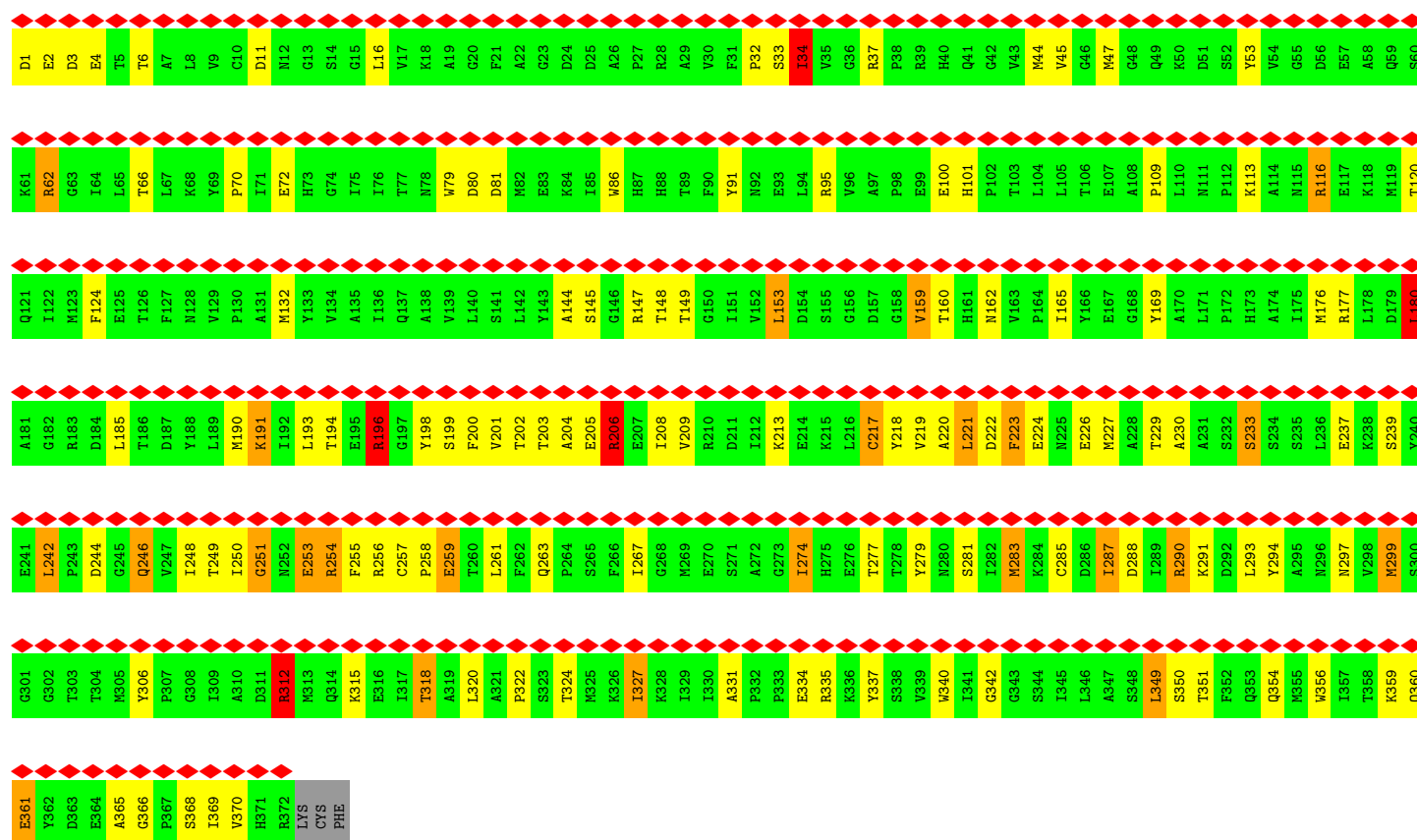


• Molecule 4: SKELETAL MUSCLE ACTIN

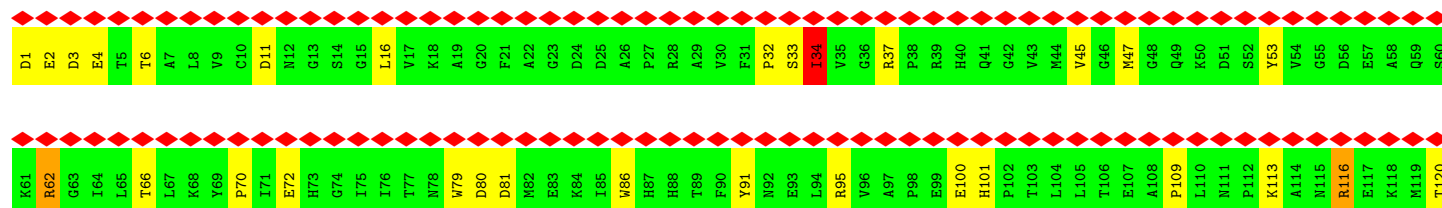


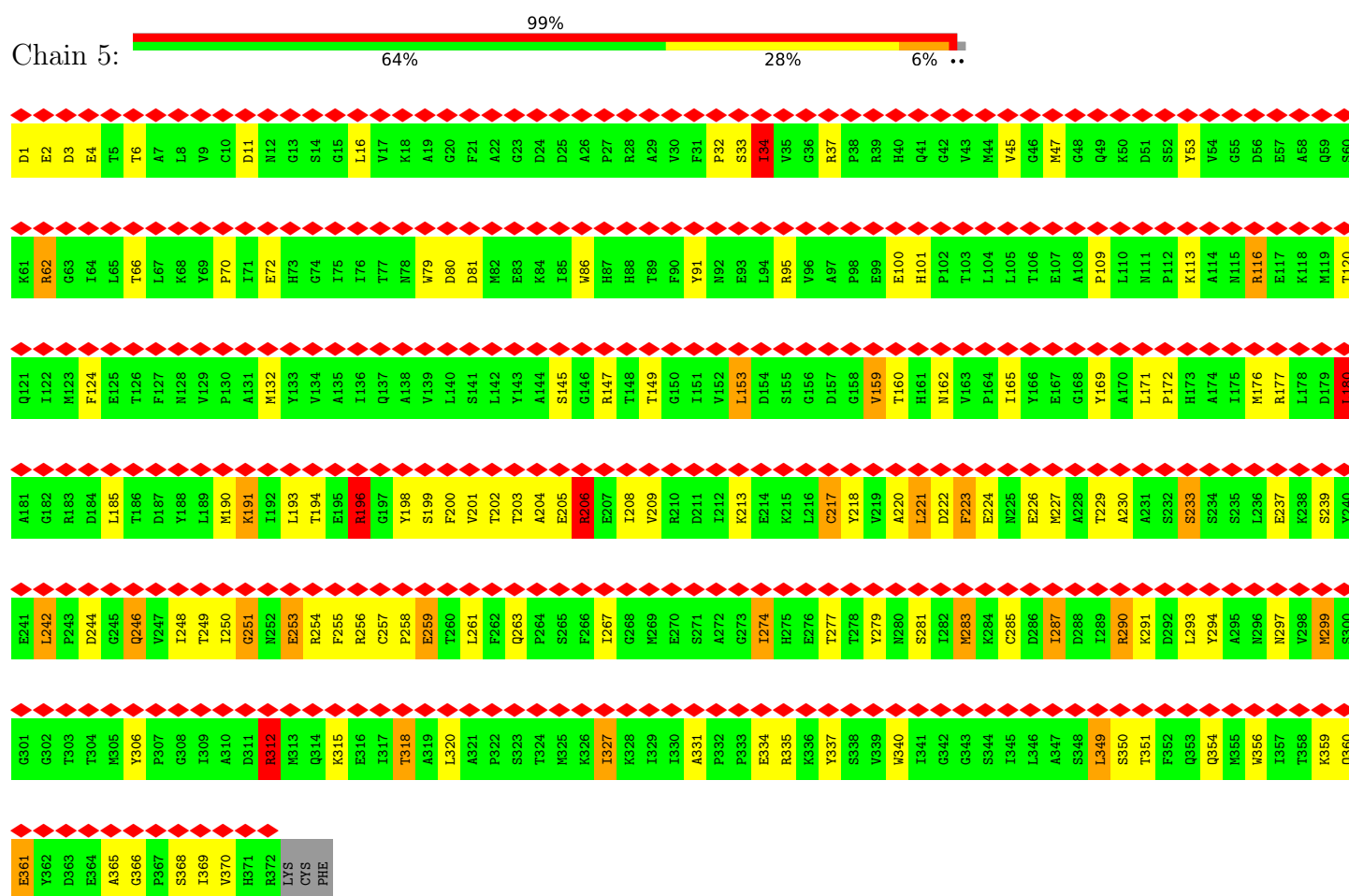
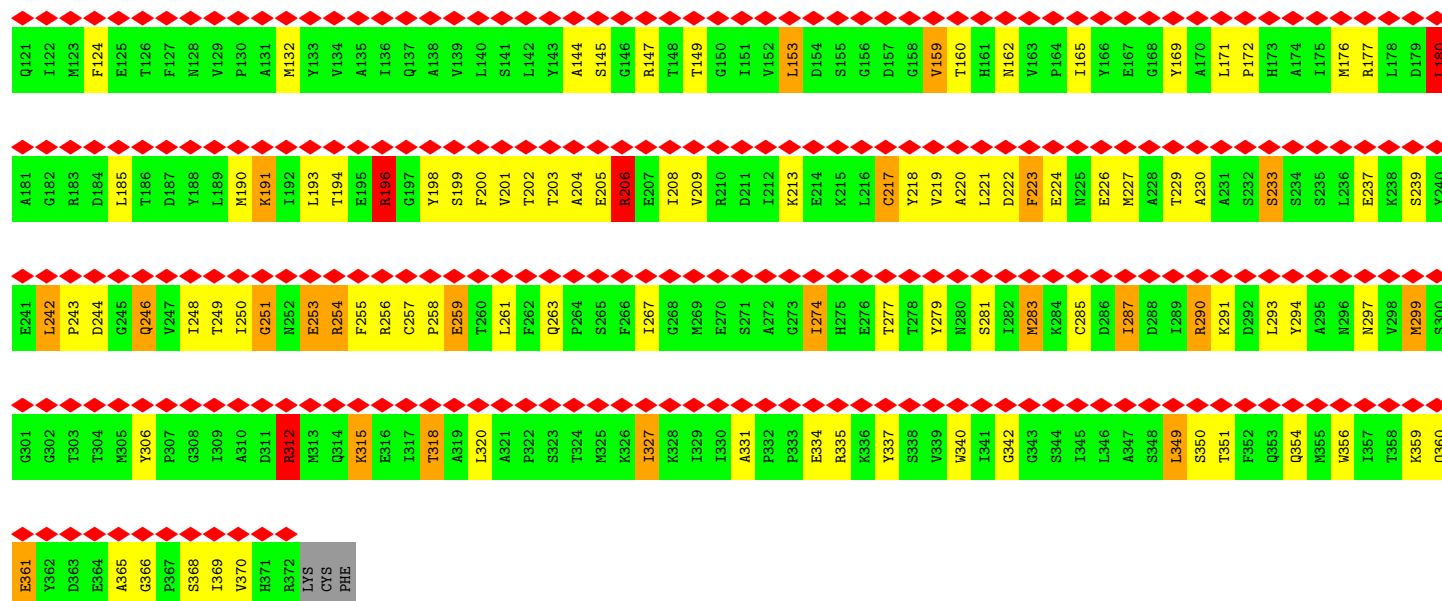


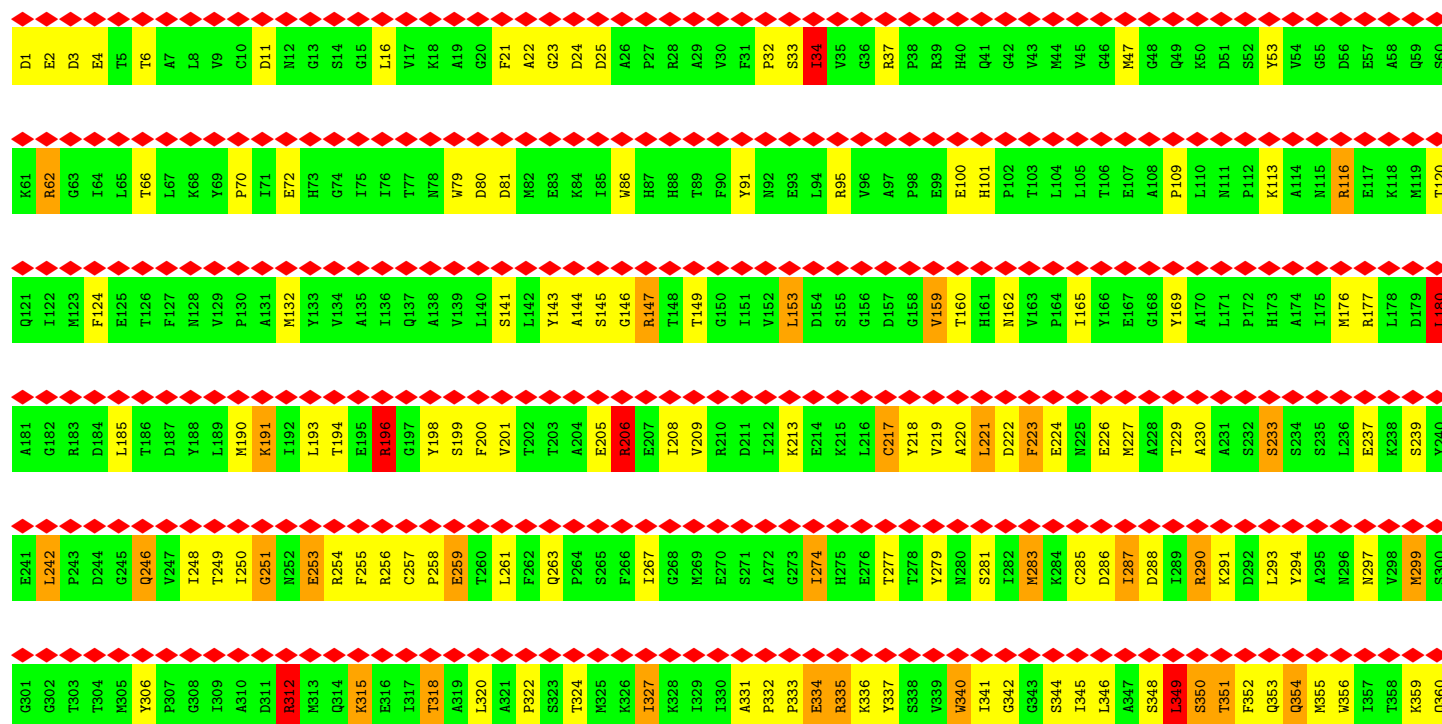
• Molecule 4: SKELETAL MUSCLE ACTIN



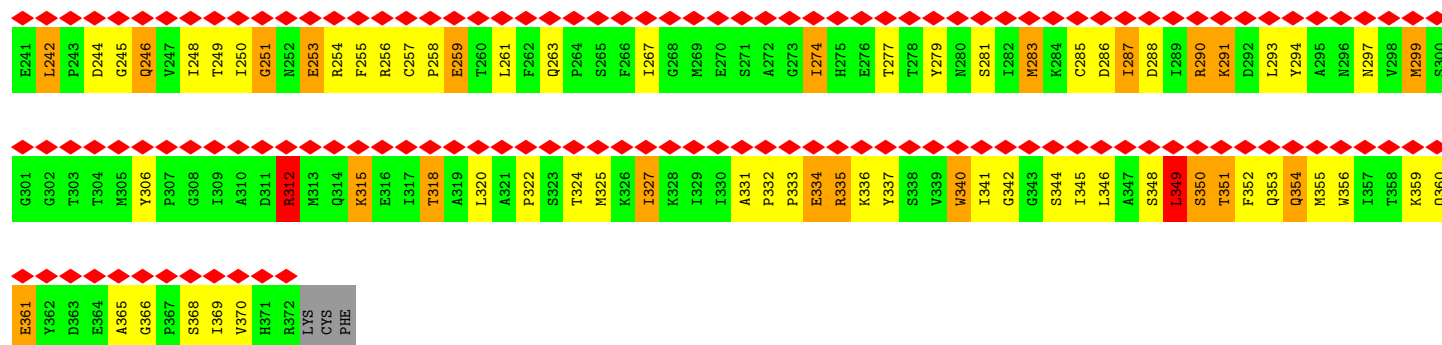
• Molecule 4: SKELETAL MUSCLE ACTIN



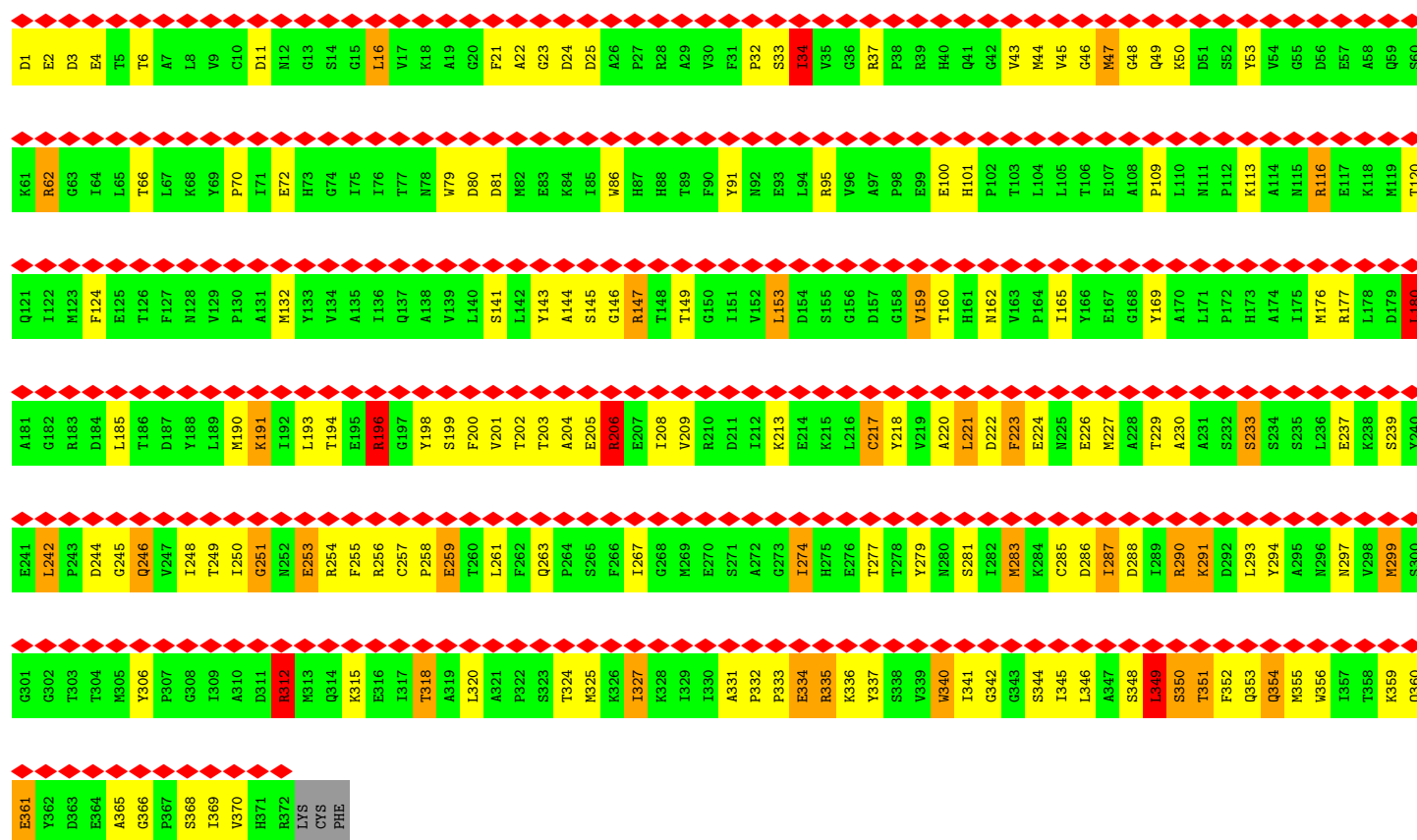




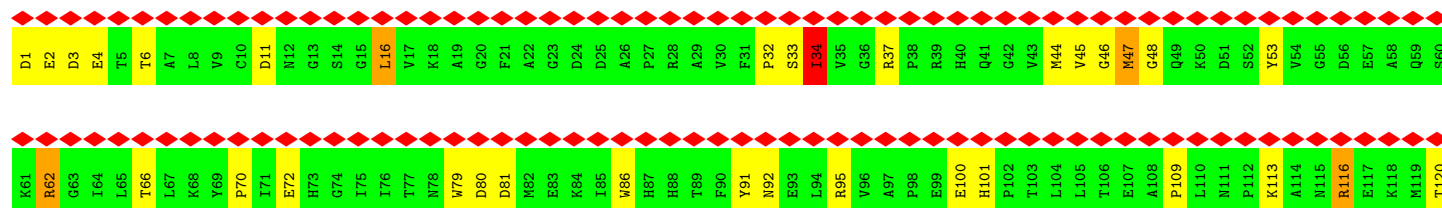
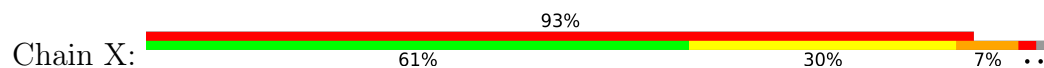


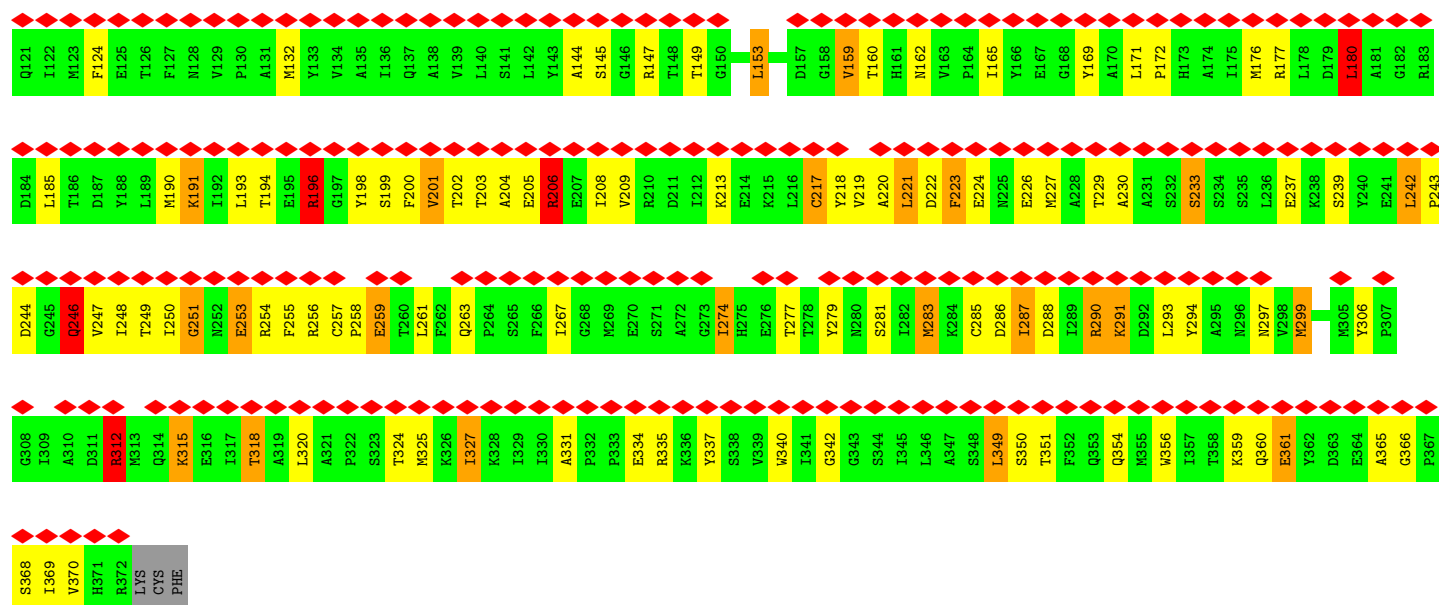


• Molecule 4: SKELETAL MUSCLE ACTIN

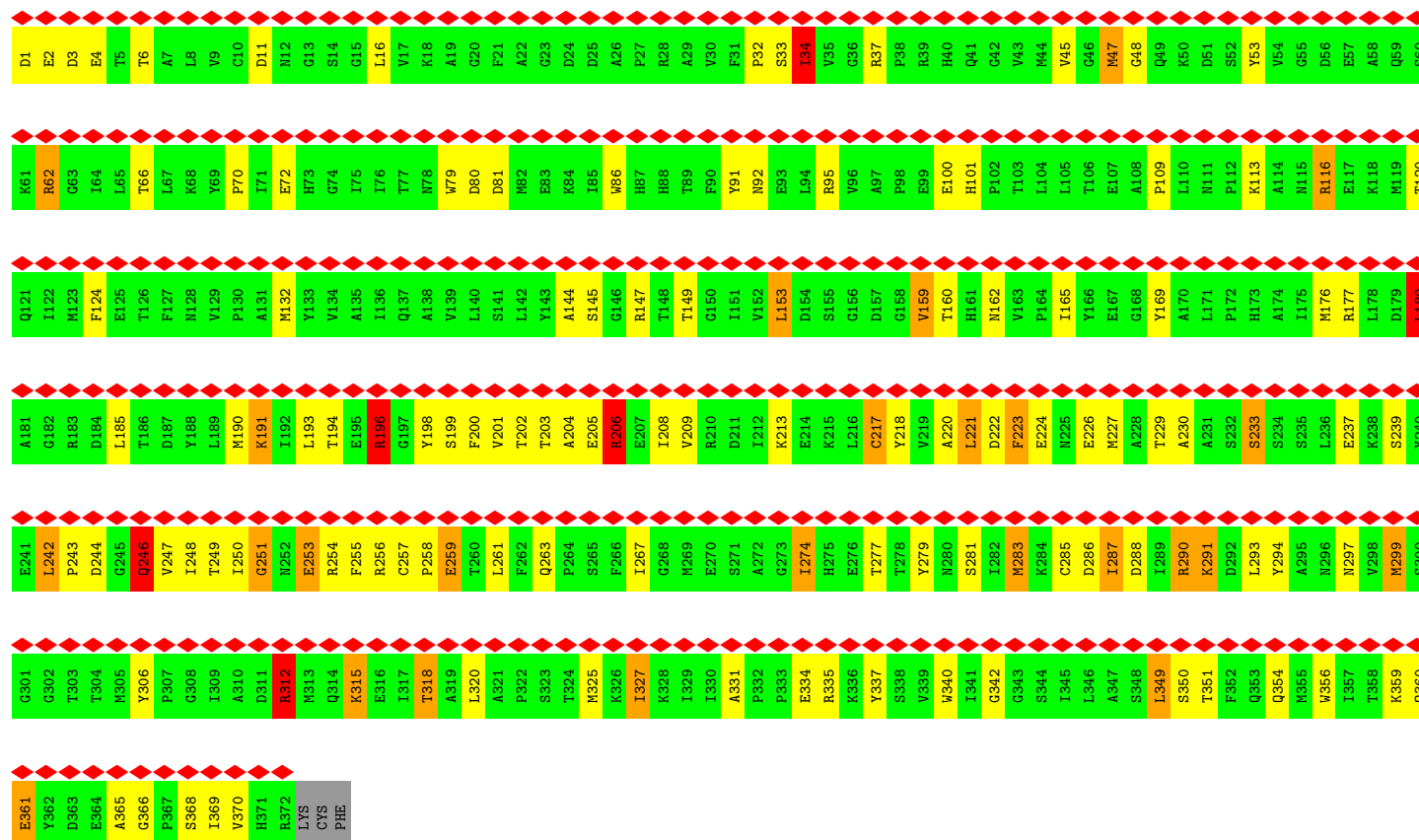


• Molecule 4: SKELETAL MUSCLE ACTIN





• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN





4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method | TOMOGRAPHY | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of tilted images used | Not provided | |
| Resolution determination method | Not provided | |
| CTF correction method | Not provided | |
| Microscope | FEI/PHILIPS EM400 | Depositor |
| Voltage (kV) | 100 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 17000 | Depositor |
| Image detector | KODAK SO-163 FILM | Depositor |
| Maximum voxel value | 366.680 | Depositor |
| Minimum voxel value | -417.992 | Depositor |
| Average voxel value | 1.860 | Depositor |
| Voxel value standard deviation | 47.792 | Depositor |
| Recommended contour level | 81.2 | Depositor |
| Tomogram size (\AA) | 9280, 9280, 464 | wwPDB |
| Tomogram dimensions | 600, 600, 30 | wwPDB |
| Tomogram angles ($^\circ$) | 90, 90, 90 | wwPDB |
| Grid spacing (\AA) | 15.4667, 15.4667, 15.4667 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 1.77 | 67/6448 (1.0%) | 1.82 | 116/8729 (1.3%) |
| 1 | D | 1.77 | 64/6448 (1.0%) | 1.82 | 115/8729 (1.3%) |
| 1 | G | 1.77 | 66/6449 (1.0%) | 1.83 | 119/8732 (1.4%) |
| 1 | J | 1.77 | 66/6449 (1.0%) | 1.86 | 118/8732 (1.4%) |
| 1 | P | 1.81 | 66/6449 (1.0%) | 1.90 | 127/8732 (1.5%) |
| 2 | B | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 2 | E | 1.22 | 10/1148 (0.9%) | 1.62 | 16/1548 (1.0%) |
| 2 | H | 1.22 | 10/1148 (0.9%) | 1.62 | 17/1548 (1.1%) |
| 2 | K | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 2 | Q | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 3 | C | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | F | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | I | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | L | 0.79 | 0/1136 | 0.94 | 4/1525 (0.3%) |
| 3 | R | 0.79 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 4 | 0 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 1 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 2 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 3 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 4 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | 5 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | 7 | 0.89 | 1/2968 (0.0%) | 1.64 | 51/4023 (1.3%) |
| 4 | 8 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 9 | 0.89 | 1/2968 (0.0%) | 1.64 | 52/4023 (1.3%) |
| 4 | V | 0.89 | 2/2968 (0.1%) | 1.64 | 50/4023 (1.2%) |
| 4 | W | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | X | 0.89 | 1/2968 (0.0%) | 1.64 | 51/4023 (1.3%) |
| 4 | Y | 0.89 | 2/2968 (0.1%) | 1.64 | 50/4023 (1.2%) |
| 4 | Z | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| All | All | 1.31 | 404/85215 (0.5%) | 1.68 | 1415/115341 (1.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 1 | 4 |
| 1 | D | 1 | 4 |
| 1 | G | 2 | 4 |
| 1 | J | 1 | 6 |
| 1 | P | 1 | 9 |
| 2 | B | 0 | 3 |
| 2 | E | 0 | 3 |
| 2 | H | 0 | 3 |
| 2 | K | 0 | 3 |
| 2 | Q | 0 | 3 |
| 3 | C | 0 | 2 |
| 3 | F | 0 | 2 |
| 3 | I | 0 | 2 |
| 3 | L | 0 | 2 |
| 3 | R | 0 | 2 |
| 4 | 0 | 0 | 1 |
| 4 | 1 | 0 | 1 |
| 4 | 2 | 0 | 1 |
| 4 | 3 | 0 | 1 |
| 4 | 4 | 0 | 1 |
| 4 | 5 | 0 | 1 |
| 4 | 7 | 0 | 1 |
| 4 | 8 | 0 | 1 |
| 4 | 9 | 0 | 1 |
| 4 | V | 0 | 1 |
| 4 | W | 0 | 1 |
| 4 | X | 0 | 1 |
| 4 | Y | 0 | 1 |
| 4 | Z | 0 | 1 |
| All | All | 6 | 66 |

The worst 5 of 404 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | P | 649 | VAL | CB-CG1 | 53.27 | 2.64 | 1.52 |
| 1 | J | 649 | VAL | CB-CG1 | 53.25 | 2.64 | 1.52 |
| 1 | A | 649 | VAL | CB-CG1 | 53.23 | 2.64 | 1.52 |
| 1 | G | 649 | VAL | CB-CG1 | 53.20 | 2.64 | 1.52 |
| 1 | D | 649 | VAL | CB-CG1 | 53.20 | 2.64 | 1.52 |

The worst 5 of 1415 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | G | 637 | LYS | O-C-N | -58.52 | 23.71 | 123.20 |
| 1 | J | 637 | LYS | O-C-N | -58.47 | 23.80 | 123.20 |
| 1 | D | 637 | LYS | O-C-N | -58.46 | 23.81 | 123.20 |
| 1 | P | 637 | LYS | O-C-N | -58.46 | 23.82 | 123.20 |
| 1 | A | 637 | LYS | O-C-N | -58.44 | 23.85 | 123.20 |

5 of 6 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 648 | THR | CB |
| 1 | D | 648 | THR | CB |
| 1 | G | 75 | ASP | CA |
| 1 | G | 648 | THR | CB |
| 1 | J | 648 | THR | CB |

5 of 66 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 623 | PHE | Sidechain |
| 1 | A | 637 | LYS | Mainchain |
| 1 | A | 649 | VAL | Mainchain |
| 1 | A | 98 | HIS | Mainchain |
| 2 | B | 22 | THR | Mainchain |

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 6797 | 0 | 6754 | 1510 | 0 |
| 1 | D | 6797 | 0 | 6755 | 1417 | 0 |
| 1 | G | 6797 | 0 | 6763 | 1561 | 0 |
| 1 | J | 6797 | 0 | 6754 | 1418 | 0 |
| 1 | P | 6797 | 0 | 6763 | 1523 | 0 |
| 2 | B | 1127 | 0 | 1085 | 239 | 0 |
| 2 | E | 1127 | 0 | 1086 | 269 | 0 |
| 2 | H | 1127 | 0 | 1088 | 298 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | K | 1127 | 0 | 1088 | 266 | 0 |
| 2 | Q | 1127 | 0 | 1088 | 261 | 0 |
| 3 | C | 1123 | 0 | 1083 | 194 | 0 |
| 3 | F | 1123 | 0 | 1083 | 168 | 0 |
| 3 | I | 1123 | 0 | 1083 | 186 | 0 |
| 3 | L | 1123 | 0 | 1083 | 161 | 0 |
| 3 | R | 1123 | 0 | 1079 | 229 | 0 |
| 4 | 0 | 2906 | 0 | 2855 | 406 | 0 |
| 4 | 1 | 2906 | 0 | 2864 | 214 | 0 |
| 4 | 2 | 2906 | 0 | 2864 | 174 | 0 |
| 4 | 3 | 2906 | 0 | 2863 | 180 | 0 |
| 4 | 4 | 2906 | 0 | 2865 | 98 | 0 |
| 4 | 5 | 2906 | 0 | 2865 | 99 | 0 |
| 4 | 7 | 2906 | 0 | 2866 | 76 | 0 |
| 4 | 8 | 2906 | 0 | 2857 | 321 | 0 |
| 4 | 9 | 2906 | 0 | 2855 | 341 | 0 |
| 4 | V | 2906 | 0 | 2851 | 385 | 0 |
| 4 | W | 2906 | 0 | 2851 | 384 | 0 |
| 4 | X | 2906 | 0 | 2862 | 212 | 0 |
| 4 | Y | 2906 | 0 | 2863 | 169 | 0 |
| 4 | Z | 2906 | 0 | 2862 | 187 | 0 |
| All | All | 85919 | 0 | 84678 | 9656 | 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 57.

The worst 5 of 9656 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:797:PHE:CE1 | 3:L:146:ILE:HG23 | 1.21 | 1.71 |
| 1:G:84:MLY:CH1 | 1:G:724:TYR:HE2 | 1.03 | 1.66 |
| 1:P:803:TYR:CD1 | 1:P:807:VAL:HG11 | 1.22 | 1.65 |
| 1:G:84:MLY:CG | 1:G:723:ARG:HD2 | 1.17 | 1.64 |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD1 | 1.26 | 1.63 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | A | 789/840 (94%) | 650 (82%) | 113 (14%) | 26 (3%) | 4 | 26 |
| 1 | D | 789/840 (94%) | 651 (82%) | 112 (14%) | 26 (3%) | 4 | 26 |
| 1 | G | 791/840 (94%) | 651 (82%) | 113 (14%) | 27 (3%) | 3 | 26 |
| 1 | J | 791/840 (94%) | 651 (82%) | 113 (14%) | 27 (3%) | 3 | 26 |
| 1 | P | 791/840 (94%) | 650 (82%) | 112 (14%) | 29 (4%) | 3 | 24 |
| 2 | B | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | E | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | H | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | K | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | Q | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 3 | C | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | F | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | I | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | L | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | R | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 4 | 0 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 1 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 2 | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| 4 | 3 | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| 4 | 4 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 5 | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| 4 | 7 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 8 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 9 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | V | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|----|
| 4 | W | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | X | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| 4 | Y | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| 4 | Z | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| All | All | 10561/10910 (97%) | 9231 (87%) | 1071 (10%) | 259 (2%) | 9 | 32 |

5 of 259 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 73 | LYS |
| 1 | A | 202 | SER |
| 1 | A | 572 | LYS |
| 1 | A | 712 | PRO |
| 1 | A | 729 | 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 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 | A | 672/672 (100%) | 512 (76%) | 160 (24%) | 0 | 4 |
| 1 | D | 672/672 (100%) | 514 (76%) | 158 (24%) | 1 | 4 |
| 1 | G | 672/672 (100%) | 513 (76%) | 159 (24%) | 1 | 4 |
| 1 | J | 672/672 (100%) | 514 (76%) | 158 (24%) | 1 | 4 |
| 1 | P | 672/672 (100%) | 514 (76%) | 158 (24%) | 1 | 4 |
| 2 | B | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 2 | E | 120/120 (100%) | 120 (100%) | 0 | 100 | 100 |
| 2 | H | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 2 | K | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 2 | Q | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 3 | C | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 3 | F | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 3 | I | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 3 | L | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 3 | R | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 4 | 0 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | 1 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 2 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 3 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 4 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 5 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 7 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 8 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 9 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | V | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | W | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | X | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | Y | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | Z | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| All | All | 8955/8997 (100%) | 7484 (84%) | 1471 (16%) | 5 | 12 |

5 of 1471 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2 | 159 | VAL |
| 4 | 8 | 34 | ILE |
| 4 | 2 | 349 | LEU |
| 4 | 2 | 153 | LEU |
| 4 | 4 | 315 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 206 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 563 | ASN |
| 4 | 2 | 354 | GLN |
| 4 | Y | 354 | GLN |
| 1 | P | 656 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 0 | 252 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

225 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 1 | MLY | A | 295 | 1 | 9,10,11 | 0.81 | 0 | 6,11,13 | 0.33 | 0 |
| 1 | MLY | D | 272 | 1 | 9,10,11 | 0.99 | 1 (11%) | 6,11,13 | 0.58 | 0 |
| 1 | MLY | J | 681 | 1 | 9,10,11 | 0.60 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | J | 369 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | A | 87 | 1 | 9,10,11 | 1.21 | 1 (11%) | 6,11,13 | 0.42 | 0 |
| 1 | MLY | J | 348 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.47 | 0 |
| 1 | MLY | J | 768 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.42 | 0 |
| 1 | MLY | P | 839 | 1 | 9,10,11 | 0.70 | 0 | 6,11,13 | 0.77 | 0 |
| 1 | MLY | D | 55 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | G | 35 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.40 | 0 |
| 1 | MLY | J | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.47 | 0 |
| 1 | MLY | D | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.47 | 0 |
| 1 | MLY | P | 833 | 1 | 9,10,11 | 1.19 | 1 (11%) | 6,11,13 | 0.31 | 0 |
| 1 | MLY | P | 19 | 1 | 9,10,11 | 1.18 | 1 (11%) | 6,11,13 | 0.57 | 0 |
| 1 | MLY | G | 415 | 1 | 9,10,11 | 0.76 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | D | 353 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | A | 833 | 1 | 9,10,11 | 1.14 | 1 (11%) | 6,11,13 | 0.32 | 0 |
| 1 | MLY | J | 598 | 1 | 9,10,11 | 0.89 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | A | 782 | 1 | 9,10,11 | 0.80 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | D | 296 | 1 | 9,10,11 | 0.66 | 0 | 6,11,13 | 0.37 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | P | 272 | 1 | 9,10,11 | 1.01 | 1 (11%) | 6,11,13 | 0.55 | 0 |
| 1 | MLY | P | 827 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | D | 190 | 1 | 9,10,11 | 1.21 | 1 (11%) | 6,11,13 | 0.54 | 0 |
| 1 | MLY | A | 385 | 1 | 9,10,11 | 1.00 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | A | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.49 | 0 |
| 1 | MLY | J | 138 | 1 | 9,10,11 | 1.33 | 1 (11%) | 6,11,13 | 0.84 | 0 |
| 1 | MLY | P | 59 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.49 | 0 |
| 1 | MLY | A | 505 | 1 | 9,10,11 | 0.90 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | P | 659 | 1 | 9,10,11 | 0.80 | 0 | 6,11,13 | 0.58 | 0 |
| 1 | MLY | J | 764 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | P | 553 | 1 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.54 | 0 |
| 1 | MLY | P | 613 | 1 | 9,10,11 | 0.56 | 0 | 6,11,13 | 0.63 | 0 |
| 1 | MLY | D | 553 | 1,4 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.55 | 0 |
| 1 | MLY | G | 598 | 1 | 9,10,11 | 0.90 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | G | 659 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.58 | 0 |
| 1 | MLY | D | 486 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | G | 190 | 1 | 9,10,11 | 1.24 | 1 (11%) | 6,11,13 | 0.52 | 0 |
| 1 | MLY | A | 827 | 1 | 9,10,11 | 0.73 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | D | 613 | 1 | 9,10,11 | 0.57 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | G | 436 | 1 | 9,10,11 | 1.07 | 1 (11%) | 6,11,13 | 0.48 | 0 |
| 1 | MLY | P | 35 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | G | 681 | 1 | 9,10,11 | 0.62 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | P | 63 | 1 | 9,10,11 | 0.90 | 0 | 6,11,13 | 0.43 | 0 |
| 1 | MLY | P | 138 | 1 | 9,10,11 | 1.33 | 1 (11%) | 6,11,13 | 0.84 | 0 |
| 1 | MLY | P | 415 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | G | 236 | 1 | 9,10,11 | 0.78 | 1 (11%) | 6,11,13 | 0.48 | 0 |
| 1 | MLY | D | 59 | 1 | 9,10,11 | 0.87 | 0 | 6,11,13 | 0.50 | 0 |
| 1 | MLY | J | 55 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.78 | 0 |
| 1 | MLY | J | 87 | 1 | 9,10,11 | 1.21 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | D | 415 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | G | 827 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.49 | 0 |
| 1 | MLY | G | 617 | 1 | 9,10,11 | 0.95 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | P | 296 | 1 | 9,10,11 | 0.66 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | P | 504 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.22 | 0 |
| 1 | MLY | P | 764 | 1 | 9,10,11 | 0.84 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | J | 837 | 1 | 9,10,11 | 0.58 | 0 | 6,11,13 | 0.55 | 0 |
| 1 | MLY | D | 504 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.21 | 0 |
| 1 | MLY | G | 130 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.76 | 0 |
| 1 | MLY | G | 296 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | G | 504 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.23 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | G | 837 | 1 | 9,10,11 | 0.59 | 0 | 6,11,13 | 0.52 | 0 |
| 1 | MLY | P | 348 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.47 | 0 |
| 1 | MLY | A | 367 | 1 | 9,10,11 | 0.62 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | J | 107 | 1 | 9,10,11 | 0.48 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | P | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.47 | 0 |
| 1 | MLY | D | 551 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | J | 35 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | P | 431 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.44 | 0 |
| 1 | MLY | A | 272 | 1 | 9,10,11 | 1.01 | 1 (11%) | 6,11,13 | 0.56 | 0 |
| 1 | MLY | J | 553 | 1 | 9,10,11 | 0.67 | 0 | 6,11,13 | 0.53 | 0 |
| 1 | MLY | J | 486 | 1 | 9,10,11 | 0.63 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | G | 348 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | A | 190 | 1 | 9,10,11 | 1.27 | 2 (22%) | 6,11,13 | 0.51 | 0 |
| 1 | MLY | P | 837 | 1 | 9,10,11 | 0.58 | 0 | 6,11,13 | 0.57 | 0 |
| 1 | MLY | D | 367 | 1 | 9,10,11 | 0.61 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | J | 296 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | A | 431 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | A | 504 | 1 | 9,10,11 | 0.90 | 0 | 6,11,13 | 0.24 | 0 |
| 1 | MLY | J | 415 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | P | 436 | 1 | 9,10,11 | 1.08 | 1 (11%) | 6,11,13 | 0.49 | 0 |
| 1 | MLY | D | 431 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | P | 681 | 1 | 9,10,11 | 0.61 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | J | 84 | 1 | 9,10,11 | 0.49 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | J | 504 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.23 | 0 |
| 1 | MLY | G | 486 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | A | 30 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.32 | 0 |
| 1 | MLY | J | 600 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | J | 613 | 1 | 9,10,11 | 0.55 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | G | 248 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.62 | 0 |
| 1 | MLY | P | 55 | 1 | 9,10,11 | 0.73 | 0 | 6,11,13 | 0.78 | 0 |
| 1 | MLY | A | 681 | 1 | 9,10,11 | 0.60 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | P | 617 | 1 | 9,10,11 | 0.97 | 1 (11%) | 6,11,13 | 0.33 | 0 |
| 1 | MLY | D | 49 | 1 | 9,10,11 | 1.08 | 1 (11%) | 6,11,13 | 0.74 | 0 |
| 1 | MLY | G | 431 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | J | 63 | 1 | 9,10,11 | 0.91 | 0 | 6,11,13 | 0.43 | 0 |
| 1 | MLY | D | 295 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | D | 827 | 1 | 9,10,11 | 0.67 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | P | 130 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.75 | 0 |
| 1 | MLY | J | 551 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.20 | 0 |
| 1 | MLY | P | 367 | 1 | 9,10,11 | 0.62 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | G | 600 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.37 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | G | 49 | 1 | 9,10,11 | 1.09 | 1 (11%) | 6,11,13 | 0.74 | 0 |
| 1 | MLY | J | 367 | 1 | 9,10,11 | 0.63 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | D | 600 | 1 | 9,10,11 | 0.51 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | A | 348 | 1 | 9,10,11 | 0.86 | 1 (11%) | 6,11,13 | 0.48 | 0 |
| 1 | MLY | D | 839 | 1 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | G | 353 | 1 | 9,10,11 | 0.86 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | G | 782 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | G | 63 | 1 | 9,10,11 | 0.90 | 0 | 6,11,13 | 0.44 | 0 |
| 1 | MLY | P | 84 | 1 | 9,10,11 | 0.48 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | G | 59 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.50 | 0 |
| 1 | MLY | D | 833 | 1 | 9,10,11 | 1.17 | 2 (22%) | 6,11,13 | 0.31 | 0 |
| 1 | MLY | J | 385 | 1 | 9,10,11 | 1.04 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | D | 138 | 1 | 9,10,11 | 1.39 | 1 (11%) | 6,11,13 | 0.85 | 0 |
| 1 | MLY | D | 19 | 1 | 9,10,11 | 1.19 | 1 (11%) | 6,11,13 | 0.56 | 0 |
| 1 | MLY | G | 528 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.66 | 0 |
| 1 | MLY | G | 551 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.20 | 0 |
| 1 | MLY | J | 659 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.57 | 0 |
| 1 | MLY | P | 551 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | P | 248 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.62 | 0 |
| 1 | MLY | A | 659 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.60 | 0 |
| 1 | MLY | D | 505 | 1 | 9,10,11 | 0.84 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | G | 367 | 1 | 9,10,11 | 0.64 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | A | 486 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | A | 768 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.41 | 0 |
| 1 | MLY | G | 613 | 1 | 9,10,11 | 0.59 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | J | 431 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | J | 436 | 1 | 9,10,11 | 1.05 | 1 (11%) | 6,11,13 | 0.49 | 0 |
| 1 | MLY | J | 505 | 1 | 9,10,11 | 0.92 | 1 (11%) | 6,11,13 | 0.33 | 0 |
| 1 | MLY | P | 30 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.30 | 0 |
| 1 | MLY | J | 49 | 1 | 9,10,11 | 1.10 | 1 (11%) | 6,11,13 | 0.74 | 0 |
| 1 | MLY | A | 84 | 1 | 9,10,11 | 0.49 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | P | 353 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | D | 782 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | G | 553 | 1,4 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.54 | 0 |
| 1 | MLY | J | 827 | 1 | 9,10,11 | 0.75 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | A | 35 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | J | 295 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | P | 528 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.65 | 0 |
| 1 | MLY | D | 385 | 1 | 9,10,11 | 0.99 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | J | 353 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.78 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | G | 369 | 1 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | D | 248 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.62 | 0 |
| 1 | MLY | G | 768 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.41 | 0 |
| 1 | MLY | A | 296 | 1 | 9,10,11 | 0.64 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | D | 63 | 1 | 9,10,11 | 0.90 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | P | 385 | 1 | 9,10,11 | 1.02 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | A | 436 | 1 | 9,10,11 | 1.06 | 1 (11%) | 6,11,13 | 0.50 | 0 |
| 1 | MLY | J | 839 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.77 | 0 |
| 1 | MLY | A | 63 | 1 | 9,10,11 | 0.93 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | D | 837 | 1 | 9,10,11 | 0.60 | 0 | 6,11,13 | 0.57 | 0 |
| 1 | MLY | G | 84 | 1 | 9,10,11 | 0.49 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | A | 415 | 1 | 9,10,11 | 0.74 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | D | 87 | 1 | 9,10,11 | 1.18 | 1 (11%) | 6,11,13 | 0.45 | 0 |
| 1 | MLY | D | 764 | 1 | 9,10,11 | 0.86 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | A | 764 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | A | 837 | 1 | 9,10,11 | 0.61 | 0 | 6,11,13 | 0.54 | 0 |
| 1 | MLY | D | 30 | 1 | 9,10,11 | 0.91 | 0 | 6,11,13 | 0.32 | 0 |
| 1 | MLY | G | 505 | 1 | 9,10,11 | 0.88 | 1 (11%) | 6,11,13 | 0.36 | 0 |
| 1 | MLY | D | 436 | 1 | 9,10,11 | 1.10 | 1 (11%) | 6,11,13 | 0.49 | 0 |
| 1 | MLY | A | 613 | 1 | 9,10,11 | 0.57 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | P | 782 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | P | 190 | 1 | 9,10,11 | 1.26 | 1 (11%) | 6,11,13 | 0.53 | 0 |
| 1 | MLY | J | 130 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.74 | 0 |
| 1 | MLY | D | 528 | 1 | 9,10,11 | 0.91 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | D | 617 | 1 | 9,10,11 | 0.96 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | J | 833 | 1 | 9,10,11 | 1.20 | 1 (11%) | 6,11,13 | 0.32 | 0 |
| 1 | MLY | G | 138 | 1 | 9,10,11 | 1.35 | 1 (11%) | 6,11,13 | 0.85 | 0 |
| 1 | MLY | G | 295 | 1 | 9,10,11 | 0.81 | 0 | 6,11,13 | 0.33 | 0 |
| 1 | MLY | A | 551 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | P | 369 | 1 | 9,10,11 | 0.70 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | A | 55 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.78 | 0 |
| 1 | MLY | P | 107 | 1 | 9,10,11 | 0.48 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | A | 617 | 1 | 9,10,11 | 0.93 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | D | 130 | 1 | 9,10,11 | 0.81 | 0 | 6,11,13 | 0.74 | 0 |
| 1 | MLY | G | 764 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | A | 553 | 1,4 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.54 | 0 |
| 1 | MLY | P | 505 | 1 | 9,10,11 | 0.92 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | A | 369 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | J | 248 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.62 | 0 |
| 1 | MLY | A | 130 | 1 | 9,10,11 | 0.81 | 0 | 6,11,13 | 0.75 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | G | 385 | 1 | 9,10,11 | 0.99 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | P | 486 | 1 | 9,10,11 | 0.64 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | A | 59 | 1 | 9,10,11 | 0.87 | 0 | 6,11,13 | 0.49 | 0 |
| 1 | MLY | P | 598 | 1 | 9,10,11 | 0.90 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | A | 528 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.67 | 0 |
| 1 | MLY | J | 272 | 1 | 9,10,11 | 1.03 | 1 (11%) | 6,11,13 | 0.55 | 0 |
| 1 | MLY | G | 833 | 1 | 9,10,11 | 1.17 | 2 (22%) | 6,11,13 | 0.32 | 0 |
| 1 | MLY | D | 84 | 1 | 9,10,11 | 0.51 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | A | 598 | 1 | 9,10,11 | 0.91 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | D | 35 | 1 | 9,10,11 | 0.73 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | G | 19 | 1 | 9,10,11 | 1.16 | 1 (11%) | 6,11,13 | 0.57 | 0 |
| 1 | MLY | D | 681 | 1 | 9,10,11 | 0.56 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | G | 87 | 1 | 9,10,11 | 1.22 | 1 (11%) | 6,11,13 | 0.42 | 0 |
| 1 | MLY | D | 369 | 1 | 9,10,11 | 0.70 | 0 | 6,11,13 | 0.44 | 0 |
| 1 | MLY | D | 348 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | D | 768 | 1 | 9,10,11 | 0.73 | 0 | 6,11,13 | 0.41 | 0 |
| 1 | MLY | D | 107 | 1 | 9,10,11 | 0.51 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | J | 30 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.31 | 0 |
| 1 | MLY | A | 19 | 1 | 9,10,11 | 1.12 | 1 (11%) | 6,11,13 | 0.58 | 0 |
| 1 | MLY | A | 107 | 1 | 9,10,11 | 0.46 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | J | 190 | 1 | 9,10,11 | 1.26 | 1 (11%) | 6,11,13 | 0.52 | 0 |
| 1 | MLY | G | 30 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.30 | 0 |
| 1 | MLY | P | 600 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | J | 782 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | G | 272 | 1 | 9,10,11 | 0.98 | 1 (11%) | 6,11,13 | 0.54 | 0 |
| 1 | MLY | J | 59 | 1 | 9,10,11 | 0.87 | 0 | 6,11,13 | 0.50 | 0 |
| 1 | MLY | A | 353 | 1 | 9,10,11 | 0.87 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | D | 598 | 1 | 9,10,11 | 0.91 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | J | 528 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.66 | 0 |
| 1 | MLY | J | 617 | 1 | 9,10,11 | 0.95 | 1 (11%) | 6,11,13 | 0.33 | 0 |
| 1 | MLY | P | 87 | 1 | 9,10,11 | 1.25 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | P | 49 | 1 | 9,10,11 | 1.10 | 1 (11%) | 6,11,13 | 0.75 | 0 |
| 1 | MLY | G | 839 | 1 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | P | 295 | 1 | 9,10,11 | 0.80 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | A | 600 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | G | 107 | 1 | 9,10,11 | 0.47 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | A | 49 | 1 | 9,10,11 | 1.05 | 1 (11%) | 6,11,13 | 0.74 | 0 |
| 1 | MLY | A | 839 | 1 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.81 | 0 |
| 1 | MLY | A | 248 | 1 | 9,10,11 | 0.84 | 0 | 6,11,13 | 0.60 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | J | 19 | 1 | 9,10,11 | 1.19 | 1 (11%) | 6,11,13 | 0.57 | 0 |
| 1 | MLY | G | 55 | 1 | 9,10,11 | 0.73 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | P | 768 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.43 | 0 |
| 1 | MLY | D | 659 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.59 | 0 |
| 1 | MLY | A | 138 | 1 | 9,10,11 | 1.33 | 1 (11%) | 6,11,13 | 0.84 | 0 |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | A | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | G | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | J | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | D | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | D | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 236 | 1 | - | 3/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | J | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | P | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 553 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 553 | 1,4 | - | 5/8/9/11 | - |
| 1 | MLY | G | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | D | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | J | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | G | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | P | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 504 | 1 | - | 4/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | G | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | P | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 553 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | P | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | A | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | D | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 431 | 1 | - | 4/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | J | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | P | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | G | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | J | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 528 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | A | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 436 | 1 | - | 4/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | J | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | P | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | G | 553 | 1,4 | - | 4/8/9/11 | - |
| 1 | MLY | J | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | A | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 528 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | G | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 782 | 1 | - | 6/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | P | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 528 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | J | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | G | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | D | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 553 | 1,4 | - | 4/8/9/11 | - |
| 1 | MLY | P | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | A | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 528 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | D | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 348 | 1 | - | 5/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | D | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | G | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 528 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | P | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | J | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 138 | 1 | - | 4/8/9/11 | - |

The worst 5 of 70 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | D | 138 | MLY | CB-CA | -3.82 | 1.48 | 1.53 |
| 1 | G | 138 | MLY | CB-CA | -3.68 | 1.48 | 1.53 |
| 1 | P | 138 | MLY | CB-CA | -3.63 | 1.48 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | A | 138 | MLY | CB-CA | -3.61 | 1.48 | 1.53 |
| 1 | J | 138 | MLY | CB-CA | -3.61 | 1.48 | 1.53 |

There are no bond angle outliers.

There are no chirality outliers.

5 of 797 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 1 | A | 19 | MLY | C-CA-CB-CG |
| 1 | A | 49 | MLY | N-CA-CB-CG |
| 1 | A | 49 | MLY | C-CA-CB-CG |
| 1 | A | 55 | MLY | N-CA-CB-CG |
| 1 | A | 55 | MLY | C-CA-CB-CG |

There are no ring outliers.

150 monomers are involved in 613 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 295 | MLY | 6 | 0 |
| 1 | D | 272 | MLY | 1 | 0 |
| 1 | A | 87 | MLY | 3 | 0 |
| 1 | J | 348 | MLY | 5 | 0 |
| 1 | J | 768 | MLY | 5 | 0 |
| 1 | P | 839 | MLY | 8 | 0 |
| 1 | D | 55 | MLY | 1 | 0 |
| 1 | G | 415 | MLY | 1 | 0 |
| 1 | A | 833 | MLY | 1 | 0 |
| 1 | J | 598 | MLY | 1 | 0 |
| 1 | A | 782 | MLY | 7 | 0 |
| 1 | D | 296 | MLY | 3 | 0 |
| 1 | P | 272 | MLY | 1 | 0 |
| 1 | D | 190 | MLY | 2 | 0 |
| 1 | J | 138 | MLY | 1 | 0 |
| 1 | P | 59 | MLY | 2 | 0 |
| 1 | A | 505 | MLY | 25 | 0 |
| 1 | P | 659 | MLY | 2 | 0 |
| 1 | J | 764 | MLY | 1 | 0 |
| 1 | P | 553 | MLY | 2 | 0 |
| 1 | D | 553 | MLY | 16 | 0 |
| 1 | G | 598 | MLY | 1 | 0 |
| 1 | G | 659 | MLY | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | D | 486 | MLY | 3 | 0 |
| 1 | G | 190 | MLY | 2 | 0 |
| 1 | G | 436 | MLY | 2 | 0 |
| 1 | P | 63 | MLY | 4 | 0 |
| 1 | P | 138 | MLY | 1 | 0 |
| 1 | P | 415 | MLY | 1 | 0 |
| 1 | D | 59 | MLY | 2 | 0 |
| 1 | J | 55 | MLY | 1 | 0 |
| 1 | J | 87 | MLY | 3 | 0 |
| 1 | D | 415 | MLY | 1 | 0 |
| 1 | G | 617 | MLY | 1 | 0 |
| 1 | P | 296 | MLY | 3 | 0 |
| 1 | P | 764 | MLY | 1 | 0 |
| 1 | J | 837 | MLY | 1 | 0 |
| 1 | G | 296 | MLY | 2 | 0 |
| 1 | G | 837 | MLY | 1 | 0 |
| 1 | P | 348 | MLY | 5 | 0 |
| 1 | J | 107 | MLY | 2 | 0 |
| 1 | D | 551 | MLY | 1 | 0 |
| 1 | A | 272 | MLY | 1 | 0 |
| 1 | J | 553 | MLY | 11 | 0 |
| 1 | J | 486 | MLY | 3 | 0 |
| 1 | G | 348 | MLY | 4 | 0 |
| 1 | A | 190 | MLY | 2 | 0 |
| 1 | P | 837 | MLY | 1 | 0 |
| 1 | J | 296 | MLY | 3 | 0 |
| 1 | J | 415 | MLY | 1 | 0 |
| 1 | P | 436 | MLY | 2 | 0 |
| 1 | J | 84 | MLY | 18 | 0 |
| 1 | G | 486 | MLY | 3 | 0 |
| 1 | A | 30 | MLY | 1 | 0 |
| 1 | J | 600 | MLY | 1 | 0 |
| 1 | G | 248 | MLY | 2 | 0 |
| 1 | P | 55 | MLY | 1 | 0 |
| 1 | P | 617 | MLY | 1 | 0 |
| 1 | D | 49 | MLY | 3 | 0 |
| 1 | J | 63 | MLY | 3 | 0 |
| 1 | D | 295 | MLY | 6 | 0 |
| 1 | G | 600 | MLY | 1 | 0 |
| 1 | G | 49 | MLY | 2 | 0 |
| 1 | D | 600 | MLY | 1 | 0 |
| 1 | A | 348 | MLY | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | D | 839 | MLY | 4 | 0 |
| 1 | G | 782 | MLY | 1 | 0 |
| 1 | G | 63 | MLY | 3 | 0 |
| 1 | P | 84 | MLY | 32 | 0 |
| 1 | G | 59 | MLY | 3 | 0 |
| 1 | D | 138 | MLY | 1 | 0 |
| 1 | G | 528 | MLY | 3 | 0 |
| 1 | J | 659 | MLY | 2 | 0 |
| 1 | P | 248 | MLY | 2 | 0 |
| 1 | A | 659 | MLY | 2 | 0 |
| 1 | A | 486 | MLY | 3 | 0 |
| 1 | A | 768 | MLY | 6 | 0 |
| 1 | J | 436 | MLY | 2 | 0 |
| 1 | J | 505 | MLY | 10 | 0 |
| 1 | P | 30 | MLY | 1 | 0 |
| 1 | J | 49 | MLY | 2 | 0 |
| 1 | D | 782 | MLY | 43 | 0 |
| 1 | G | 553 | MLY | 27 | 0 |
| 1 | J | 295 | MLY | 6 | 0 |
| 1 | P | 528 | MLY | 2 | 0 |
| 1 | G | 369 | MLY | 1 | 0 |
| 1 | D | 248 | MLY | 2 | 0 |
| 1 | G | 768 | MLY | 2 | 0 |
| 1 | A | 296 | MLY | 2 | 0 |
| 1 | D | 63 | MLY | 3 | 0 |
| 1 | A | 436 | MLY | 2 | 0 |
| 1 | J | 839 | MLY | 9 | 0 |
| 1 | A | 63 | MLY | 4 | 0 |
| 1 | D | 837 | MLY | 1 | 0 |
| 1 | G | 84 | MLY | 33 | 0 |
| 1 | A | 415 | MLY | 1 | 0 |
| 1 | D | 87 | MLY | 3 | 0 |
| 1 | D | 764 | MLY | 7 | 0 |
| 1 | A | 764 | MLY | 10 | 0 |
| 1 | A | 837 | MLY | 12 | 0 |
| 1 | D | 30 | MLY | 1 | 0 |
| 1 | G | 505 | MLY | 16 | 0 |
| 1 | D | 436 | MLY | 2 | 0 |
| 1 | P | 782 | MLY | 1 | 0 |
| 1 | P | 190 | MLY | 2 | 0 |
| 1 | D | 528 | MLY | 3 | 0 |
| 1 | D | 617 | MLY | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | G | 138 | MLY | 1 | 0 |
| 1 | G | 295 | MLY | 6 | 0 |
| 1 | A | 551 | MLY | 2 | 0 |
| 1 | A | 55 | MLY | 1 | 0 |
| 1 | P | 107 | MLY | 3 | 0 |
| 1 | A | 617 | MLY | 1 | 0 |
| 1 | G | 764 | MLY | 20 | 0 |
| 1 | A | 553 | MLY | 18 | 0 |
| 1 | P | 505 | MLY | 8 | 0 |
| 1 | A | 369 | MLY | 1 | 0 |
| 1 | J | 248 | MLY | 2 | 0 |
| 1 | P | 486 | MLY | 3 | 0 |
| 1 | A | 59 | MLY | 2 | 0 |
| 1 | P | 598 | MLY | 1 | 0 |
| 1 | A | 528 | MLY | 2 | 0 |
| 1 | J | 272 | MLY | 1 | 0 |
| 1 | A | 598 | MLY | 1 | 0 |
| 1 | G | 87 | MLY | 2 | 0 |
| 1 | D | 348 | MLY | 6 | 0 |
| 1 | D | 107 | MLY | 2 | 0 |
| 1 | J | 30 | MLY | 1 | 0 |
| 1 | A | 107 | MLY | 3 | 0 |
| 1 | J | 190 | MLY | 2 | 0 |
| 1 | G | 30 | MLY | 1 | 0 |
| 1 | P | 600 | MLY | 1 | 0 |
| 1 | J | 782 | MLY | 1 | 0 |
| 1 | G | 272 | MLY | 1 | 0 |
| 1 | J | 59 | MLY | 3 | 0 |
| 1 | D | 598 | MLY | 1 | 0 |
| 1 | J | 528 | MLY | 3 | 0 |
| 1 | J | 617 | MLY | 1 | 0 |
| 1 | P | 87 | MLY | 3 | 0 |
| 1 | P | 49 | MLY | 3 | 0 |
| 1 | G | 839 | MLY | 4 | 0 |
| 1 | P | 295 | MLY | 6 | 0 |
| 1 | A | 600 | MLY | 1 | 0 |
| 1 | G | 107 | MLY | 3 | 0 |
| 1 | A | 49 | MLY | 3 | 0 |
| 1 | A | 839 | MLY | 8 | 0 |
| 1 | A | 248 | MLY | 2 | 0 |
| 1 | G | 55 | MLY | 1 | 0 |
| 1 | D | 659 | MLY | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 138 | MLY | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | P | 5 |
| 1 | D | 4 |
| 1 | A | 4 |
| 1 | J | 3 |
| 1 | G | 3 |
| 3 | C | 1 |
| 3 | F | 1 |
| 3 | I | 1 |
| 3 | L | 1 |
| 3 | R | 1 |
| 2 | B | 1 |
| 2 | E | 1 |
| 2 | H | 1 |
| 2 | K | 1 |
| 2 | Q | 1 |

The worst 5 of 29 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | J | 769:ALA | C | 770:GLY | N | 5.57 |

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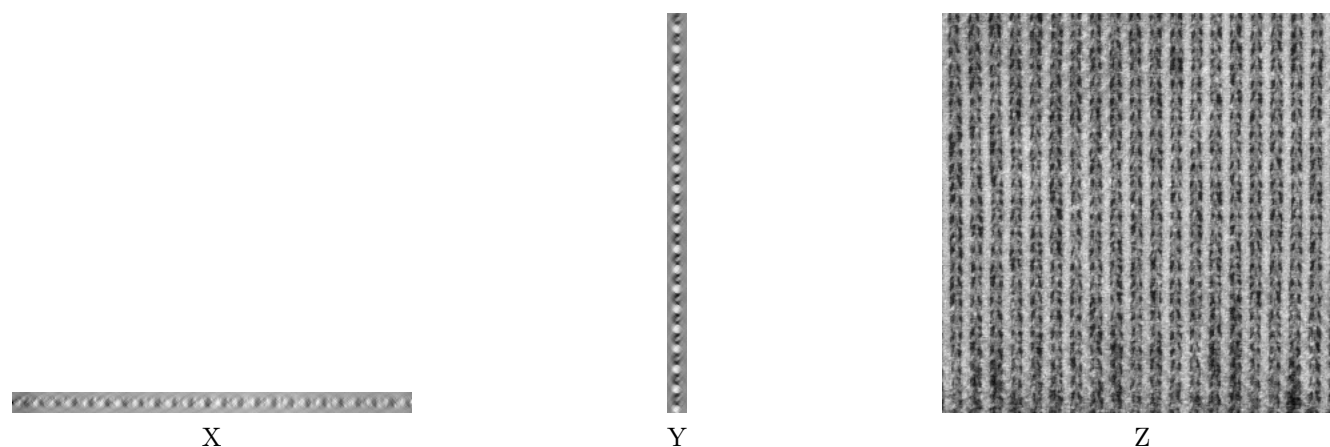
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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | D | 769:ALA | C | 770:GLY | N | 4.97 |
| 1 | G | 769:ALA | C | 770:GLY | N | 4.52 |
| 1 | P | 786:ILE | C | 787:ILE | N | 4.06 |
| 1 | D | 709:LYS | C | 710:GLY | N | 3.41 |

6 Tomogram visualisation [i](#)

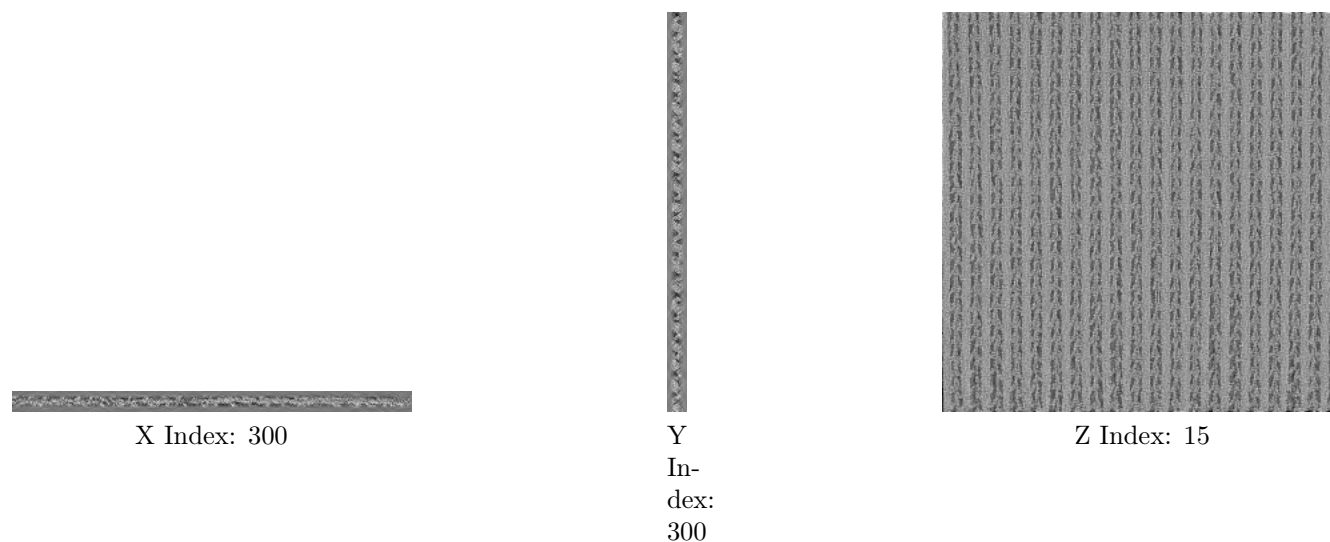
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



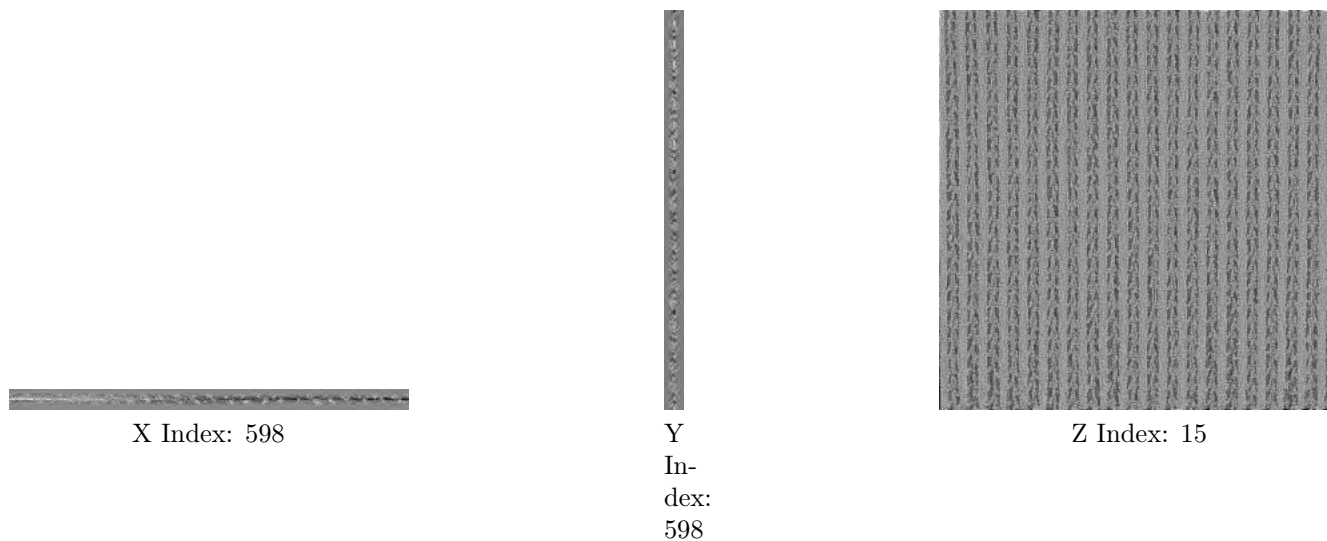
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



The images above show the largest variance slices of the tomogram in three orthogonal directions.

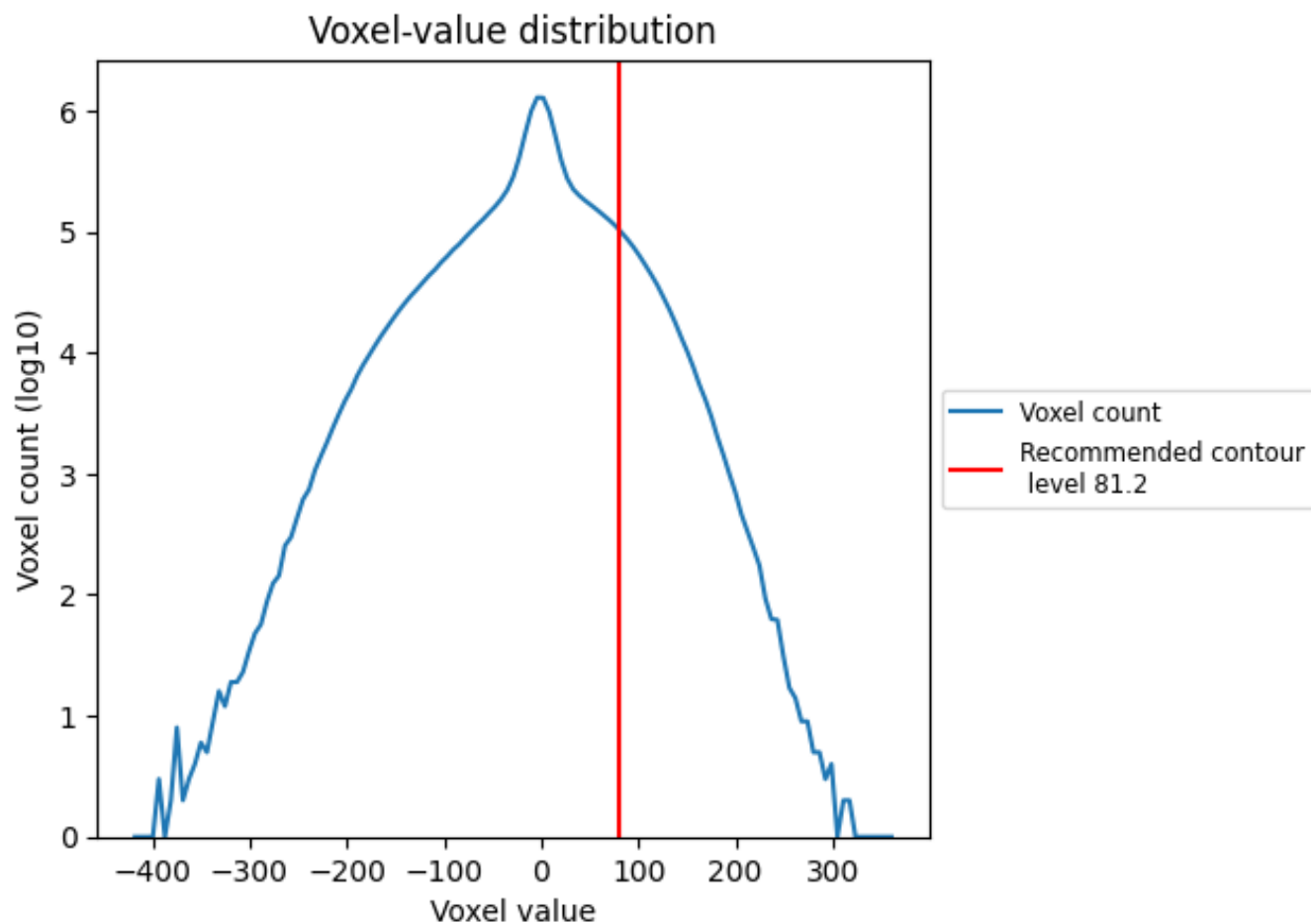
6.4 Mask visualisation [i](#)

This section was not generated.

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

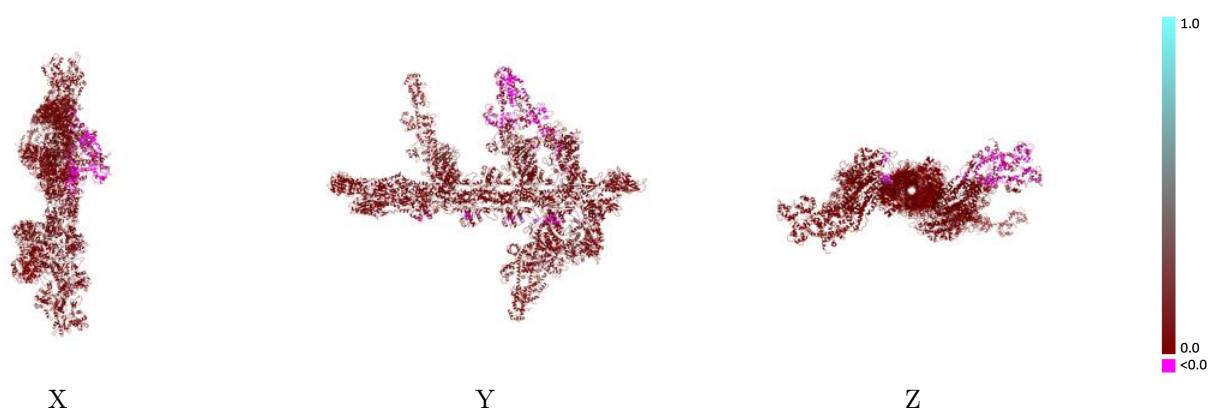
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1C. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay [i](#)

This section was not generated.

8.2 Q-score mapped to coordinate model [i](#)

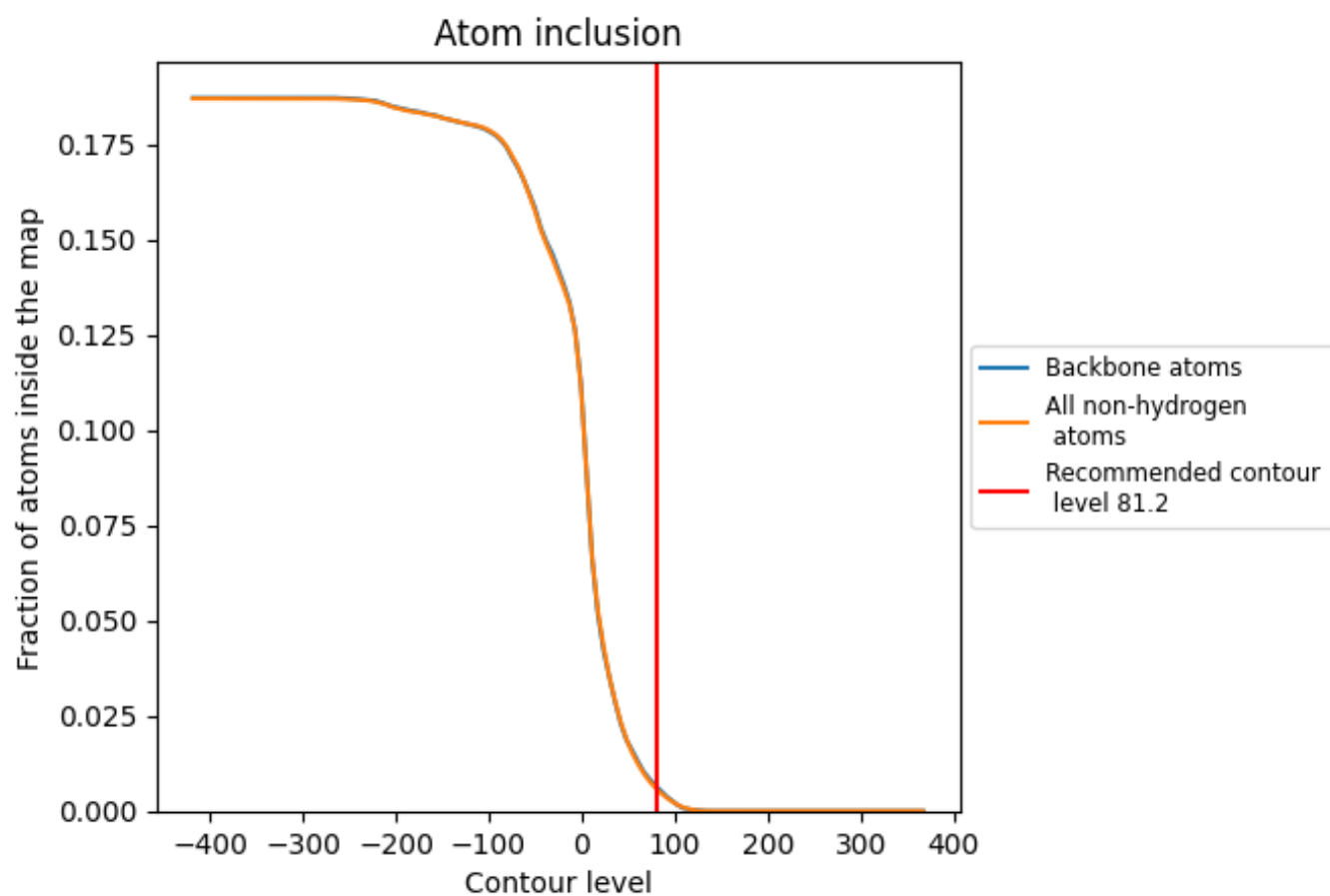


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.





























































8.4 Atom inclusion [i](#)



At the recommended contour level, 1% of all backbone atoms, 1% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (81.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|---|
| All |  0.0055 |  -0.0000 |
| 0 |  0.0000 |  0.0000 |
| 1 |  0.0147 |  0.0010 |
| 2 |  0.0000 |  0.0000 |
| 3 |  0.0000 |  0.0000 |
| 4 |  0.0000 |  -0.0000 |
| 5 |  0.0000 |  0.0000 |
| 7 |  0.0000 |  0.0000 |
| 8 |  0.0000 |  -0.0010 |
| 9 |  0.0000 |  0.0010 |
| A |  0.0000 |  -0.0010 |
| B |  0.0000 |  0.0000 |
| C |  0.0000 |  0.0000 |
| D |  0.0000 |  0.0030 |
| E |  0.0000 |  -0.0080 |
| F |  0.1517 |  0.0060 |
| G |  0.0000 |  -0.0020 |
| H |  0.0000 |  0.0000 |
| I |  0.0000 |  0.0000 |
| J |  0.0000 |  -0.0010 |
| K |  0.0331 |  0.0020 |
| L |  0.0000 |  -0.0040 |
| P |  0.0000 |  0.0000 |
| Q |  0.0000 |  0.0000 |
| R |  0.0000 |  0.0000 |
| V |  0.0000 |  -0.0020 |
| W |  0.0000 |  -0.0000 |
| X |  0.0688 |  -0.0030 |
| Y |  0.0000 |  0.0000 |
| Z |  0.0074 |  0.0060 |

