# Full wwPDB EM Validation Report

Dec 11, 2022 – 03:48 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 6SO3 |
| EMDB ID | : | EMD-7029 |
| Title | : | The interacting head motif in insect flight muscle myosin thick filaments |
| Authors | : | Morris, E.P.; Knupp, C.; Squire, J.M. |
| Deposited on | : | 2019-08-28 |
| Resolution | : | 6.20 Å(reported) |

This is a Full wwPDB EM Validation 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 (i) symbol.

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

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

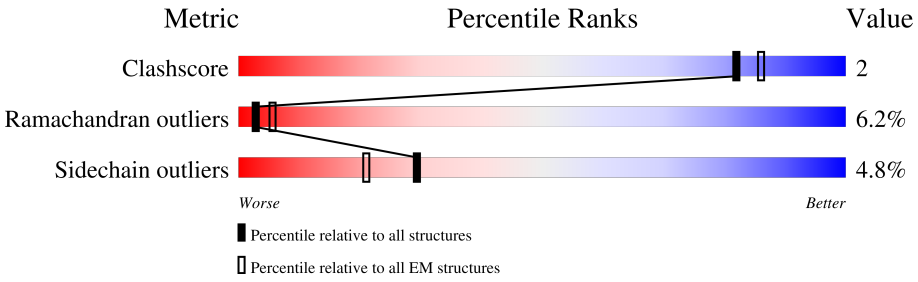
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 6.20 Å.

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




| Metric | 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 <=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 | 1953 | 43% 29% 12% 57% |
| 1 | B | 1953 | 43% 30% 10% 57% |
| 2 | C | 156 | 100% 71% 26% |
| 2 | D | 156 | 100% 69% 25% 6% |
| 3 | E | 196 | 100% 68% 23% 8% |
| 3 | F | 196 | 100% 69% 24% 7% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37957 atoms, of which 18956 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 Myosin 2 heavy chain striated muscle.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | B | 840 | Total | C | H | N | O | S | 0 | 0 |
| | | | 13499 | 4302 | 6760 | 1164 | 1245 | 28 | | |
| 1 | A | 840 | Total | C | H | N | O | S | 0 | 0 |
| | | | 13498 | 4302 | 6760 | 1164 | 1244 | 28 | | |

- Molecule 2 is a protein called Myosin 2 essential light chain striated muscle.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | D | 156 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2460 | 779 | 1227 | 199 | 247 | 8 | | |
| 2 | C | 156 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2460 | 779 | 1227 | 199 | 247 | 8 | | |

- Molecule 3 is a protein called Myosin 2 regulatory light chain striated muscle.

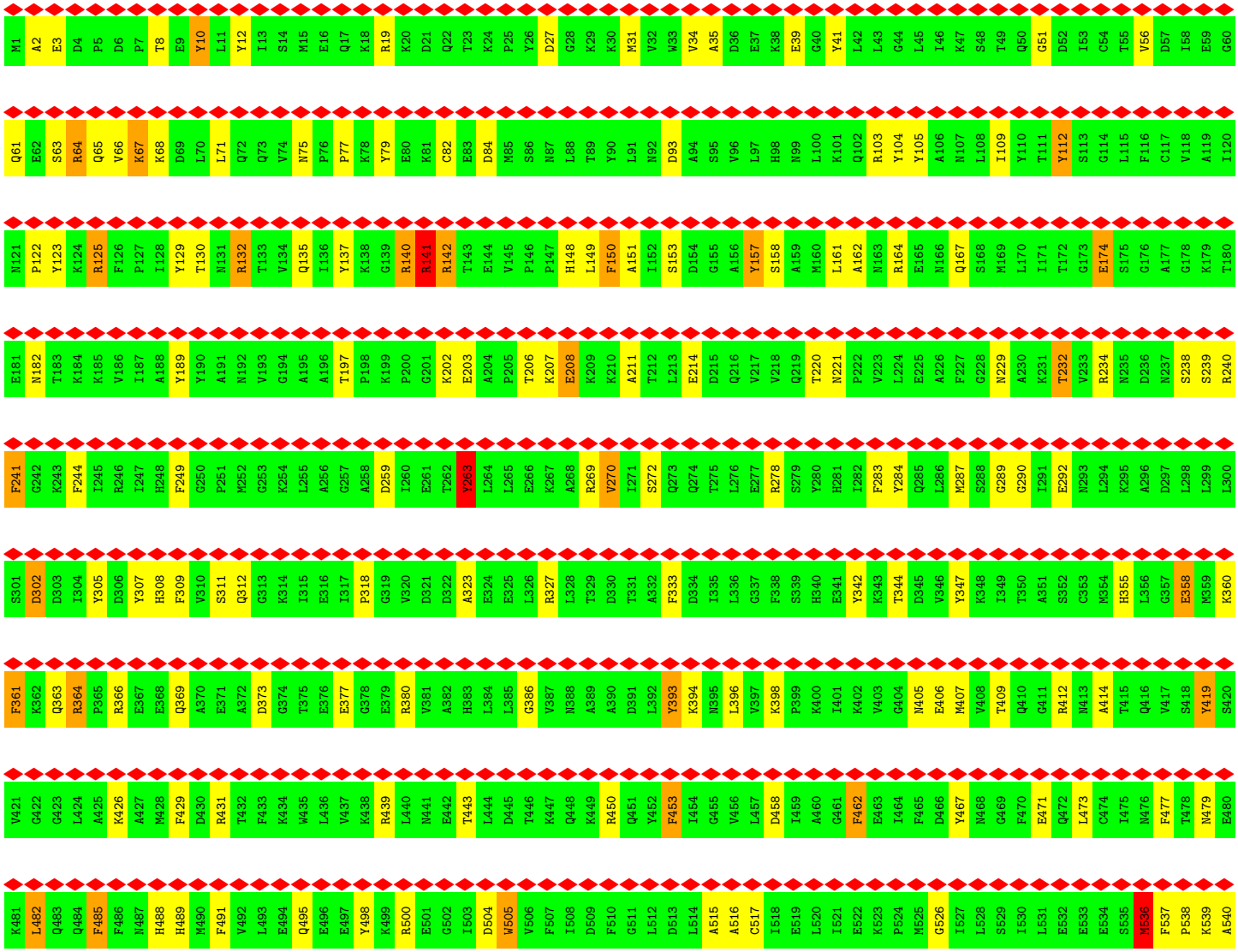
| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | F | 196 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3020 | 952 | 1491 | 257 | 314 | 6 | | |
| 3 | E | 196 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3020 | 952 | 1491 | 257 | 314 | 6 | | |

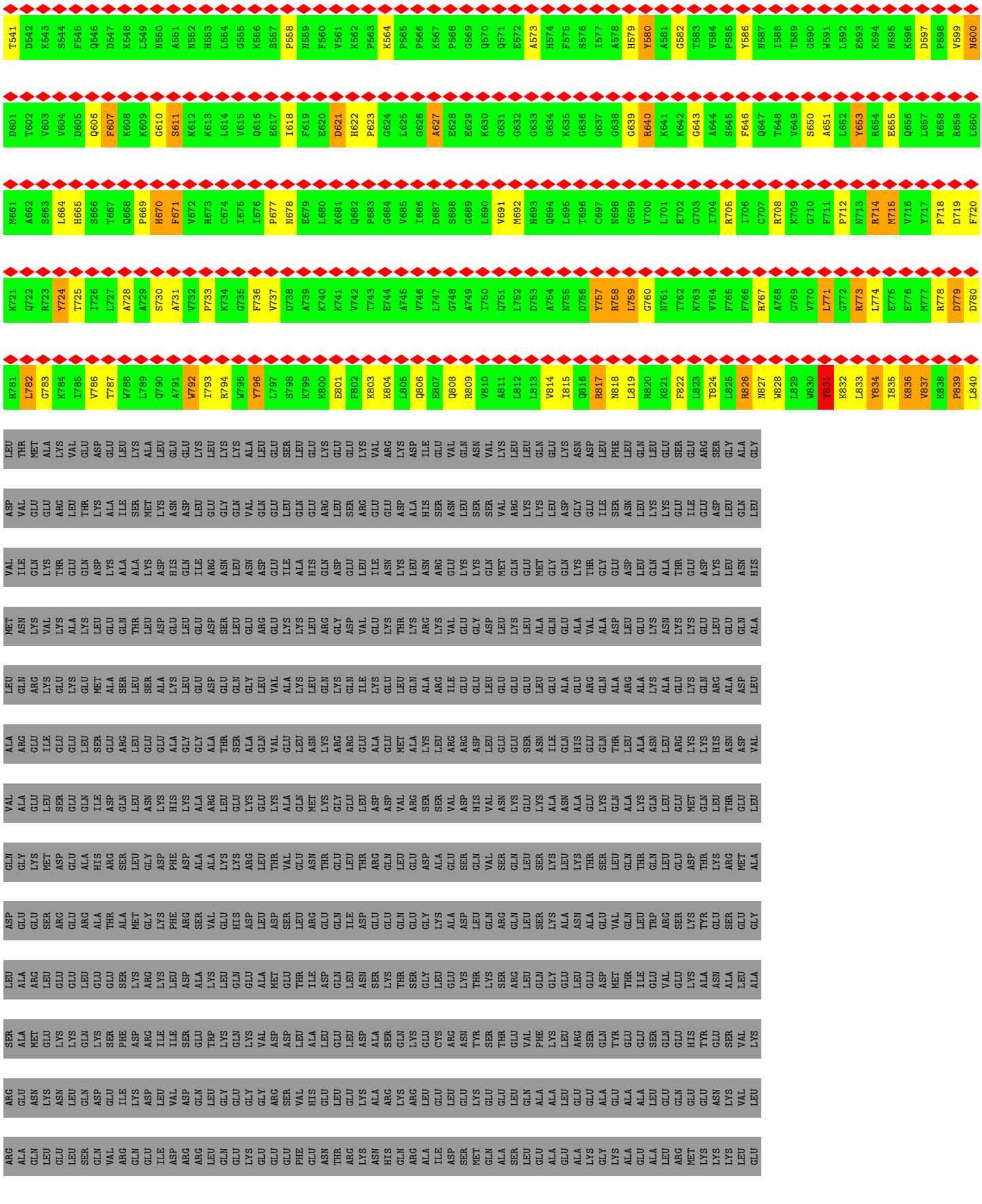
# 3 Residue-property plots (i)

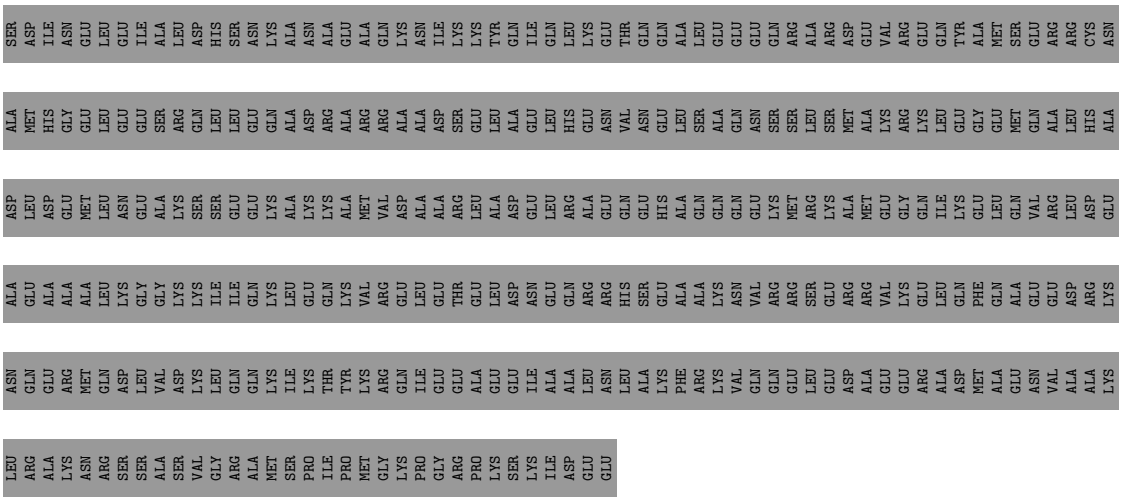
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Myosin 2 heavy chain striated muscle

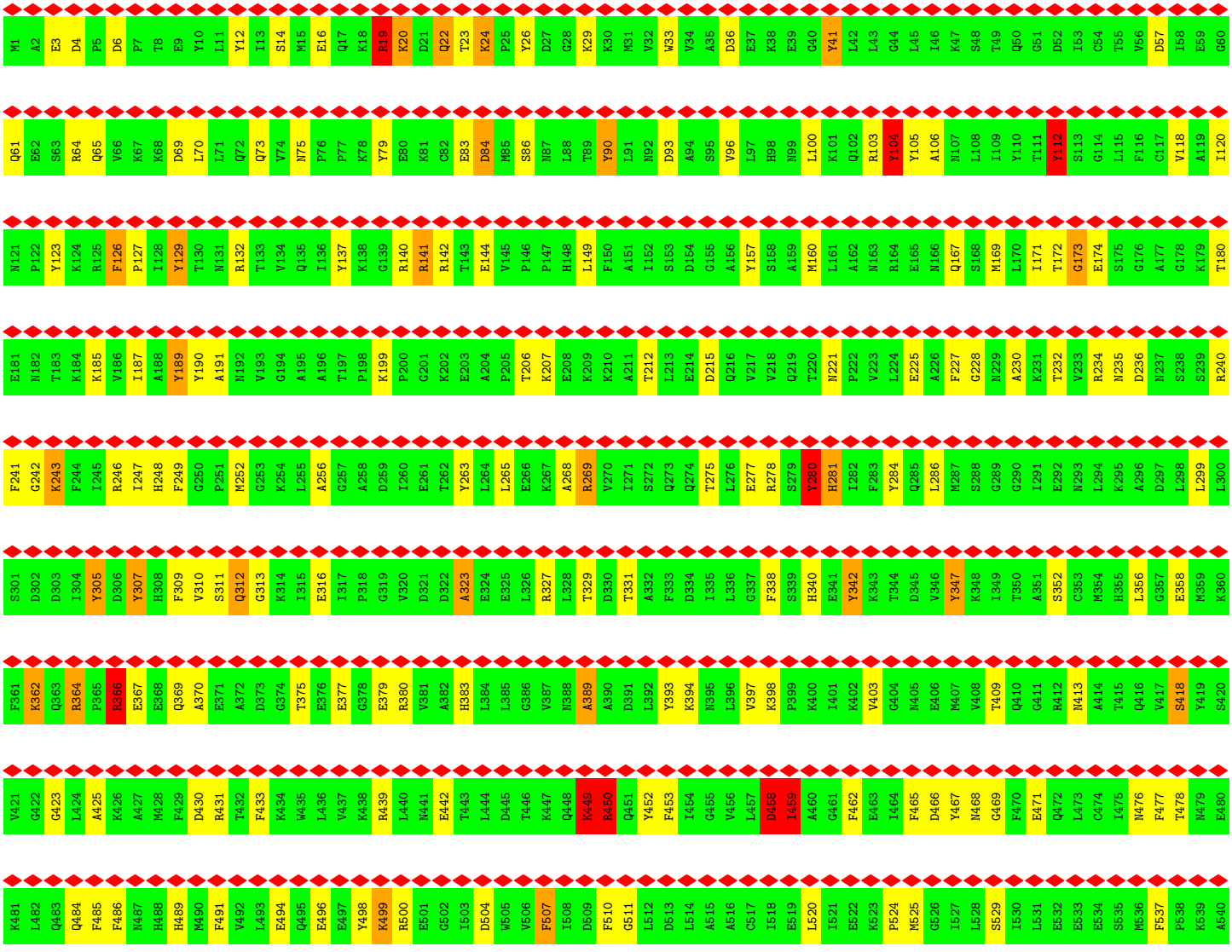
Chain B:

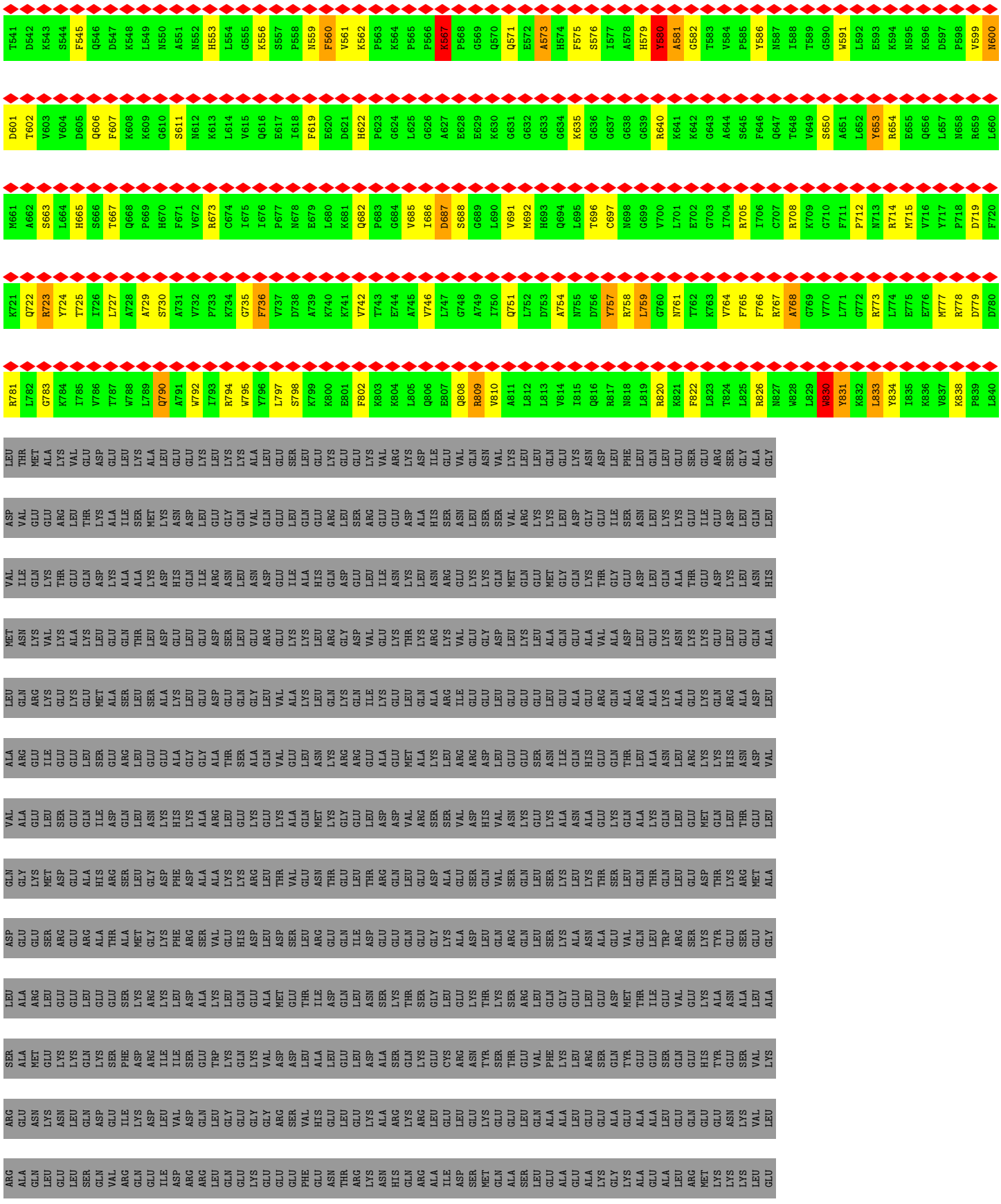



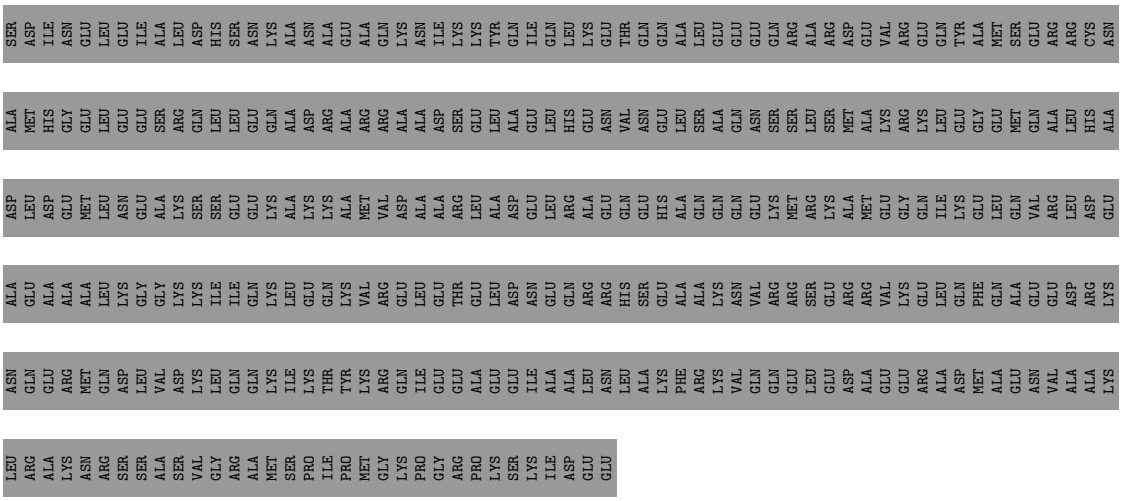

T541 D542 K543 S544 F545 Q546 D547 K548 L549 N550 A551 N552 H553 L554 G555 K556 S557 P558 N559 F560 V561 K562 P563 K564 P565 P566 K567 P568 G569 Q570 Q571 E572 A573 H574 F575 S576 I577 A578 H579 Y580 A581 G582 T583 V584 P585 Y586 N587 I588 T589 G590 W591 L592 E593 K594 N595 K596 D597 P598 V599 N600
D601 T602 V603 V604 D605 Q606 F607 K608 K609 G610 S611 N612 K613 L614 V615 Q616 E617 I618 F619 E620 D621 H622 P623 G624 L625 G626 A627 E628 E629 K630 G631 G632 G633 G634 K635 G636 G637 G638 G639 R640 K641 K642 G643 A644 S645 F646 Q647 T648 V649 S650 A651 L652 Y653 R654 E655 Q656 L657 N658 R659 L660
M661 A662 S663 L664 H665 S666 T667 Q668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 L680 K681 Q682 P683 G684 V685 I686 D687 S688 G689 L690 V691 M692 H693 Q694 L695 T696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 N713 R714 M715 V716 Y717 P718 D719 F720
K721 Q722 R723 Y724 T725 I726 L727 A728 A729 S730 A731 V732 P733 K734 G735 F736 V737 D738 A739 K740 K741 V742 T743 E744 A745 V746 L747 G748 A749 I750 Q751 L752 D753 A754 N755 D756 Y757 R758 L759 G760 N761 T762 K763 V764 F765 F766 R767 A768 G769 V770 L771 G772 R773 L774 E775 E776 M777 R778 D779 D780
R781 L782 G783 K784 I785 V786 T787 W788 L789 Q790 A791 W792 I793 R794 W795 Y796 L797 S798 K799 K800 E801 F802 K803 K804 L805 Q806 E807 Q808 R809 V810 A811 L812 L813 V814 I815 Q816 R817 N818 L819 R820 K821 F822 L823 T824 L825 R826 N827 W828 L829 W830 Y831 K832 L833 Y834 I835 K836 V837 K838 P839 L840



• Molecule 1: Myosin 2 heavy chain striated muscle

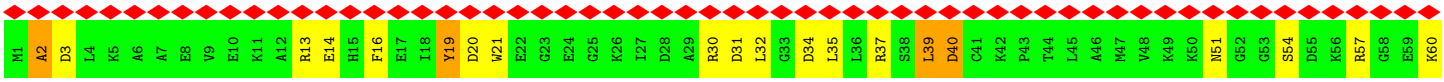



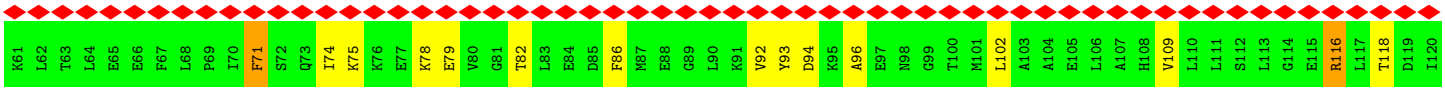

T541 D542 K543 S544 F545 Q546 D547 K548 L549 N550 A551 N552 H553 L554 G555 K556 S557 P558 N559 F560 V561 K562 P563 K564 P565 P566 K567 P568 G569 Q570 Q571 E572 A573 H574 F575 S576 I577 A578 H579 Y580 A581 G582 T583 V584 P585 Y586 N587 I588 T589 G590 W591 L592 E593 K594 N595 K596 D597 P598 V599 N600
D601 T602 V603 V604 D605 Q606 F607 K608 K609 G610 S611 N612 K613 L614 V615 Q616 E617 I618 F619 E620 D621 H622 P623 G624 L625 G626 A627 E628 E629 K630 G631 G632 G633 G634 K635 G636 G637 G638 G639 R640 K641 K642 G643 A644 S645 F646 Q647 T648 V649 S650 A651 L652 Y653 R654 E655 Q656 L657 N658 R659 L660
M661 A662 S663 L664 H665 S666 T667 Q668 P669 H670 F671 V672 R673 C674 I675 I676 P677 N678 E679 L680 K681 Q682 P683 G684 V685 I686 D687 S688 G689 L690 V691 M692 H693 Q694 L695 T696 C697 N698 G699 V700 L701 E702 G703 I704 R705 I706 C707 R708 K709 G710 F711 P712 N713 R714 M715 V716 Y717 P718 D719 F720
K721 Q722 R723 Y724 T725 I726 L727 A728 A729 S730 A731 V732 P733 K734 G735 F736 V737 D738 A739 K740 K741 V742 T743 E744 A745 V746 L747 G748 A749 I750 Q751 L752 D753 A754 N755 D756 Y757 R758 L759 G760 N761 T762 K763 V764 F765 F766 R767 A768 G769 V770 L771 G772 R773 L774 E775 E776 M777 R778 D779 D780
R781 L782 G783 K784 I785 V786 T787 W788 L789 Q790 A791 W792 T793 R794 W795 Y796 L797 S798 K799 K800 E801 F802 K803 K804 L805 Q806 E807 Q808 R809 V810 A811 L812 L813 V814 I815 Q816 R817 N818 L819 R820 K821 F822 L823 T824 L825 R826 N827 W828 L829 W830 Y831 K832 L833 Y834 I835 K836 V837 K838 P839 L840

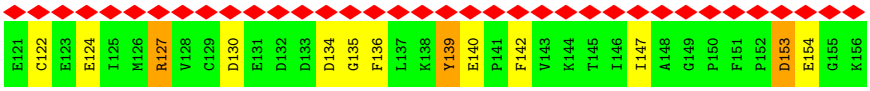



• Molecule 2: Myosin 2 essential light chain striated muscle

Chain D:

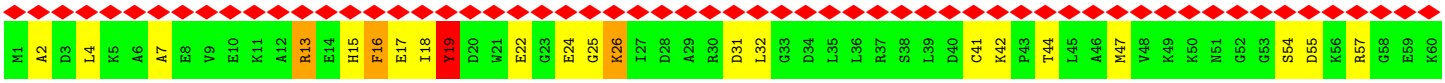



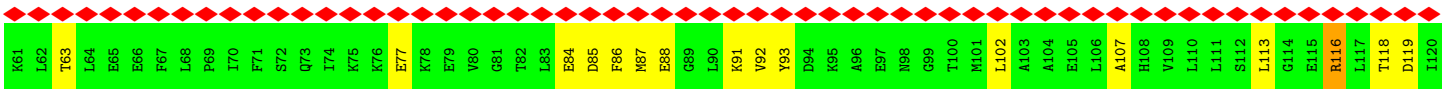



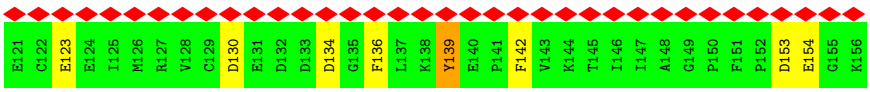




• Molecule 2: Myosin 2 essential light chain striated muscle

Chain C:

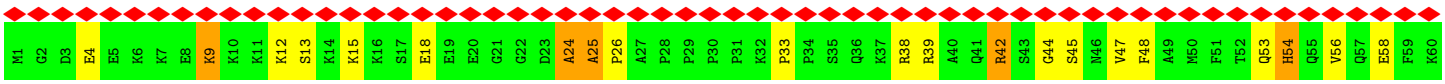




• Molecule 3: Myosin 2 regulatory light chain striated muscle

Chain F:


• Molecule 3: Myosin 2 regulatory light chain striated muscle

Chain E:


# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | HELICAL | Depositor |
| Imposed symmetry | HELICAL, twist=33.98°, rise=145 Å, axial sym=C4 | Depositor |
| Number of segments used | 24000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 65 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | DIRECT ELECTRON DE-20 (5k x 3k) | Depositor |
| Maximum map value | 0.181 | Depositor |
| Minimum map value | -0.056 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.009 | Depositor |
| Recommended contour level | 0.032 | Depositor |
| Map size (Å) | 528.336, 528.336, 528.336 | wwPDB |
| Map dimensions | 432, 432, 432 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.223, 1.223, 1.223 | 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 | A | 1.70 | 50/6882 (0.7%) | 2.01 | 194/9279 (2.1%) |
| 1 | B | 1.70 | 56/6883 (0.8%) | 1.98 | 158/9280 (1.7%) |
| 2 | C | 1.70 | 9/1251 (0.7%) | 1.94 | 26/1674 (1.6%) |
| 2 | D | 1.65 | 6/1251 (0.5%) | 1.99 | 43/1674 (2.6%) |
| 3 | E | 1.66 | 8/1554 (0.5%) | 1.94 | 38/2081 (1.8%) |
| 3 | F | 1.68 | 8/1554 (0.5%) | 1.98 | 33/2081 (1.6%) |
| All | All | 1.69 | 137/19375 (0.7%) | 1.99 | 492/26069 (1.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 18 |
| 1 | B | 0 | 31 |
| 2 | C | 0 | 6 |
| 2 | D | 0 | 1 |
| 3 | E | 0 | 3 |
| 3 | F | 0 | 3 |
| All | All | 0 | 62 |

All (137) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | F | 42 | ARG | CZ-NH2 | 8.38 | 1.44 | 1.33 |
| 1 | B | 796 | TYR | CE2-CZ | 8.13 | 1.49 | 1.38 |
| 1 | A | 342 | TYR | CG-CD1 | 7.94 | 1.49 | 1.39 |
| 1 | B | 834 | TYR | CE2-CZ | 7.80 | 1.48 | 1.38 |
| 3 | F | 13 | SER | CA-CB | 7.50 | 1.64 | 1.52 |
| 1 | A | 366 | ARG | CZ-NH1 | 7.36 | 1.42 | 1.33 |
| 1 | A | 347 | TYR | CE2-CZ | 7.34 | 1.48 | 1.38 |
| 1 | A | 735 | GLY | N-CA | -7.33 | 1.35 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 453 | PHE | CG-CD1 | 7.30 | 1.49 | 1.38 |
| 1 | B | 142 | ARG | NE-CZ | 7.19 | 1.42 | 1.33 |
| 1 | B | 358 | GLU | CG-CD | 7.04 | 1.62 | 1.51 |
| 2 | D | 139 | TYR | CZ-OH | 6.91 | 1.49 | 1.37 |
| 1 | B | 412 | ARG | CD-NE | 6.88 | 1.58 | 1.46 |
| 1 | A | 781 | ARG | CZ-NH2 | 6.87 | 1.42 | 1.33 |
| 1 | B | 537 | PHE | CE2-CZ | 6.87 | 1.50 | 1.37 |
| 1 | B | 653 | TYR | CG-CD2 | 6.83 | 1.48 | 1.39 |
| 1 | A | 450 | ARG | CZ-NH2 | 6.80 | 1.41 | 1.33 |
| 2 | C | 25 | GLY | CA-C | -6.75 | 1.41 | 1.51 |
| 1 | A | 576 | SER | CA-CB | 6.74 | 1.63 | 1.52 |
| 1 | B | 269 | ARG | NE-CZ | 6.73 | 1.41 | 1.33 |
| 1 | B | 263 | TYR | CZ-OH | 6.66 | 1.49 | 1.37 |
| 3 | F | 47 | VAL | CA-CB | -6.65 | 1.40 | 1.54 |
| 1 | B | 125 | ARG | CD-NE | 6.61 | 1.57 | 1.46 |
| 1 | A | 727 | LEU | N-CA | 6.55 | 1.59 | 1.46 |
| 1 | A | 157 | TYR | CE2-CZ | 6.34 | 1.46 | 1.38 |
| 1 | A | 757 | TYR | CE1-CZ | 6.34 | 1.46 | 1.38 |
| 1 | B | 104 | TYR | CZ-OH | 6.31 | 1.48 | 1.37 |
| 1 | A | 783 | GLY | CA-C | 6.26 | 1.61 | 1.51 |
| 1 | A | 757 | TYR | CB-CG | -6.25 | 1.42 | 1.51 |
| 1 | A | 798 | SER | CA-CB | 6.25 | 1.62 | 1.52 |
| 1 | B | 249 | PHE | CG-CD1 | 6.14 | 1.48 | 1.38 |
| 1 | B | 730 | SER | CA-CB | 6.12 | 1.62 | 1.52 |
| 1 | B | 203 | GLU | CB-CG | 6.12 | 1.63 | 1.52 |
| 1 | A | 83 | GLU | CD-OE1 | 6.11 | 1.32 | 1.25 |
| 1 | B | 540 | ALA | CA-CB | 6.06 | 1.65 | 1.52 |
| 1 | A | 418 | SER | CA-CB | 6.02 | 1.61 | 1.52 |
| 1 | A | 708 | ARG | NE-CZ | 6.02 | 1.40 | 1.33 |
| 1 | A | 137 | TYR | CB-CG | -6.00 | 1.42 | 1.51 |
| 1 | B | 174 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | A | 352 | SER | CA-CB | 5.97 | 1.61 | 1.52 |
| 1 | B | 643 | GLY | N-CA | -5.95 | 1.37 | 1.46 |
| 1 | B | 826 | ARG | NE-CZ | 5.94 | 1.40 | 1.33 |
| 2 | C | 54 | SER | CA-CB | 5.94 | 1.61 | 1.52 |
| 1 | A | 189 | TYR | CB-CG | 5.94 | 1.60 | 1.51 |
| 2 | D | 14 | GLU | CG-CD | 5.92 | 1.60 | 1.51 |
| 1 | A | 724 | TYR | CB-CG | 5.92 | 1.60 | 1.51 |
| 3 | E | 168 | SER | CA-CB | 5.92 | 1.61 | 1.52 |
| 1 | A | 379 | GLU | CD-OE1 | 5.92 | 1.32 | 1.25 |
| 1 | A | 611 | SER | CA-CB | 5.91 | 1.61 | 1.52 |
| 1 | A | 453 | PHE | CE1-CZ | 5.88 | 1.48 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 640 | ARG | CD-NE | 5.88 | 1.56 | 1.46 |
| 1 | B | 278 | ARG | CD-NE | 5.87 | 1.56 | 1.46 |
| 1 | B | 12 | TYR | CZ-OH | 5.86 | 1.47 | 1.37 |
| 1 | A | 140 | ARG | CZ-NH2 | 5.84 | 1.40 | 1.33 |
| 1 | A | 529 | SER | CA-CB | 5.83 | 1.61 | 1.52 |
| 1 | A | 307 | TYR | CE2-CZ | 5.82 | 1.46 | 1.38 |
| 1 | B | 10 | TYR | CG-CD1 | 5.78 | 1.46 | 1.39 |
| 1 | B | 439 | ARG | CZ-NH1 | 5.77 | 1.40 | 1.33 |
| 1 | A | 367 | GLU | CG-CD | 5.76 | 1.60 | 1.51 |
| 1 | B | 167 | GLN | CG-CD | 5.76 | 1.64 | 1.51 |
| 1 | A | 24 | LYS | CA-CB | 5.76 | 1.66 | 1.53 |
| 1 | A | 157 | TYR | CD2-CE2 | 5.75 | 1.48 | 1.39 |
| 2 | C | 139 | TYR | CB-CG | 5.73 | 1.60 | 1.51 |
| 3 | E | 150 | SER | N-CA | -5.65 | 1.35 | 1.46 |
| 3 | F | 161 | ASP | CA-CB | 5.63 | 1.66 | 1.53 |
| 3 | E | 61 | GLU | CG-CD | 5.62 | 1.60 | 1.51 |
| 3 | F | 118 | ARG | CZ-NH1 | 5.58 | 1.40 | 1.33 |
| 3 | E | 162 | GLU | CG-CD | 5.58 | 1.60 | 1.51 |
| 3 | F | 25 | ALA | CA-CB | 5.57 | 1.64 | 1.52 |
| 3 | F | 174 | GLY | CA-C | -5.56 | 1.43 | 1.51 |
| 1 | A | 141 | ARG | NE-CZ | 5.51 | 1.40 | 1.33 |
| 1 | A | 173 | GLY | CA-C | -5.49 | 1.43 | 1.51 |
| 2 | C | 77 | GLU | CD-OE2 | 5.47 | 1.31 | 1.25 |
| 1 | B | 63 | SER | CB-OG | 5.47 | 1.49 | 1.42 |
| 1 | A | 498 | TYR | CZ-OH | 5.46 | 1.47 | 1.37 |
| 1 | B | 450 | ARG | NE-CZ | 5.45 | 1.40 | 1.33 |
| 2 | D | 124 | GLU | CG-CD | 5.43 | 1.60 | 1.51 |
| 1 | A | 242 | GLY | N-CA | -5.43 | 1.37 | 1.46 |
| 2 | C | 24 | GLU | CB-CG | 5.43 | 1.62 | 1.52 |
| 3 | E | 42 | ARG | CZ-NH1 | 5.42 | 1.40 | 1.33 |
| 2 | C | 17 | GLU | CG-CD | 5.41 | 1.60 | 1.51 |
| 1 | A | 313 | GLY | N-CA | -5.41 | 1.38 | 1.46 |
| 1 | A | 191 | ALA | CA-CB | 5.39 | 1.63 | 1.52 |
| 1 | B | 724 | TYR | CD2-CE2 | 5.36 | 1.47 | 1.39 |
| 1 | B | 122 | PRO | C-N | 5.32 | 1.46 | 1.34 |
| 1 | A | 247 | ILE | C-N | 5.31 | 1.46 | 1.34 |
| 1 | B | 239 | SER | CA-CB | 5.30 | 1.60 | 1.52 |
| 1 | A | 174 | GLU | CD-OE2 | 5.29 | 1.31 | 1.25 |
| 1 | B | 431 | ARG | CZ-NH1 | 5.29 | 1.40 | 1.33 |
| 1 | B | 162 | ALA | CA-CB | 5.24 | 1.63 | 1.52 |
| 1 | B | 610 | GLY | CA-C | -5.24 | 1.43 | 1.51 |
| 1 | B | 51 | GLY | CA-C | -5.24 | 1.43 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 606 | GLN | CG-CD | 5.24 | 1.63 | 1.51 |
| 1 | B | 214 | GLU | CB-CG | 5.23 | 1.62 | 1.52 |
| 1 | B | 129 | TYR | CE2-CZ | 5.22 | 1.45 | 1.38 |
| 1 | B | 495 | GLN | CG-CD | 5.22 | 1.63 | 1.51 |
| 2 | D | 139 | TYR | CE1-CZ | 5.22 | 1.45 | 1.38 |
| 1 | A | 236 | ASP | CA-CB | 5.22 | 1.65 | 1.53 |
| 1 | A | 171 | ILE | CA-CB | 5.22 | 1.66 | 1.54 |
| 1 | B | 182 | ASN | CB-CG | 5.22 | 1.63 | 1.51 |
| 1 | B | 373 | ASP | C-N | 5.21 | 1.42 | 1.33 |
| 3 | E | 94 | GLU | CD-OE2 | -5.20 | 1.20 | 1.25 |
| 1 | A | 284 | TYR | CE2-CZ | 5.20 | 1.45 | 1.38 |
| 1 | B | 477 | PHE | CB-CG | 5.18 | 1.60 | 1.51 |
| 3 | E | 124 | GLU | CD-OE2 | 5.18 | 1.31 | 1.25 |
| 1 | B | 289 | GLY | C-N | 5.18 | 1.42 | 1.33 |
| 1 | B | 309 | PHE | CG-CD2 | 5.17 | 1.46 | 1.38 |
| 2 | C | 154 | GLU | CB-CG | 5.17 | 1.61 | 1.52 |
| 2 | D | 34 | ASP | CB-CG | 5.17 | 1.62 | 1.51 |
| 3 | E | 85 | SER | CB-OG | 5.17 | 1.49 | 1.42 |
| 1 | B | 505 | TRP | CD2-CE3 | -5.16 | 1.32 | 1.40 |
| 1 | B | 311 | SER | CA-CB | 5.16 | 1.60 | 1.52 |
| 1 | B | 129 | TYR | CE1-CZ | 5.15 | 1.45 | 1.38 |
| 1 | A | 79 | TYR | CE2-CZ | 5.14 | 1.45 | 1.38 |
| 1 | B | 364 | ARG | CD-NE | 5.13 | 1.55 | 1.46 |
| 1 | B | 419 | TYR | CG-CD2 | 5.12 | 1.45 | 1.39 |
| 1 | A | 12 | TYR | CE2-CZ | 5.11 | 1.45 | 1.38 |
| 1 | B | 839 | PRO | CA-C | -5.10 | 1.42 | 1.52 |
| 1 | B | 655 | GLU | CB-CG | 5.10 | 1.61 | 1.52 |
| 1 | B | 238 | SER | CA-CB | 5.08 | 1.60 | 1.52 |
| 1 | B | 539 | LYS | N-CA | -5.08 | 1.36 | 1.46 |
| 3 | F | 4 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 2 | C | 13 | ARG | CD-NE | 5.08 | 1.55 | 1.46 |
| 1 | A | 70 | LEU | CA-CB | 5.07 | 1.65 | 1.53 |
| 1 | A | 104 | TYR | CE2-CZ | 5.07 | 1.45 | 1.38 |
| 1 | A | 575 | PHE | CE2-CZ | 5.07 | 1.47 | 1.37 |
| 1 | B | 640 | ARG | CZ-NH2 | 5.05 | 1.39 | 1.33 |
| 2 | C | 123 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 2 | D | 57 | ARG | CD-NE | 5.04 | 1.55 | 1.46 |
| 1 | A | 225 | GLU | CG-CD | 5.04 | 1.59 | 1.51 |
| 1 | B | 363 | GLN | C-N | 5.04 | 1.45 | 1.34 |
| 1 | A | 397 | VAL | CB-CG1 | 5.03 | 1.63 | 1.52 |
| 1 | B | 377 | GLU | N-CA | -5.03 | 1.36 | 1.46 |
| 1 | A | 442 | GLU | CD-OE1 | -5.02 | 1.20 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 783 | GLY | N-CA | -5.02 | 1.38 | 1.46 |
| 1 | A | 380 | ARG | CZ-NH1 | 5.01 | 1.39 | 1.33 |
| 1 | B | 500 | ARG | NE-CZ | 5.01 | 1.39 | 1.33 |

All (492) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 809 | ARG | NE-CZ-NH1 | 17.57 | 129.08 | 120.30 |
| 3 | F | 38 | ARG | NE-CZ-NH2 | 17.39 | 128.99 | 120.30 |
| 3 | F | 149 | ARG | NE-CZ-NH2 | 16.97 | 128.78 | 120.30 |
| 1 | A | 767 | ARG | NE-CZ-NH2 | 16.62 | 128.61 | 120.30 |
| 1 | B | 809 | ARG | NE-CZ-NH2 | -16.00 | 112.30 | 120.30 |
| 1 | B | 708 | ARG | NE-CZ-NH1 | 15.82 | 128.21 | 120.30 |
| 1 | B | 767 | ARG | NE-CZ-NH1 | -15.31 | 112.65 | 120.30 |
| 1 | A | 41 | TYR | CB-CG-CD1 | -15.21 | 111.88 | 121.00 |
| 1 | B | 758 | ARG | NE-CZ-NH1 | -14.72 | 112.94 | 120.30 |
| 1 | A | 767 | ARG | NE-CZ-NH1 | -14.44 | 113.08 | 120.30 |
| 1 | A | 305 | TYR | CB-CG-CD2 | 14.36 | 129.62 | 121.00 |
| 1 | A | 132 | ARG | NE-CZ-NH2 | 14.18 | 127.39 | 120.30 |
| 1 | A | 809 | ARG | NE-CZ-NH2 | 13.91 | 127.26 | 120.30 |
| 1 | A | 327 | ARG | NE-CZ-NH1 | -13.83 | 113.38 | 120.30 |
| 2 | D | 86 | PHE | CB-CG-CD2 | 13.36 | 130.15 | 120.80 |
| 1 | B | 640 | ARG | NE-CZ-NH1 | 13.25 | 126.92 | 120.30 |
| 1 | B | 283 | PHE | CB-CG-CD2 | 13.17 | 130.02 | 120.80 |
| 2 | C | 139 | TYR | CB-CG-CD1 | -12.78 | 113.33 | 121.00 |
| 1 | B | 498 | TYR | CB-CG-CD1 | -12.38 | 113.57 | 121.00 |
| 3 | E | 59 | PHE | CB-CG-CD1 | -12.33 | 112.17 | 120.80 |
| 1 | B | 342 | TYR | CB-CG-CD1 | 12.07 | 128.24 | 121.00 |
| 1 | A | 778 | ARG | NE-CZ-NH2 | 12.03 | 126.32 | 120.30 |
| 1 | B | 141 | ARG | NE-CZ-NH2 | 11.96 | 126.28 | 120.30 |
| 2 | D | 37 | ARG | NE-CZ-NH2 | 11.78 | 126.19 | 120.30 |
| 2 | C | 139 | TYR | CB-CG-CD2 | 11.77 | 128.06 | 121.00 |
| 3 | F | 118 | ARG | NE-CZ-NH1 | -11.72 | 114.44 | 120.30 |
| 2 | D | 19 | TYR | CB-CG-CD2 | -11.63 | 114.02 | 121.00 |
| 1 | A | 305 | TYR | CB-CG-CD1 | -11.47 | 114.12 | 121.00 |
| 1 | A | 431 | ARG | NE-CZ-NH1 | -11.38 | 114.61 | 120.30 |
| 1 | B | 64 | ARG | NE-CZ-NH2 | 11.26 | 125.93 | 120.30 |
| 1 | B | 342 | TYR | CB-CG-CD2 | -11.21 | 114.28 | 121.00 |
| 1 | B | 439 | ARG | NE-CZ-NH2 | 11.17 | 125.88 | 120.30 |
| 1 | B | 364 | ARG | NE-CZ-NH2 | 11.15 | 125.88 | 120.30 |
| 2 | C | 116 | ARG | NE-CZ-NH1 | -11.12 | 114.74 | 120.30 |
| 1 | B | 580 | TYR | CB-CG-CD2 | 11.12 | 127.67 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 439 | ARG | NE-CZ-NH2 | 11.10 | 125.85 | 120.30 |
| 1 | B | 580 | TYR | CB-CG-CD1 | -10.78 | 114.53 | 121.00 |
| 1 | B | 283 | PHE | CB-CG-CD1 | -10.75 | 113.27 | 120.80 |
| 1 | B | 498 | TYR | CB-CG-CD2 | 10.73 | 127.44 | 121.00 |
| 1 | B | 129 | TYR | CB-CG-CD1 | -10.69 | 114.59 | 121.00 |
| 3 | E | 118 | ARG | NE-CZ-NH1 | -10.51 | 115.05 | 120.30 |
| 3 | E | 83 | PHE | CB-CG-CD1 | -10.31 | 113.58 | 120.80 |
| 1 | A | 104 | TYR | CB-CG-CD1 | -10.29 | 114.83 | 121.00 |
| 1 | A | 654 | ARG | NE-CZ-NH1 | -10.19 | 115.21 | 120.30 |
| 1 | A | 773 | ARG | NE-CZ-NH2 | 10.05 | 125.33 | 120.30 |
| 1 | A | 280 | TYR | CB-CG-CD2 | -10.04 | 114.97 | 121.00 |
| 1 | B | 778 | ARG | NE-CZ-NH2 | 10.04 | 125.32 | 120.30 |
| 1 | A | 607 | PHE | CB-CG-CD2 | -9.78 | 113.96 | 120.80 |
| 1 | B | 736 | PHE | CB-CG-CD2 | 9.74 | 127.62 | 120.80 |
| 2 | D | 71 | PHE | CB-CG-CD2 | -9.73 | 113.99 | 120.80 |
| 1 | B | 794 | ARG | NE-CZ-NH1 | -9.66 | 115.47 | 120.30 |
| 2 | D | 30 | ARG | NE-CZ-NH2 | 9.66 | 125.13 | 120.30 |
| 1 | B | 431 | ARG | NE-CZ-NH1 | -9.65 | 115.47 | 120.30 |
| 1 | A | 705 | ARG | NE-CZ-NH1 | -9.62 | 115.49 | 120.30 |
| 1 | A | 342 | TYR | CB-CG-CD1 | -9.59 | 115.25 | 121.00 |
| 1 | B | 671 | PHE | CB-CG-CD2 | 9.57 | 127.50 | 120.80 |
| 2 | D | 116 | ARG | NE-CZ-NH1 | -9.53 | 115.53 | 120.30 |
| 1 | B | 327 | ARG | NE-CZ-NH2 | -9.50 | 115.55 | 120.30 |
| 1 | A | 507 | PHE | CB-CG-CD1 | -9.48 | 114.17 | 120.80 |
| 1 | A | 323 | ALA | N-CA-CB | 9.46 | 123.35 | 110.10 |
| 2 | D | 86 | PHE | CB-CG-CD1 | -9.39 | 114.23 | 120.80 |
| 1 | A | 504 | ASP | CB-CG-OD2 | 9.32 | 126.69 | 118.30 |
| 1 | B | 64 | ARG | NE-CZ-NH1 | -9.31 | 115.65 | 120.30 |
| 3 | E | 118 | ARG | NE-CZ-NH2 | 9.28 | 124.94 | 120.30 |
| 2 | D | 93 | TYR | CB-CG-CD1 | -9.28 | 115.44 | 121.00 |
| 1 | A | 673 | ARG | NE-CZ-NH1 | -9.25 | 115.67 | 120.30 |
| 1 | B | 361 | PHE | CB-CG-CD1 | -9.22 | 114.34 | 120.80 |
| 1 | A | 736 | PHE | CB-CG-CD2 | -9.21 | 114.35 | 120.80 |
| 1 | A | 640 | ARG | NE-CZ-NH2 | -9.17 | 115.71 | 120.30 |
| 1 | B | 129 | TYR | CB-CG-CD2 | 9.09 | 126.45 | 121.00 |
| 2 | C | 63 | THR | CA-CB-CG2 | -9.09 | 99.68 | 112.40 |
| 1 | A | 280 | TYR | CB-CG-CD1 | 9.06 | 126.44 | 121.00 |
| 1 | B | 19 | ARG | NE-CZ-NH1 | -9.01 | 115.80 | 120.30 |
| 1 | B | 31 | MET | CG-SD-CE | -9.01 | 85.79 | 100.20 |
| 1 | B | 736 | PHE | CB-CG-CD1 | -8.97 | 114.52 | 120.80 |
| 2 | C | 19 | TYR | CB-CG-CD2 | 8.85 | 126.31 | 121.00 |
| 1 | A | 673 | ARG | NE-CZ-NH2 | 8.85 | 124.72 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 431 | ARG | NE-CZ-NH2 | 8.78 | 124.69 | 120.30 |
| 1 | A | 778 | ARG | NE-CZ-NH1 | -8.72 | 115.94 | 120.30 |
| 3 | E | 158 | PHE | CB-CG-CD1 | -8.72 | 114.70 | 120.80 |
| 3 | F | 149 | ARG | NE-CZ-NH1 | -8.72 | 115.94 | 120.30 |
| 1 | A | 132 | ARG | NE-CZ-NH1 | -8.70 | 115.95 | 120.30 |
| 1 | A | 765 | PHE | CB-CG-CD1 | -8.65 | 114.74 | 120.80 |
| 1 | B | 103 | ARG | NE-CZ-NH2 | 8.65 | 124.62 | 120.30 |
| 1 | B | 758 | ARG | NE-CZ-NH2 | 8.65 | 124.62 | 120.30 |
| 1 | A | 389 | ALA | N-CA-CB | 8.59 | 122.12 | 110.10 |
| 1 | A | 826 | ARG | NE-CZ-NH1 | -8.57 | 116.02 | 120.30 |
| 1 | A | 103 | ARG | NE-CZ-NH2 | 8.52 | 124.56 | 120.30 |
| 1 | B | 485 | PHE | CB-CG-CD1 | -8.50 | 114.85 | 120.80 |
| 1 | B | 132 | ARG | NE-CZ-NH1 | -8.49 | 116.06 | 120.30 |
| 1 | B | 10 | TYR | CB-CG-CD2 | 8.46 | 126.08 | 121.00 |
| 3 | E | 59 | PHE | CB-CG-CD2 | 8.44 | 126.71 | 120.80 |
| 3 | F | 24 | ALA | N-CA-CB | 8.40 | 121.86 | 110.10 |
| 1 | A | 269 | ARG | NE-CZ-NH1 | -8.40 | 116.10 | 120.30 |
| 1 | A | 41 | TYR | CB-CG-CD2 | 8.38 | 126.03 | 121.00 |
| 1 | B | 234 | ARG | NE-CZ-NH1 | 8.37 | 124.48 | 120.30 |
| 3 | F | 42 | ARG | NE-CZ-NH1 | 8.36 | 124.48 | 120.30 |
| 1 | A | 140 | ARG | NE-CZ-NH1 | -8.34 | 116.13 | 120.30 |
| 1 | A | 19 | ARG | NE-CZ-NH1 | -8.31 | 116.15 | 120.30 |
| 1 | A | 794 | ARG | NE-CZ-NH1 | -8.30 | 116.15 | 120.30 |
| 1 | B | 396 | LEU | CB-CG-CD2 | 8.27 | 125.06 | 111.00 |
| 1 | B | 157 | TYR | CB-CG-CD1 | -8.25 | 116.05 | 121.00 |
| 1 | B | 705 | ARG | NE-CZ-NH2 | -8.18 | 116.21 | 120.30 |
| 1 | A | 347 | TYR | CB-CG-CD2 | -8.18 | 116.09 | 121.00 |
| 2 | D | 2 | ALA | N-CA-CB | 8.17 | 121.54 | 110.10 |
| 1 | B | 132 | ARG | NE-CZ-NH2 | 8.12 | 124.36 | 120.30 |
| 1 | A | 545 | PHE | CB-CG-CD2 | -8.03 | 115.18 | 120.80 |
| 3 | F | 83 | PHE | CB-CG-CD2 | -8.00 | 115.20 | 120.80 |
| 2 | D | 19 | TYR | CB-CG-CD1 | 8.00 | 125.80 | 121.00 |
| 1 | A | 736 | PHE | CB-CG-CD1 | 7.98 | 126.39 | 120.80 |
| 3 | F | 118 | ARG | NE-CZ-NH2 | 7.98 | 124.29 | 120.30 |
| 1 | B | 627 | ALA | N-CA-CB | 7.92 | 121.19 | 110.10 |
| 2 | D | 20 | ASP | CB-CG-OD1 | 7.88 | 125.40 | 118.30 |
| 1 | B | 123 | TYR | CB-CG-CD1 | -7.79 | 116.33 | 121.00 |
| 2 | C | 116 | ARG | NE-CZ-NH2 | 7.78 | 124.19 | 120.30 |
| 1 | A | 777 | MET | CG-SD-CE | -7.77 | 87.77 | 100.20 |
| 1 | B | 767 | ARG | NE-CZ-NH2 | 7.77 | 124.18 | 120.30 |
| 3 | F | 82 | THR | CA-CB-CG2 | -7.76 | 101.53 | 112.40 |
| 1 | B | 249 | PHE | CB-CG-CD2 | 7.75 | 126.23 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | F | 48 | PHE | CB-CG-CD2 | -7.73 | 115.39 | 120.80 |
| 1 | A | 157 | TYR | CB-CG-CD2 | 7.70 | 125.62 | 121.00 |
| 1 | A | 327 | ARG | NE-CZ-NH2 | 7.69 | 124.15 | 120.30 |
| 1 | A | 537 | PHE | CB-CG-CD1 | -7.68 | 115.42 | 120.80 |
| 1 | B | 104 | TYR | N-CA-CB | 7.67 | 124.40 | 110.60 |
| 1 | A | 573 | ALA | N-CA-CB | 7.57 | 120.70 | 110.10 |
| 1 | B | 65 | GLN | N-CA-CB | 7.55 | 124.18 | 110.60 |
| 2 | D | 154 | GLU | N-CA-CB | 7.54 | 124.18 | 110.60 |
| 1 | A | 504 | ASP | CB-CG-OD1 | -7.54 | 111.51 | 118.30 |
| 2 | C | 16 | PHE | CB-CG-CD2 | -7.52 | 115.54 | 120.80 |
| 2 | C | 7 | ALA | N-CA-CB | 7.52 | 120.63 | 110.10 |
| 1 | A | 822 | PHE | CB-CG-CD1 | 7.45 | 126.02 | 120.80 |
| 1 | B | 831 | TYR | N-CA-CB | 7.43 | 123.97 | 110.60 |
| 3 | E | 173 | ASP | CB-CG-OD2 | -7.40 | 111.64 | 118.30 |
| 1 | A | 766 | PHE | CB-CG-CD2 | -7.35 | 115.66 | 120.80 |
| 1 | A | 765 | PHE | CB-CG-CD2 | 7.34 | 125.94 | 120.80 |
| 1 | A | 500 | ARG | NE-CZ-NH1 | -7.32 | 116.64 | 120.30 |
| 1 | B | 671 | PHE | CB-CG-CD1 | -7.31 | 115.69 | 120.80 |
| 1 | A | 364 | ARG | NE-CZ-NH1 | -7.30 | 116.65 | 120.30 |
| 1 | B | 189 | TYR | CB-CG-CD2 | -7.30 | 116.62 | 121.00 |
| 1 | B | 105 | TYR | CB-CG-CD2 | -7.29 | 116.62 | 121.00 |
| 1 | B | 307 | TYR | CB-CG-CD2 | 7.25 | 125.35 | 121.00 |
| 1 | B | 607 | PHE | CB-CG-CD1 | 7.20 | 125.84 | 120.80 |
| 1 | A | 452 | TYR | CG-CD2-CE2 | 7.19 | 127.06 | 121.30 |
| 1 | B | 792 | TRP | CG-CD2-CE3 | 7.19 | 140.37 | 133.90 |
| 2 | C | 4 | LEU | CB-CA-C | -7.19 | 96.54 | 110.20 |
| 1 | A | 41 | TYR | CG-CD2-CE2 | -7.17 | 115.57 | 121.30 |
| 1 | B | 302 | ASP | CB-CG-OD1 | 7.16 | 124.75 | 118.30 |
| 1 | A | 779 | ASP | CB-CG-OD2 | 7.16 | 124.74 | 118.30 |
| 1 | A | 809 | ARG | NE-CZ-NH1 | -7.15 | 116.72 | 120.30 |
| 1 | A | 545 | PHE | CB-CG-CD1 | 7.14 | 125.80 | 120.80 |
| 1 | A | 307 | TYR | CB-CG-CD2 | 7.12 | 125.27 | 121.00 |
| 1 | A | 430 | ASP | CB-CG-OD2 | -7.12 | 111.90 | 118.30 |
| 2 | D | 92 | VAL | CG1-CB-CG2 | -7.11 | 99.52 | 110.90 |
| 1 | B | 796 | TYR | CB-CG-CD1 | 7.10 | 125.26 | 121.00 |
| 1 | A | 586 | TYR | CB-CG-CD1 | 7.08 | 125.25 | 121.00 |
| 1 | B | 366 | ARG | NE-CZ-NH1 | -7.07 | 116.76 | 120.30 |
| 3 | F | 38 | ARG | NE-CZ-NH1 | -7.05 | 116.77 | 120.30 |
| 2 | D | 31 | ASP | CB-CG-OD1 | 7.05 | 124.64 | 118.30 |
| 1 | A | 607 | PHE | CB-CG-CD1 | 7.04 | 125.73 | 120.80 |
| 3 | E | 161 | ASP | CB-CG-OD2 | -7.01 | 111.99 | 118.30 |
| 3 | E | 83 | PHE | CB-CG-CD2 | 7.01 | 125.70 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 393 | TYR | CB-CG-CD2 | -6.93 | 116.84 | 121.00 |
| 1 | A | 580 | TYR | CB-CG-CD1 | -6.93 | 116.84 | 121.00 |
| 3 | F | 98 | MET | CG-SD-CE | -6.92 | 89.13 | 100.20 |
| 1 | A | 234 | ARG | NE-CZ-NH1 | -6.91 | 116.84 | 120.30 |
| 1 | B | 651 | ALA | N-CA-CB | 6.83 | 119.67 | 110.10 |
| 1 | A | 458 | ASP | CB-CG-OD1 | -6.82 | 112.16 | 118.30 |
| 3 | F | 80 | ARG | NE-CZ-NH1 | 6.82 | 123.71 | 120.30 |
| 2 | C | 153 | ASP | CB-CG-OD1 | -6.81 | 112.17 | 118.30 |
| 1 | A | 90 | TYR | CB-CG-CD1 | -6.80 | 116.92 | 121.00 |
| 1 | B | 284 | TYR | CB-CG-CD2 | -6.80 | 116.92 | 121.00 |
| 1 | A | 129 | TYR | CB-CG-CD2 | -6.78 | 116.93 | 121.00 |
| 3 | E | 88 | ARG | NE-CZ-NH1 | -6.77 | 116.92 | 120.30 |
| 3 | F | 25 | ALA | N-CA-CB | 6.73 | 119.53 | 110.10 |
| 1 | A | 342 | TYR | CB-CG-CD2 | 6.72 | 125.03 | 121.00 |
| 3 | E | 139 | GLU | OE1-CD-OE2 | -6.71 | 115.25 | 123.30 |
| 1 | B | 439 | ARG | NH1-CZ-NH2 | -6.71 | 112.02 | 119.40 |
| 1 | A | 466 | ASP | CB-CG-OD1 | 6.67 | 124.30 | 118.30 |
| 1 | A | 79 | TYR | CB-CG-CD2 | -6.66 | 117.00 | 121.00 |
| 1 | A | 826 | ARG | NE-CZ-NH2 | 6.66 | 123.63 | 120.30 |
| 1 | A | 491 | PHE | CB-CG-CD2 | 6.64 | 125.45 | 120.80 |
| 1 | B | 692 | MET | CG-SD-CE | -6.64 | 89.58 | 100.20 |
| 1 | B | 333 | PHE | CB-CG-CD1 | -6.62 | 116.17 | 120.80 |
| 1 | A | 241 | PHE | CB-CG-CD2 | -6.62 | 116.17 | 120.80 |
| 1 | B | 259 | ASP | N-CA-CB | 6.60 | 122.48 | 110.60 |
| 1 | A | 696 | THR | N-CA-CB | 6.58 | 122.80 | 110.30 |
| 1 | A | 797 | LEU | CB-CG-CD1 | 6.57 | 122.17 | 111.00 |
| 3 | F | 80 | ARG | NE-CZ-NH2 | 6.55 | 123.58 | 120.30 |
| 1 | B | 241 | PHE | CB-CG-CD1 | -6.55 | 116.22 | 120.80 |
| 3 | F | 108 | PHE | CB-CG-CD2 | -6.54 | 116.22 | 120.80 |
| 1 | A | 307 | TYR | CG-CD1-CE1 | 6.53 | 126.52 | 121.30 |
| 1 | A | 275 | THR | CA-CB-CG2 | -6.49 | 103.32 | 112.40 |
| 1 | A | 601 | ASP | CB-CG-OD2 | -6.49 | 112.46 | 118.30 |
| 1 | A | 794 | ARG | NE-CZ-NH2 | 6.48 | 123.54 | 120.30 |
| 1 | B | 361 | PHE | CB-CG-CD2 | 6.47 | 125.33 | 120.80 |
| 1 | A | 284 | TYR | CB-CG-CD1 | -6.46 | 117.12 | 121.00 |
| 3 | F | 131 | ALA | CB-CA-C | -6.46 | 100.41 | 110.10 |
| 2 | D | 116 | ARG | NE-CZ-NH2 | 6.46 | 123.53 | 120.30 |
| 2 | C | 19 | TYR | CB-CG-CD1 | -6.44 | 117.14 | 121.00 |
| 1 | B | 140 | ARG | NE-CZ-NH2 | 6.43 | 123.52 | 120.30 |
| 1 | B | 834 | TYR | CB-CG-CD2 | 6.40 | 124.84 | 121.00 |
| 2 | D | 71 | PHE | CB-CG-CD1 | 6.39 | 125.28 | 120.80 |
| 2 | D | 136 | PHE | CB-CG-CD1 | -6.38 | 116.33 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 323 | ALA | N-CA-CB | 6.38 | 119.03 | 110.10 |
| 1 | A | 278 | ARG | NE-CZ-NH2 | 6.38 | 123.49 | 120.30 |
| 1 | A | 96 | VAL | CA-CB-CG1 | -6.38 | 101.33 | 110.90 |
| 1 | A | 458 | ASP | CA-CB-CG | 6.37 | 127.41 | 113.40 |
| 3 | F | 88 | ARG | NE-CZ-NH2 | 6.33 | 123.47 | 120.30 |
| 1 | A | 367 | GLU | C-N-CA | 6.33 | 137.53 | 121.70 |
| 2 | D | 79 | GLU | N-CA-CB | 6.33 | 121.99 | 110.60 |
| 1 | B | 618 | ILE | O-C-N | -6.33 | 112.58 | 122.70 |
| 1 | A | 241 | PHE | CB-CG-CD1 | 6.33 | 125.23 | 120.80 |
| 1 | A | 714 | ARG | NE-CZ-NH1 | 6.33 | 123.46 | 120.30 |
| 1 | A | 234 | ARG | NE-CZ-NH2 | 6.32 | 123.46 | 120.30 |
| 1 | B | 757 | TYR | CG-CD1-CE1 | -6.31 | 116.25 | 121.30 |
| 3 | E | 131 | ALA | CB-CA-C | -6.28 | 100.68 | 110.10 |
| 1 | B | 241 | PHE | CB-CG-CD2 | 6.27 | 125.19 | 120.80 |
| 1 | A | 768 | ALA | N-CA-CB | 6.25 | 118.85 | 110.10 |
| 1 | B | 462 | PHE | N-CA-C | -6.25 | 94.12 | 111.00 |
| 1 | B | 482 | LEU | CB-CG-CD2 | -6.25 | 100.38 | 111.00 |
| 1 | A | 142 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 3 | E | 39 | ARG | NE-CZ-NH1 | -6.20 | 117.20 | 120.30 |
| 2 | D | 16 | PHE | CB-CG-CD2 | -6.18 | 116.47 | 120.80 |
| 1 | A | 377 | GLU | O-C-N | -6.18 | 112.69 | 123.20 |
| 3 | E | 65 | LEU | CB-CG-CD1 | 6.18 | 121.51 | 111.00 |
| 1 | B | 691 | VAL | CG1-CB-CG2 | -6.18 | 101.02 | 110.90 |
| 1 | A | 347 | TYR | CZ-CE2-CD2 | -6.18 | 114.24 | 119.80 |
| 3 | F | 120 | ALA | N-CA-CB | 6.17 | 118.74 | 110.10 |
| 1 | B | 19 | ARG | NE-CZ-NH2 | 6.16 | 123.38 | 120.30 |
| 1 | B | 834 | TYR | CB-CG-CD1 | -6.15 | 117.31 | 121.00 |
| 1 | B | 720 | PHE | CG-CD2-CE2 | -6.14 | 114.05 | 120.80 |
| 1 | B | 586 | TYR | CB-CG-CD2 | -6.10 | 117.34 | 121.00 |
| 3 | F | 80 | ARG | NH1-CZ-NH2 | -6.08 | 112.71 | 119.40 |
| 1 | B | 208 | GLU | N-CA-CB | 6.06 | 121.52 | 110.60 |
| 3 | E | 137 | GLU | N-CA-C | -6.06 | 94.64 | 111.00 |
| 1 | A | 469 | GLY | N-CA-C | -6.06 | 97.96 | 113.10 |
| 1 | A | 41 | TYR | CZ-CE2-CD2 | 6.05 | 125.25 | 119.80 |
| 1 | B | 141 | ARG | NE-CZ-NH1 | -6.05 | 117.27 | 120.30 |
| 1 | B | 650 | SER | O-C-N | -6.05 | 113.03 | 122.70 |
| 1 | A | 64 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 1 | A | 467 | TYR | O-C-N | 6.04 | 132.35 | 122.70 |
| 1 | B | 708 | ARG | NH1-CZ-NH2 | -6.03 | 112.77 | 119.40 |
| 1 | B | 360 | LYS | N-CA-CB | 6.02 | 121.44 | 110.60 |
| 3 | F | 56 | VAL | CA-CB-CG1 | 6.02 | 119.93 | 110.90 |
| 1 | A | 781 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 708 | ARG | NE-CZ-NH1 | -6.01 | 117.29 | 120.30 |
| 3 | E | 112 | LEU | N-CA-CB | 5.99 | 122.38 | 110.40 |
| 2 | D | 30 | ARG | NH1-CZ-NH2 | -5.98 | 112.82 | 119.40 |
| 1 | B | 783 | GLY | N-CA-C | -5.98 | 98.15 | 113.10 |
| 1 | A | 452 | TYR | CB-CG-CD2 | 5.98 | 124.59 | 121.00 |
| 2 | D | 130 | ASP | CB-CG-OD1 | 5.97 | 123.67 | 118.30 |
| 3 | E | 59 | PHE | N-CA-CB | 5.96 | 121.32 | 110.60 |
| 3 | E | 161 | ASP | CB-CG-OD1 | 5.94 | 123.64 | 118.30 |
| 1 | A | 685 | VAL | N-CA-C | -5.92 | 95.00 | 111.00 |
| 1 | B | 232 | THR | N-CA-C | -5.92 | 95.02 | 111.00 |
| 1 | A | 640 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | A | 580 | TYR | CG-CD2-CE2 | -5.90 | 116.58 | 121.30 |
| 1 | A | 601 | ASP | CB-CG-OD1 | 5.90 | 123.61 | 118.30 |
| 1 | B | 211 | ALA | N-CA-CB | 5.90 | 118.36 | 110.10 |
| 1 | A | 246 | ARG | NE-CZ-NH2 | 5.90 | 123.25 | 120.30 |
| 1 | A | 494 | GLU | CB-CA-C | -5.90 | 98.59 | 110.40 |
| 1 | A | 215 | ASP | CB-CG-OD2 | 5.89 | 123.60 | 118.30 |
| 1 | B | 824 | THR | CA-CB-CG2 | -5.89 | 104.16 | 112.40 |
| 1 | A | 830 | TRP | N-CA-CB | 5.89 | 121.20 | 110.60 |
| 2 | D | 153 | ASP | N-CA-CB | 5.88 | 121.19 | 110.60 |
| 3 | F | 188 | THR | N-CA-CB | 5.88 | 121.48 | 110.30 |
| 2 | D | 3 | ASP | CB-CG-OD2 | 5.87 | 123.58 | 118.30 |
| 1 | A | 409 | THR | CA-CB-CG2 | -5.86 | 104.19 | 112.40 |
| 1 | A | 268 | ALA | C-N-CA | 5.86 | 136.35 | 121.70 |
| 1 | A | 106 | ALA | CB-CA-C | -5.85 | 101.32 | 110.10 |
| 1 | B | 10 | TYR | CB-CG-CD1 | -5.85 | 117.49 | 121.00 |
| 1 | A | 453 | PHE | CB-CG-CD1 | -5.84 | 116.71 | 120.80 |
| 1 | B | 792 | TRP | CD2-CE3-CZ3 | 5.83 | 126.38 | 118.80 |
| 1 | B | 621 | ASP | N-CA-CB | 5.83 | 121.09 | 110.60 |
| 1 | A | 452 | TYR | CG-CD1-CE1 | 5.82 | 125.95 | 121.30 |
| 1 | A | 510 | PHE | N-CA-CB | 5.82 | 121.07 | 110.60 |
| 1 | A | 591 | TRP | CD1-NE1-CE2 | -5.81 | 103.77 | 109.00 |
| 1 | A | 795 | TRP | CA-CB-CG | 5.81 | 124.73 | 113.70 |
| 1 | A | 423 | GLY | N-CA-C | -5.80 | 98.59 | 113.10 |
| 2 | D | 140 | GLU | OE1-CD-OE2 | 5.80 | 130.26 | 123.30 |
| 3 | E | 103 | PRO | N-CA-CB | 5.79 | 110.25 | 103.30 |
| 1 | A | 834 | TYR | CB-CG-CD1 | -5.79 | 117.53 | 121.00 |
| 1 | B | 817 | ARG | NE-CZ-NH2 | -5.75 | 117.42 | 120.30 |
| 1 | A | 383 | HIS | CA-CB-CG | 5.75 | 123.38 | 113.60 |
| 1 | B | 35 | ALA | N-CA-CB | 5.74 | 118.14 | 110.10 |
| 1 | A | 126 | PHE | CB-CG-CD2 | 5.74 | 124.82 | 120.80 |
| 1 | A | 520 | LEU | CB-CG-CD1 | 5.73 | 120.74 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 86 | PHE | CB-CG-CD1 | -5.73 | 116.79 | 120.80 |
| 1 | A | 190 | TYR | CB-CG-CD2 | 5.72 | 124.43 | 121.00 |
| 1 | A | 653 | TYR | CD1-CE1-CZ | -5.72 | 114.65 | 119.80 |
| 1 | B | 573 | ALA | N-CA-CB | 5.71 | 118.10 | 110.10 |
| 2 | D | 2 | ALA | O-C-N | 5.71 | 131.84 | 122.70 |
| 2 | D | 127 | ARG | NE-CZ-NH2 | 5.70 | 123.15 | 120.30 |
| 1 | B | 600 | ASN | C-N-CA | 5.69 | 135.93 | 121.70 |
| 3 | E | 135 | PHE | CB-CG-CD1 | -5.69 | 116.82 | 120.80 |
| 1 | B | 164 | ARG | NE-CZ-NH2 | 5.68 | 123.14 | 120.30 |
| 2 | D | 31 | ASP | CB-CG-OD2 | -5.68 | 113.19 | 118.30 |
| 1 | A | 331 | THR | CA-CB-CG2 | 5.68 | 120.35 | 112.40 |
| 1 | B | 278 | ARG | N-CA-CB | 5.67 | 120.80 | 110.60 |
| 1 | B | 622 | HIS | CA-CB-CG | -5.66 | 103.98 | 113.60 |
| 1 | B | 364 | ARG | NE-CZ-NH1 | -5.66 | 117.47 | 120.30 |
| 1 | A | 510 | PHE | CB-CA-C | -5.66 | 99.08 | 110.40 |
| 3 | E | 166 | ALA | N-CA-CB | 5.66 | 118.02 | 110.10 |
| 1 | B | 599 | VAL | C-N-CA | 5.65 | 135.83 | 121.70 |
| 1 | A | 16 | GLU | OE1-CD-OE2 | 5.64 | 130.07 | 123.30 |
| 1 | A | 64 | ARG | NH1-CZ-NH2 | -5.63 | 113.20 | 119.40 |
| 1 | B | 640 | ARG | NH1-CZ-NH2 | -5.63 | 113.21 | 119.40 |
| 1 | B | 536 | MET | C-N-CA | 5.62 | 135.76 | 121.70 |
| 1 | A | 665 | HIS | N-CA-CB | 5.62 | 120.72 | 110.60 |
| 1 | B | 150 | PHE | CB-CG-CD2 | -5.62 | 116.87 | 120.80 |
| 3 | F | 48 | PHE | CB-CG-CD1 | 5.62 | 124.73 | 120.80 |
| 1 | A | 73 | GLN | N-CA-CB | 5.62 | 120.71 | 110.60 |
| 1 | A | 792 | TRP | CB-CG-CD2 | -5.62 | 119.30 | 126.60 |
| 3 | E | 99 | VAL | CA-CB-CG1 | 5.62 | 119.32 | 110.90 |
| 1 | A | 394 | LYS | N-CA-CB | 5.61 | 120.70 | 110.60 |
| 1 | A | 246 | ARG | NE-CZ-NH1 | -5.60 | 117.50 | 120.30 |
| 1 | B | 787 | THR | CA-CB-OG1 | 5.60 | 120.76 | 109.00 |
| 1 | A | 433 | PHE | CB-CG-CD1 | 5.60 | 124.72 | 120.80 |
| 2 | C | 26 | LYS | N-CA-CB | 5.59 | 120.67 | 110.60 |
| 3 | F | 58 | GLU | O-C-N | -5.59 | 113.76 | 122.70 |
| 1 | A | 227 | PHE | CB-CG-CD2 | -5.59 | 116.89 | 120.80 |
| 1 | B | 801 | GLU | OE1-CD-OE2 | 5.58 | 130.00 | 123.30 |
| 2 | D | 102 | LEU | CB-CA-C | -5.57 | 99.62 | 110.20 |
| 1 | B | 398 | LYS | N-CA-CB | 5.57 | 120.62 | 110.60 |
| 1 | A | 468 | ASN | N-CA-CB | 5.55 | 120.60 | 110.60 |
| 1 | A | 307 | TYR | N-CA-CB | 5.55 | 120.59 | 110.60 |
| 3 | E | 25 | ALA | N-CA-CB | 5.55 | 117.87 | 110.10 |
| 2 | D | 142 | PHE | CB-CG-CD2 | 5.54 | 124.68 | 120.80 |
| 1 | B | 719 | ASP | C-N-CA | 5.54 | 135.54 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 55 | ASP | CB-CG-OD1 | 5.54 | 123.28 | 118.30 |
| 3 | E | 195 | GLY | N-CA-C | 5.54 | 126.94 | 113.10 |
| 1 | A | 84 | ASP | N-CA-CB | 5.54 | 120.56 | 110.60 |
| 1 | A | 802 | PHE | CB-CG-CD1 | -5.53 | 116.93 | 120.80 |
| 1 | A | 433 | PHE | CB-CG-CD2 | -5.52 | 116.94 | 120.80 |
| 2 | D | 109 | VAL | CB-CA-C | -5.51 | 100.92 | 111.40 |
| 1 | A | 581 | ALA | CB-CA-C | -5.51 | 101.83 | 110.10 |
| 1 | A | 157 | TYR | CB-CG-CD1 | -5.51 | 117.69 | 121.00 |
| 2 | C | 102 | LEU | CB-CG-CD2 | 5.51 | 120.36 | 111.00 |
| 1 | A | 347 | TYR | CB-CG-CD1 | 5.51 | 124.30 | 121.00 |
| 3 | E | 42 | ARG | NE-CZ-NH1 | -5.50 | 117.55 | 120.30 |
| 1 | A | 724 | TYR | CD1-CE1-CZ | -5.50 | 114.85 | 119.80 |
| 1 | A | 57 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | A | 69 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | A | 560 | PHE | N-CA-CB | 5.49 | 120.48 | 110.60 |
| 2 | D | 93 | TYR | CG-CD1-CE1 | -5.49 | 116.91 | 121.30 |
| 1 | A | 792 | TRP | CB-CG-CD1 | 5.48 | 134.12 | 127.00 |
| 3 | E | 88 | ARG | NE-CZ-NH2 | 5.48 | 123.04 | 120.30 |
| 1 | A | 232 | THR | N-CA-C | -5.47 | 96.22 | 111.00 |
| 1 | A | 462 | PHE | CB-CG-CD1 | -5.47 | 116.97 | 120.80 |
| 1 | B | 305 | TYR | CB-CG-CD2 | 5.47 | 124.28 | 121.00 |
| 1 | B | 458 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 3 | F | 170 | ALA | CB-CA-C | -5.46 | 101.91 | 110.10 |
| 3 | E | 57 | GLN | N-CA-C | -5.46 | 96.25 | 111.00 |
| 3 | F | 15 | LYS | N-CA-C | -5.46 | 96.26 | 111.00 |
| 2 | C | 119 | ASP | CB-CG-OD1 | -5.46 | 113.39 | 118.30 |
| 2 | C | 142 | PHE | CB-CG-CD1 | -5.45 | 116.99 | 120.80 |
| 1 | B | 817 | ARG | O-C-N | -5.43 | 114.01 | 122.70 |
| 1 | B | 287 | MET | CB-CA-C | -5.43 | 99.54 | 110.40 |
| 1 | A | 83 | GLU | OE1-CD-OE2 | -5.43 | 116.79 | 123.30 |
| 1 | A | 602 | THR | N-CA-C | -5.42 | 96.37 | 111.00 |
| 1 | B | 12 | TYR | CB-CA-C | -5.41 | 99.57 | 110.40 |
| 1 | B | 148 | HIS | C-N-CA | 5.41 | 135.23 | 121.70 |
| 1 | B | 779 | ASP | CB-CG-OD2 | -5.41 | 113.43 | 118.30 |
| 1 | A | 105 | TYR | O-C-N | 5.41 | 131.36 | 122.70 |
| 2 | D | 19 | TYR | N-CA-CB | 5.41 | 120.33 | 110.60 |
| 3 | E | 117 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 2 | C | 86 | PHE | CG-CD1-CE1 | -5.39 | 114.87 | 120.80 |
| 1 | A | 19 | ARG | N-CA-CB | 5.39 | 120.30 | 110.60 |
| 1 | B | 66 | VAL | C-N-CA | 5.38 | 135.14 | 121.70 |
| 1 | A | 553 | HIS | CA-CB-CG | -5.38 | 104.46 | 113.60 |
| 2 | C | 41 | CYS | N-CA-CB | 5.37 | 120.27 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 505 | TRP | CE2-CD2-CE3 | 5.37 | 125.14 | 118.70 |
| 1 | A | 212 | THR | N-CA-CB | 5.37 | 120.50 | 110.30 |
| 1 | A | 486 | PHE | CB-CG-CD2 | 5.37 | 124.56 | 120.80 |
| 1 | A | 802 | PHE | CB-CG-CD2 | 5.37 | 124.56 | 120.80 |
| 1 | A | 810 | VAL | CG1-CB-CG2 | 5.36 | 119.48 | 110.90 |
| 1 | B | 757 | TYR | CB-CG-CD2 | -5.36 | 117.79 | 121.00 |
| 3 | F | 67 | ASP | CB-CG-OD2 | -5.36 | 113.48 | 118.30 |
| 1 | B | 56 | VAL | CA-CB-CG1 | -5.35 | 102.88 | 110.90 |
| 2 | D | 13 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 1 | B | 485 | PHE | CB-CG-CD2 | 5.34 | 124.54 | 120.80 |
| 2 | C | 113 | LEU | N-CA-C | -5.33 | 96.59 | 111.00 |
| 2 | D | 136 | PHE | CB-CA-C | -5.33 | 99.73 | 110.40 |
| 1 | B | 471 | GLU | OE1-CD-OE2 | 5.33 | 129.70 | 123.30 |
| 1 | A | 838 | LYS | CA-C-N | 5.33 | 132.02 | 117.10 |
| 1 | A | 653 | TYR | CB-CG-CD1 | 5.33 | 124.20 | 121.00 |
| 1 | B | 82 | CYS | N-CA-CB | 5.32 | 120.18 | 110.60 |
| 1 | B | 393 | TYR | CZ-CE2-CD2 | 5.32 | 124.59 | 119.80 |
| 1 | B | 787 | THR | CA-CB-CG2 | -5.32 | 104.95 | 112.40 |
| 2 | D | 37 | ARG | NH1-CZ-NH2 | -5.32 | 113.55 | 119.40 |
| 3 | E | 78 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | A | 263 | TYR | CB-CG-CD2 | 5.29 | 124.17 | 121.00 |
| 3 | F | 42 | ARG | NH1-CZ-NH2 | -5.29 | 113.59 | 119.40 |
| 1 | B | 151 | ALA | N-CA-CB | 5.28 | 117.50 | 110.10 |
| 1 | B | 782 | LEU | C-N-CA | 5.28 | 133.39 | 122.30 |
| 2 | D | 40 | ASP | N-CA-CB | 5.28 | 120.10 | 110.60 |
| 1 | A | 189 | TYR | CG-CD2-CE2 | -5.27 | 117.08 | 121.30 |
| 1 | B | 793 | ILE | CB-CA-C | -5.26 | 101.08 | 111.60 |
| 1 | B | 366 | ARG | NH1-CZ-NH2 | 5.26 | 125.18 | 119.40 |
| 2 | D | 78 | LYS | CA-CB-CG | 5.26 | 124.97 | 113.40 |
| 1 | A | 370 | ALA | N-CA-CB | 5.25 | 117.45 | 110.10 |
| 2 | D | 136 | PHE | CB-CG-CD2 | 5.25 | 124.47 | 120.80 |
| 3 | F | 175 | ASN | CB-CA-C | 5.25 | 120.90 | 110.40 |
| 1 | B | 307 | TYR | CB-CG-CD1 | -5.24 | 117.85 | 121.00 |
| 3 | E | 21 | GLY | C-N-CA | 5.24 | 133.30 | 122.30 |
| 1 | B | 221 | ASN | N-CA-CB | 5.24 | 120.03 | 110.60 |
| 1 | B | 774 | LEU | N-CA-CB | 5.24 | 120.87 | 110.40 |
| 1 | A | 833 | LEU | N-CA-C | -5.24 | 96.87 | 111.00 |
| 3 | E | 51 | PHE | CB-CG-CD1 | 5.24 | 124.46 | 120.80 |
| 1 | A | 687 | ASP | N-CA-C | -5.23 | 96.88 | 111.00 |
| 1 | A | 380 | ARG | NE-CZ-NH1 | -5.23 | 117.69 | 120.30 |
| 3 | F | 170 | ALA | N-CA-CB | 5.22 | 117.42 | 110.10 |
| 1 | B | 229 | ASN | N-CA-CB | 5.22 | 120.00 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | E | 85 | SER | N-CA-CB | -5.22 | 102.68 | 110.50 |
| 1 | B | 305 | TYR | CB-CG-CD1 | -5.20 | 117.88 | 121.00 |
| 1 | B | 691 | VAL | CA-CB-CG1 | 5.20 | 118.71 | 110.90 |
| 3 | E | 122 | THR | N-CA-CB | 5.20 | 120.19 | 110.30 |
| 2 | D | 39 | LEU | CB-CG-CD1 | 5.20 | 119.84 | 111.00 |
| 1 | A | 567 | LYS | N-CA-CB | 5.20 | 119.96 | 110.60 |
| 3 | E | 73 | PHE | CB-CG-CD2 | -5.20 | 117.16 | 120.80 |
| 1 | B | 344 | THR | CA-CB-CG2 | -5.20 | 105.13 | 112.40 |
| 1 | B | 728 | ALA | N-CA-CB | 5.20 | 117.37 | 110.10 |
| 1 | A | 715 | MET | CG-SD-CE | -5.19 | 91.89 | 100.20 |
| 1 | A | 452 | TYR | CD1-CG-CD2 | -5.19 | 112.19 | 117.90 |
| 1 | A | 263 | TYR | CZ-CE2-CD2 | 5.18 | 124.46 | 119.80 |
| 1 | B | 538 | PRO | N-CD-CG | 5.16 | 110.94 | 103.20 |
| 2 | D | 122 | CYS | O-C-N | -5.16 | 114.44 | 122.70 |
| 1 | A | 790 | GLN | CA-CB-CG | 5.16 | 124.76 | 113.40 |
| 1 | A | 653 | TYR | CG-CD1-CE1 | 5.16 | 125.43 | 121.30 |
| 2 | D | 135 | GLY | N-CA-C | -5.16 | 100.20 | 113.10 |
| 1 | B | 504 | ASP | CB-CG-OD2 | -5.15 | 113.66 | 118.30 |
| 1 | B | 780 | ASP | CB-CG-OD2 | 5.15 | 122.94 | 118.30 |
| 3 | F | 177 | LEU | CB-CG-CD1 | -5.15 | 102.24 | 111.00 |
| 1 | A | 265 | LEU | N-CA-C | -5.15 | 97.09 | 111.00 |
| 1 | B | 394 | LYS | N-CA-CB | -5.15 | 101.33 | 110.60 |
| 1 | A | 169 | MET | CG-SD-CE | -5.15 | 91.96 | 100.20 |
| 1 | B | 153 | SER | N-CA-CB | 5.14 | 118.21 | 110.50 |
| 1 | B | 290 | GLY | O-C-N | 5.14 | 130.93 | 122.70 |
| 3 | E | 123 | ASP | C-N-CA | 5.14 | 134.55 | 121.70 |
| 1 | B | 792 | TRP | CE2-CD2-CE3 | -5.14 | 112.53 | 118.70 |
| 1 | A | 838 | LYS | CA-C-O | -5.14 | 109.31 | 120.10 |
| 1 | A | 485 | PHE | CB-CG-CD2 | 5.13 | 124.39 | 120.80 |
| 1 | A | 413 | ASN | N-CA-CB | 5.13 | 119.83 | 110.60 |
| 1 | A | 757 | TYR | CB-CG-CD1 | 5.12 | 124.08 | 121.00 |
| 1 | A | 759 | LEU | CB-CG-CD2 | 5.12 | 119.71 | 111.00 |
| 1 | B | 840 | LEU | N-CA-CB | 5.12 | 120.64 | 110.40 |
| 1 | A | 459 | ILE | CA-CB-CG2 | -5.12 | 100.66 | 110.90 |
| 1 | A | 6 | ASP | CB-CG-OD1 | 5.12 | 122.91 | 118.30 |
| 1 | A | 112 | TYR | CG-CD1-CE1 | 5.12 | 125.39 | 121.30 |
| 1 | A | 280 | TYR | CZ-CE2-CD2 | 5.12 | 124.41 | 119.80 |
| 1 | A | 723 | ARG | CD-NE-CZ | 5.11 | 130.75 | 123.60 |
| 1 | B | 342 | TYR | CZ-CE2-CD2 | -5.11 | 115.21 | 119.80 |
| 2 | C | 87 | MET | CG-SD-CE | -5.11 | 92.03 | 100.20 |
| 1 | A | 277 | GLU | N-CA-CB | 5.10 | 119.78 | 110.60 |
| 1 | B | 670 | HIS | N-CA-C | -5.10 | 97.23 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 134 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 1 | A | 157 | TYR | CG-CD1-CE1 | 5.10 | 125.38 | 121.30 |
| 1 | A | 403 | VAL | CA-CB-CG1 | 5.09 | 118.54 | 110.90 |
| 2 | C | 44 | THR | CA-C-O | 5.09 | 130.79 | 120.10 |
| 3 | E | 140 | GLY | N-CA-C | -5.09 | 100.38 | 113.10 |
| 3 | E | 142 | CYS | O-C-N | -5.08 | 114.56 | 122.70 |
| 2 | C | 130 | ASP | N-CA-CB | 5.08 | 119.75 | 110.60 |
| 1 | A | 820 | ARG | C-N-CA | 5.08 | 134.39 | 121.70 |
| 1 | B | 302 | ASP | CB-CG-OD2 | -5.07 | 113.74 | 118.30 |
| 3 | F | 18 | GLU | N-CA-CB | 5.06 | 119.71 | 110.60 |
| 2 | C | 136 | PHE | CB-CG-CD1 | -5.06 | 117.26 | 120.80 |
| 1 | B | 794 | ARG | NH1-CZ-NH2 | 5.06 | 124.96 | 119.40 |
| 1 | A | 820 | ARG | NE-CZ-NH2 | 5.06 | 122.83 | 120.30 |
| 3 | F | 33 | PRO | N-CA-CB | 5.05 | 109.36 | 103.30 |
| 1 | B | 125 | ARG | CG-CD-NE | -5.05 | 101.19 | 111.80 |
| 1 | B | 249 | PHE | CB-CG-CD1 | -5.05 | 117.26 | 120.80 |
| 1 | A | 26 | TYR | CB-CG-CD2 | -5.05 | 117.97 | 121.00 |
| 1 | B | 79 | TYR | CA-CB-CG | -5.05 | 103.81 | 113.40 |
| 1 | B | 599 | VAL | CA-C-N | -5.05 | 106.10 | 117.20 |
| 2 | D | 118 | THR | CA-CB-CG2 | -5.05 | 105.33 | 112.40 |
| 2 | D | 127 | ARG | NE-CZ-NH1 | -5.05 | 117.78 | 120.30 |
| 1 | B | 473 | LEU | CB-CG-CD1 | 5.04 | 119.58 | 111.00 |
| 1 | A | 141 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |
| 1 | B | 130 | THR | CA-CB-CG2 | -5.04 | 105.34 | 112.40 |
| 1 | B | 831 | TYR | CZ-CE2-CD2 | -5.03 | 115.27 | 119.80 |
| 1 | A | 830 | TRP | O-C-N | 5.03 | 130.75 | 122.70 |
| 2 | C | 47 | MET | CA-CB-CG | 5.03 | 121.85 | 113.30 |
| 1 | B | 75 | ASN | N-CA-CB | 5.03 | 119.65 | 110.60 |
| 1 | B | 443 | THR | N-CA-CB | 5.03 | 119.85 | 110.30 |
| 1 | A | 499 | LYS | N-CA-C | -5.03 | 97.43 | 111.00 |
| 3 | E | 48 | PHE | CB-CG-CD2 | -5.03 | 117.28 | 120.80 |
| 1 | A | 496 | GLU | CG-CD-OE1 | -5.02 | 108.26 | 118.30 |
| 1 | B | 714 | ARG | NE-CZ-NH2 | 5.02 | 122.81 | 120.30 |
| 1 | A | 449 | LYS | N-CA-CB | 5.02 | 119.63 | 110.60 |
| 1 | B | 778 | ARG | CG-CD-NE | -5.01 | 101.27 | 111.80 |
| 1 | B | 270 | VAL | CG1-CB-CG2 | 5.01 | 118.92 | 110.90 |
| 1 | A | 33 | TRP | N-CA-CB | 5.00 | 119.60 | 110.60 |

There are no chirality outliers.

All (62) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 104 | TYR | Sidechain |
| 1 | A | 112 | TYR | Sidechain |
| 1 | A | 123 | TYR | Sidechain |
| 1 | A | 129 | TYR | Sidechain |
| 1 | A | 189 | TYR | Sidechain |
| 1 | A | 240 | ARG | Sidechain |
| 1 | A | 249 | PHE | Sidechain |
| 1 | A | 338 | PHE | Sidechain |
| 1 | A | 340 | HIS | Sidechain |
| 1 | A | 342 | TYR | Sidechain |
| 1 | A | 347 | TYR | Sidechain |
| 1 | A | 477 | PHE | Sidechain |
| 1 | A | 489 | HIS | Sidechain |
| 1 | A | 567 | LYS | Peptide |
| 1 | A | 580 | TYR | Sidechain |
| 1 | A | 619 | PHE | Sidechain |
| 1 | A | 831 | TYR | Sidechain |
| 1 | A | 90 | TYR | Sidechain |
| 1 | B | 10 | TYR | Sidechain |
| 1 | B | 112 | TYR | Sidechain |
| 1 | B | 125 | ARG | Sidechain |
| 1 | B | 132 | ARG | Sidechain |
| 1 | B | 240 | ARG | Sidechain,Peptide |
| 1 | B | 263 | TYR | Sidechain |
| 1 | B | 318 | PRO | Peptide |
| 1 | B | 347 | TYR | Sidechain |
| 1 | B | 369 | GLN | Mainchain |
| 1 | B | 393 | TYR | Sidechain |
| 1 | B | 419 | TYR | Sidechain |
| 1 | B | 429 | PHE | Sidechain |
| 1 | B | 453 | PHE | Sidechain |
| 1 | B | 467 | TYR | Peptide |
| 1 | B | 491 | PHE | Peptide |
| 1 | B | 526 | GLY | Peptide |
| 1 | B | 621 | ASP | Peptide |
| 1 | B | 627 | ALA | Peptide |
| 1 | B | 639 | GLY | Peptide |
| 1 | B | 64 | ARG | Sidechain |
| 1 | B | 640 | ARG | Sidechain |
| 1 | B | 653 | TYR | Sidechain |
| 1 | B | 669 | PRO | Peptide |
| 1 | B | 670 | HIS | Sidechain |
| 1 | B | 714 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 724 | TYR | Sidechain |
| 1 | B | 757 | TYR | Sidechain |
| 1 | B | 796 | TYR | Sidechain |
| 1 | B | 831 | TYR | Sidechain |
| 1 | B | 84 | ASP | Peptide |
| 2 | C | 116 | ARG | Sidechain |
| 2 | C | 139 | TYR | Sidechain |
| 2 | C | 16 | PHE | Sidechain |
| 2 | C | 19 | TYR | Sidechain |
| 2 | C | 57 | ARG | Sidechain |
| 2 | C | 93 | TYR | Sidechain |
| 2 | D | 19 | TYR | Sidechain |
| 3 | E | 38 | ARG | Sidechain |
| 3 | E | 39 | ARG | Sidechain |
| 3 | E | 63 | PHE | Sidechain |
| 3 | F | 113 | THR | Peptide |
| 3 | F | 88 | ARG | Sidechain |
| 3 | F | 9 | LYS | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 6738 | 6760 | 6760 | 41 | 0 |
| 1 | B | 6739 | 6760 | 6760 | 36 | 0 |
| 2 | C | 1233 | 1227 | 1227 | 4 | 0 |
| 2 | D | 1233 | 1227 | 1227 | 5 | 0 |
| 3 | E | 1529 | 1491 | 1491 | 10 | 0 |
| 3 | F | 1529 | 1491 | 1491 | 13 | 0 |
| All | All | 19001 | 18956 | 18956 | 94 | 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 2.

All (94) 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) |
|---|---|---|---|
| 3:E:32:LYS:H | 3:E:33:PRO:HD2 | 1.44 | 0.81 |
| 1:A:20:LYS:HG2 | 1:A:22:GLN:H | 1.58 | 0.68 |
| 1:B:67:LYS:HD2 | 1:B:67:LYS:H | 1.62 | 0.65 |
| 1:B:815:ILE:HG23 | 3:F:147:LEU:HD22 | 1.81 | 0.63 |
| 1:A:729:ALA:HB1 | 2:C:88:GLU:HG3 | 1.85 | 0.58 |
| 3:F:80:ARG:HE | 3:F:99:VAL:HG23 | 1.69 | 0.58 |
| 1:B:773:ARG:HD3 | 1:B:773:ARG:H | 1.69 | 0.58 |
| 3:E:23:ASP:H | 3:E:31:PRO:HA | 1.69 | 0.56 |
| 1:A:256:ALA:HB3 | 1:A:450:ARG:HH12 | 1.71 | 0.56 |
| 1:A:758:ARG:HE | 1:A:759:LEU:H | 1.53 | 0.55 |
| 1:B:197:THR:HG22 | 2:D:127:ARG:HH12 | 1.70 | 0.55 |
| 1:A:206:THR:HB | 1:A:207:LYS:HB2 | 1.89 | 0.55 |
| 1:A:187:ILE:HD12 | 1:A:221:ASN:HD21 | 1.72 | 0.55 |
| 1:B:135:GLN:HB3 | 1:B:140:ARG:HH11 | 1.72 | 0.54 |
| 1:B:814:VAL:HG21 | 3:F:39:ARG:HH21 | 1.73 | 0.54 |
| 1:B:773:ARG:H | 1:B:773:ARG:CD | 2.20 | 0.54 |
| 1:A:160:MET:HB2 | 1:A:167:GLN:HB2 | 1.89 | 0.54 |
| 3:E:32:LYS:H | 3:E:33:PRO:CD | 2.18 | 0.54 |
| 2:D:51:ASN:HD21 | 2:D:74:ILE:HD11 | 1.73 | 0.53 |
| 3:F:42:ARG:H | 3:F:123:ASP:H | 1.56 | 0.53 |
| 1:A:356:LEU:HD13 | 1:A:425:ALA:HB2 | 1.91 | 0.52 |
| 1:A:663:SER:O | 1:A:667:THR:HG23 | 2.09 | 0.52 |
| 3:E:178:ILE:HG22 | 3:E:180:ILE:H | 1.75 | 0.51 |
| 1:A:830:TRP:CH2 | 3:E:111:PHE:CE1 | 2.99 | 0.51 |
| 1:B:833:LEU:HD21 | 3:F:171:PRO:HB3 | 1.91 | 0.51 |
| 1:A:4:ASP:HB3 | 1:A:14:SER:HA | 1.94 | 0.50 |
| 3:F:54:HIS:O | 3:F:54:HIS:CG | 2.65 | 0.48 |
| 1:A:248:HIS:CE1 | 1:A:449:LYS:HA | 2.48 | 0.48 |
| 1:A:581:ALA:HA | 1:A:697:CYS:SG | 2.53 | 0.48 |
| 1:B:815:ILE:HG22 | 1:B:819:LEU:HD12 | 1.95 | 0.48 |
| 1:B:826:ARG:HH11 | 3:F:170:ALA:HA | 1.79 | 0.47 |
| 1:B:244:PHE:CZ | 1:B:664:LEU:HD21 | 2.49 | 0.47 |
| 3:F:44:GLY:H | 3:F:120:ALA:HA | 1.80 | 0.47 |
| 1:B:137:TYR:CE2 | 1:B:150:PHE:CE2 | 3.02 | 0.47 |
| 1:B:792:TRP:CH2 | 2:D:147:ILE:HD12 | 2.49 | 0.47 |
| 3:F:96:ASP:HA | 3:F:99:VAL:HG12 | 1.96 | 0.47 |
| 1:A:100:LEU:HD22 | 1:A:118:VAL:HG23 | 1.96 | 0.47 |
| 2:C:15:HIS:HA | 2:C:18:ILE:HD12 | 1.96 | 0.47 |
| 1:A:650:SER:HA | 1:A:653:TYR:CD2 | 2.50 | 0.46 |
| 1:B:828:TRP:CD1 | 3:F:186:ILE:HG22 | 2.50 | 0.46 |
| 1:A:172:THR:HG22 | 1:A:173:GLY:H | 1.81 | 0.45 |
| 3:E:24:ALA:O | 3:E:25:ALA:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:356:LEU:HD12 | 1:A:356:LEU:H | 1.82 | 0.45 |
| 1:B:386:GLY:HA3 | 1:A:736:PHE:HA | 1.99 | 0.45 |
| 1:A:230:ALA:HB1 | 1:A:281:HIS:H | 1.82 | 0.45 |
| 1:A:398:LYS:HB2 | 1:A:398:LYS:NZ | 2.32 | 0.45 |
| 1:B:488:HIS:CD2 | 1:B:665:HIS:CE1 | 3.04 | 0.45 |
| 1:A:687:ASP:O | 1:A:691:VAL:HG23 | 2.17 | 0.45 |
| 1:A:312:GLN:HE21 | 1:A:362:LYS:HB3 | 1.81 | 0.44 |
| 1:A:808:GLN:HE22 | 3:E:141:LYS:NZ | 2.16 | 0.44 |
| 1:A:751:GLN:HE21 | 1:A:751:GLN:HA | 1.83 | 0.44 |
| 2:D:39:LEU:HD13 | 2:D:71:PHE:CZ | 2.52 | 0.44 |
| 1:A:20:LYS:HA | 1:A:24:LYS:HG3 | 1.99 | 0.44 |
| 1:B:488:HIS:O | 1:B:488:HIS:CG | 2.71 | 0.44 |
| 3:F:9:LYS:HA | 3:F:12:LYS:HB2 | 2.00 | 0.44 |
| 1:A:104:TYR:CE1 | 1:A:120:ILE:HG22 | 2.52 | 0.43 |
| 1:B:579:HIS:CG | 1:B:580:TYR:H | 2.36 | 0.43 |
| 1:A:459:ILE:HD12 | 1:A:459:ILE:H | 1.83 | 0.43 |
| 1:B:611:SER:HA | 1:A:730:SER:HA | 2.01 | 0.43 |
| 1:B:759:LEU:HD12 | 1:B:760:GLY:H | 1.83 | 0.43 |
| 1:B:827:ASN:HD21 | 1:B:831:TYR:HA | 1.84 | 0.43 |
| 1:B:771:LEU:H | 1:B:771:LEU:HD22 | 1.84 | 0.43 |
| 1:A:20:LYS:HA | 1:A:24:LYS:CG | 2.48 | 0.43 |
| 1:B:158:SER:HB3 | 1:B:715:MET:HA | 2.00 | 0.43 |
| 1:A:230:ALA:HB3 | 1:A:280:TYR:HA | 2.00 | 0.43 |
| 1:B:479:ASN:HA | 1:B:482:LEU:HG | 2.01 | 0.43 |
| 1:B:833:LEU:HG | 1:B:837:VAL:HG22 | 2.00 | 0.43 |
| 1:A:243:LYS:HZ2 | 1:A:243:LYS:HB3 | 1.84 | 0.43 |
| 3:F:86:LEU:HD21 | 3:E:31:PRO:HB2 | 2.01 | 0.42 |
| 1:B:361:PHE:HB2 | 1:B:414:ALA:HA | 2.01 | 0.42 |
| 1:B:485:PHE:HB3 | 1:B:489:HIS:CE1 | 2.55 | 0.42 |
| 3:F:107:ASN:H | 3:F:110:MET:HB2 | 1.84 | 0.42 |
| 3:E:151:LEU:HD23 | 3:E:151:LEU:HA | 1.87 | 0.42 |
| 1:B:406:GLU:HG2 | 1:B:407:MET:H | 1.85 | 0.42 |
| 1:A:230:ALA:CB | 1:A:281:HIS:H | 2.33 | 0.42 |
| 1:B:41:TYR:CE1 | 1:B:93:ASP:HB2 | 2.54 | 0.42 |
| 1:B:718:PRO:HB3 | 2:D:94:ASP:H | 1.85 | 0.42 |
| 1:B:804:LYS:HA | 1:B:808:GLN:HG3 | 2.01 | 0.41 |
| 1:A:459:ILE:HG21 | 1:A:478:THR:HB | 2.02 | 0.41 |
| 1:A:561:VAL:HG12 | 1:A:562:LYS:N | 2.34 | 0.41 |
| 2:C:19:TYR:CD2 | 2:C:31:ASP:HB3 | 2.55 | 0.41 |
| 1:A:831:TYR:HA | 3:E:115:PHE:CE1 | 2.55 | 0.41 |
| 1:B:782:LEU:HD13 | 1:B:786:VAL:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:104:TYR:CD2 | 1:A:686:ILE:HD11 | 2.56 | 0.41 |
| 1:A:126:PHE:HB3 | 1:A:127:PRO:HD2 | 2.02 | 0.41 |
| 1:A:243:LYS:HZ2 | 1:A:458:ASP:HB3 | 1.86 | 0.41 |
| 1:A:41:TYR:CZ | 1:A:688:SER:HB3 | 2.56 | 0.41 |
| 2:C:85:ASP:H | 2:C:88:GLU:HB2 | 1.86 | 0.41 |
| 1:B:834:TYR:H | 1:B:835:ILE:HG13 | 1.86 | 0.40 |
| 1:B:827:ASN:OD1 | 1:B:831:TYR:CE1 | 2.73 | 0.40 |
| 1:B:355:HIS:CG | 1:B:380:ARG:HD2 | 2.56 | 0.40 |
| 1:B:157:TYR:CZ | 1:B:161:LEU:HD22 | 2.56 | 0.40 |
| 1:A:84:ASP:H | 1:A:112:TYR:HB2 | 1.87 | 0.40 |
| 1:A:476:ASN:HB3 | 1:A:579:HIS:CD2 | 2.57 | 0.40 |

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 | A | 838/1953 (43%) | 675 (80%) | 106 (13%) | 57 (7%) | 1 15 |
| 1 | B | 838/1953 (43%) | 705 (84%) | 89 (11%) | 44 (5%) | 2 19 |
| 2 | C | 154/156 (99%) | 130 (84%) | 16 (10%) | 8 (5%) | 2 19 |
| 2 | D | 154/156 (99%) | 132 (86%) | 15 (10%) | 7 (4%) | 2 21 |
| 3 | E | 194/196 (99%) | 148 (76%) | 31 (16%) | 15 (8%) | 1 13 |
| 3 | F | 194/196 (99%) | 149 (77%) | 28 (14%) | 17 (9%) | 1 11 |
| All | All | 2372/4610 (52%) | 1939 (82%) | 285 (12%) | 148 (6%) | 3 16 |

All (148) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 149 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 206 | THR |
| 1 | B | 208 | GLU |
| 1 | B | 270 | VAL |
| 1 | B | 358 | GLU |
| 1 | B | 462 | PHE |
| 1 | B | 505 | TRP |
| 1 | B | 515 | ALA |
| 1 | B | 536 | MET |
| 1 | B | 558 | PRO |
| 1 | B | 600 | ASN |
| 1 | B | 731 | ALA |
| 1 | B | 759 | LEU |
| 1 | B | 806 | GLN |
| 1 | B | 836 | LYS |
| 3 | F | 24 | ALA |
| 3 | F | 93 | GLN |
| 3 | F | 127 | VAL |
| 3 | F | 136 | ASP |
| 3 | F | 144 | GLU |
| 1 | A | 369 | GLN |
| 1 | A | 418 | SER |
| 1 | A | 465 | PHE |
| 1 | A | 507 | PHE |
| 1 | A | 511 | GLY |
| 1 | A | 559 | ASN |
| 1 | A | 573 | ALA |
| 1 | A | 600 | ASN |
| 1 | A | 606 | GLN |
| 1 | A | 622 | HIS |
| 1 | A | 768 | ALA |
| 1 | A | 830 | TRP |
| 1 | A | 833 | LEU |
| 2 | C | 22 | GLU |
| 2 | C | 26 | LYS |
| 2 | C | 84 | GLU |
| 2 | C | 92 | VAL |
| 2 | C | 118 | THR |
| 3 | E | 25 | ALA |
| 3 | E | 32 | LYS |
| 3 | E | 139 | GLU |
| 3 | E | 188 | THR |
| 1 | B | 61 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 68 | LYS |
| 1 | B | 141 | ARG |
| 1 | B | 202 | LYS |
| 1 | B | 207 | LYS |
| 1 | B | 516 | ALA |
| 1 | B | 582 | GLY |
| 2 | D | 21 | TRP |
| 2 | D | 153 | ASP |
| 3 | F | 67 | ASP |
| 3 | F | 86 | LEU |
| 1 | A | 3 | GLU |
| 1 | A | 65 | GLN |
| 1 | A | 86 | SER |
| 1 | A | 144 | GLU |
| 1 | A | 269 | ARG |
| 1 | A | 307 | TYR |
| 1 | A | 310 | VAL |
| 1 | A | 311 | SER |
| 1 | A | 316 | GLU |
| 1 | A | 323 | ALA |
| 1 | A | 366 | ARG |
| 1 | A | 471 | GLU |
| 1 | A | 499 | LYS |
| 1 | A | 556 | LYS |
| 1 | A | 560 | PHE |
| 1 | A | 723 | ARG |
| 3 | E | 51 | PHE |
| 3 | E | 159 | SER |
| 3 | E | 195 | GLY |
| 1 | B | 3 | GLU |
| 1 | B | 292 | GLU |
| 1 | B | 611 | SER |
| 1 | B | 646 | PHE |
| 1 | B | 677 | PRO |
| 1 | B | 712 | PRO |
| 1 | B | 839 | PRO |
| 2 | D | 2 | ALA |
| 2 | D | 96 | ALA |
| 3 | F | 45 | SER |
| 3 | F | 63 | PHE |
| 3 | F | 103 | PRO |
| 1 | A | 29 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 299 | LEU |
| 1 | A | 449 | LYS |
| 1 | A | 525 | MET |
| 1 | A | 567 | LYS |
| 1 | A | 580 | TYR |
| 1 | A | 635 | LYS |
| 1 | A | 719 | ASP |
| 1 | A | 722 | GLN |
| 1 | A | 754 | ALA |
| 2 | C | 2 | ALA |
| 3 | E | 16 | LYS |
| 3 | E | 37 | LYS |
| 3 | E | 48 | PHE |
| 3 | E | 73 | PHE |
| 3 | E | 131 | ALA |
| 3 | E | 166 | ALA |
| 3 | E | 169 | GLU |
| 1 | B | 27 | ASP |
| 1 | B | 263 | TYR |
| 1 | B | 272 | SER |
| 1 | B | 308 | HIS |
| 1 | B | 405 | ASN |
| 1 | B | 597 | ASP |
| 1 | B | 725 | THR |
| 1 | B | 733 | PRO |
| 1 | B | 803 | LYS |
| 2 | D | 134 | ASP |
| 3 | F | 90 | CYS |
| 3 | F | 172 | ILE |
| 1 | A | 19 | ARG |
| 1 | A | 22 | GLN |
| 1 | A | 23 | THR |
| 1 | A | 199 | LYS |
| 1 | A | 235 | ASN |
| 1 | A | 309 | PHE |
| 1 | A | 389 | ALA |
| 1 | A | 682 | GLN |
| 2 | C | 107 | ALA |
| 3 | E | 152 | THR |
| 1 | B | 2 | ALA |
| 1 | B | 39 | GLU |
| 1 | B | 312 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 40 | ASP |
| 3 | F | 26 | PRO |
| 3 | F | 54 | HIS |
| 3 | F | 91 | THR |
| 3 | F | 95 | LEU |
| 1 | A | 61 | GLN |
| 1 | A | 358 | GLU |
| 1 | A | 450 | ARG |
| 1 | A | 582 | GLY |
| 1 | A | 761 | ASN |
| 2 | C | 91 | LYS |
| 1 | B | 77 | PRO |
| 2 | D | 116 | ARG |
| 3 | F | 25 | ALA |
| 1 | A | 228 | GLY |
| 1 | A | 375 | THR |
| 1 | A | 571 | GLN |
| 1 | B | 623 | PRO |
| 1 | A | 712 | PRO |
| 1 | B | 737 | VAL |
| 1 | A | 524 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 721/1689 (43%) | 686 (95%) | 35 (5%) | 25 50 |
| 1 | B | 721/1689 (43%) | 686 (95%) | 35 (5%) | 25 50 |
| 2 | C | 132/132 (100%) | 129 (98%) | 3 (2%) | 50 70 |
| 2 | D | 132/132 (100%) | 125 (95%) | 7 (5%) | 22 47 |
| 3 | E | 164/164 (100%) | 153 (93%) | 11 (7%) | 16 41 |
| 3 | F | 164/164 (100%) | 157 (96%) | 7 (4%) | 29 53 |
| All | All | 2034/3970 (51%) | 1936 (95%) | 98 (5%) | 29 51 |

All (98) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 8 | THR |
| 1 | B | 34 | VAL |
| 1 | B | 67 | LYS |
| 1 | B | 71 | LEU |
| 1 | B | 109 | ILE |
| 1 | B | 112 | TYR |
| 1 | B | 141 | ARG |
| 1 | B | 142 | ARG |
| 1 | B | 174 | GLU |
| 1 | B | 220 | THR |
| 1 | B | 232 | THR |
| 1 | B | 241 | PHE |
| 1 | B | 302 | ASP |
| 1 | B | 364 | ARG |
| 1 | B | 409 | THR |
| 1 | B | 426 | LYS |
| 1 | B | 517 | CYS |
| 1 | B | 536 | MET |
| 1 | B | 541 | THR |
| 1 | B | 564 | LYS |
| 1 | B | 607 | PHE |
| 1 | B | 671 | PHE |
| 1 | B | 678 | ASN |
| 1 | B | 715 | MET |
| 1 | B | 758 | ARG |
| 1 | B | 771 | LEU |
| 1 | B | 773 | ARG |
| 1 | B | 779 | ASP |
| 1 | B | 817 | ARG |
| 1 | B | 818 | ASN |
| 1 | B | 822 | PHE |
| 1 | B | 831 | TYR |
| 1 | B | 832 | LYS |
| 1 | B | 836 | LYS |
| 1 | B | 837 | VAL |
| 2 | D | 32 | LEU |
| 2 | D | 35 | LEU |
| 2 | D | 54 | SER |
| 2 | D | 60 | LYS |
| 2 | D | 75 | LYS |
| 2 | D | 82 | THR |
| 2 | D | 139 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | F | 53 | GLN |
| 3 | F | 64 | GLN |
| 3 | F | 93 | GLN |
| 3 | F | 99 | VAL |
| 3 | F | 143 | LYS |
| 3 | F | 182 | LYS |
| 3 | F | 186 | ILE |
| 1 | A | 19 | ARG |
| 1 | A | 20 | LYS |
| 1 | A | 36 | ASP |
| 1 | A | 75 | ASN |
| 1 | A | 93 | ASP |
| 1 | A | 141 | ARG |
| 1 | A | 149 | LEU |
| 1 | A | 180 | THR |
| 1 | A | 185 | LYS |
| 1 | A | 243 | LYS |
| 1 | A | 252 | MET |
| 1 | A | 280 | TYR |
| 1 | A | 281 | HIS |
| 1 | A | 286 | LEU |
| 1 | A | 305 | TYR |
| 1 | A | 312 | GLN |
| 1 | A | 329 | THR |
| 1 | A | 362 | LYS |
| 1 | A | 364 | ARG |
| 1 | A | 366 | ARG |
| 1 | A | 450 | ARG |
| 1 | A | 458 | ASP |
| 1 | A | 459 | ILE |
| 1 | A | 484 | GLN |
| 1 | A | 567 | LYS |
| 1 | A | 599 | VAL |
| 1 | A | 600 | ASN |
| 1 | A | 692 | MET |
| 1 | A | 725 | THR |
| 1 | A | 742 | VAL |
| 1 | A | 746 | VAL |
| 1 | A | 757 | TYR |
| 1 | A | 764 | VAL |
| 1 | A | 790 | GLN |
| 1 | A | 809 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 13 | ARG |
| 2 | C | 32 | LEU |
| 2 | C | 42 | LYS |
| 3 | E | 1 | MET |
| 3 | E | 14 | LYS |
| 3 | E | 16 | LYS |
| 3 | E | 42 | ARG |
| 3 | E | 54 | HIS |
| 3 | E | 59 | PHE |
| 3 | E | 75 | SER |
| 3 | E | 108 | PHE |
| 3 | E | 112 | LEU |
| 3 | E | 141 | LYS |
| 3 | E | 188 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 73 | GLN |
| 1 | B | 98 | HIS |
| 1 | B | 219 | GLN |
| 1 | B | 281 | HIS |
| 1 | B | 285 | GLN |
| 1 | B | 340 | HIS |
| 1 | B | 479 | ASN |
| 1 | B | 488 | HIS |
| 1 | B | 489 | HIS |
| 1 | B | 495 | GLN |
| 1 | B | 550 | ASN |
| 1 | B | 665 | HIS |
| 1 | B | 678 | ASN |
| 1 | B | 698 | ASN |
| 1 | B | 722 | GLN |
| 1 | B | 806 | GLN |
| 1 | B | 818 | ASN |
| 1 | B | 827 | ASN |
| 2 | D | 108 | HIS |
| 1 | A | 22 | GLN |
| 1 | A | 50 | GLN |
| 1 | A | 216 | GLN |
| 1 | A | 221 | ASN |
| 1 | A | 293 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 552 | ASN |
| 1 | A | 579 | HIS |
| 1 | A | 622 | HIS |
| 1 | A | 698 | ASN |
| 1 | A | 751 | GLN |
| 1 | A | 808 | GLN |
| 1 | A | 816 | GLN |

#### 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 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)

There are no chain breaks in this entry.

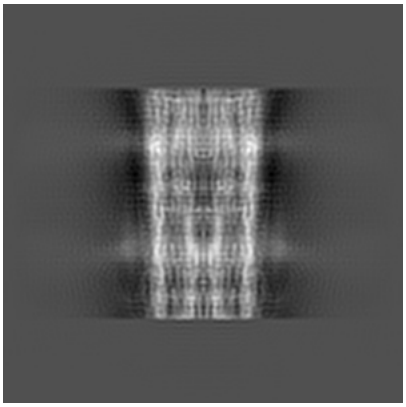
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7029. These allow visual inspection of the internal detail of the map and identification of artifacts.

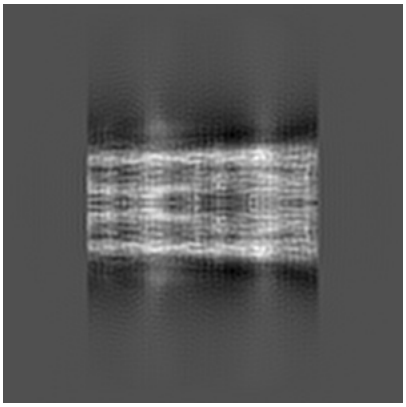
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

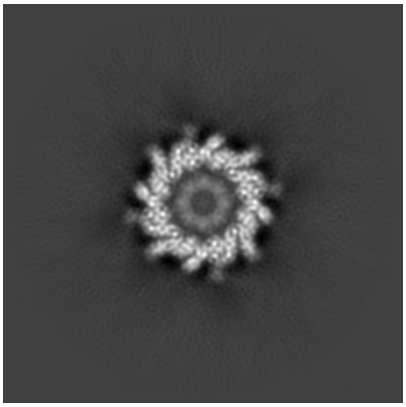
### 6.1.1 Primary map



X



Y

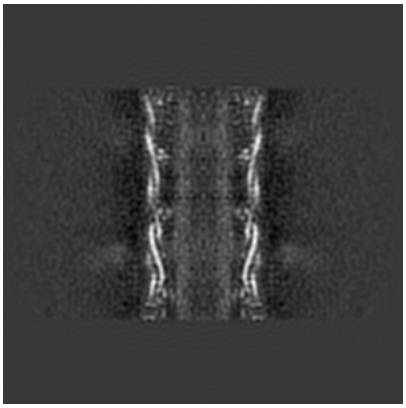


Z

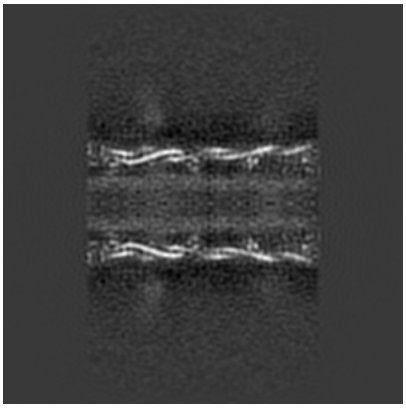
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

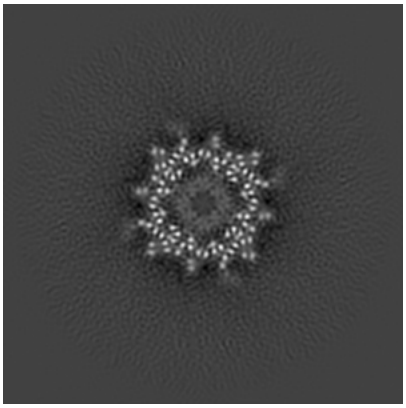
### 6.2.1 Primary map



X Index: 216



Y Index: 216

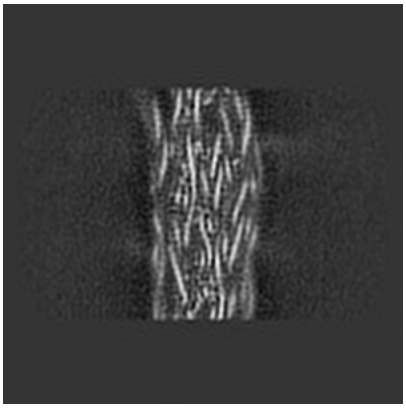


Z Index: 216

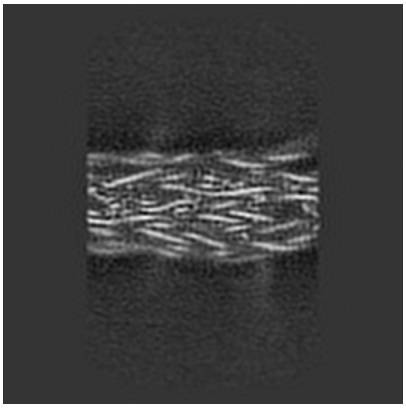
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

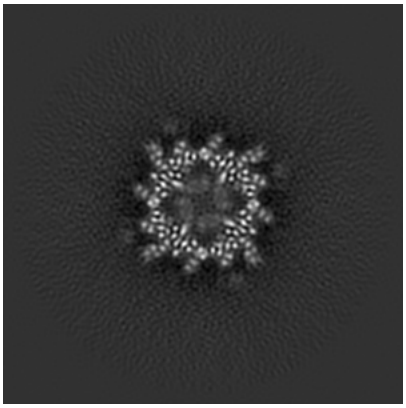
### 6.3.1 Primary map



X Index: 167



Y Index: 167



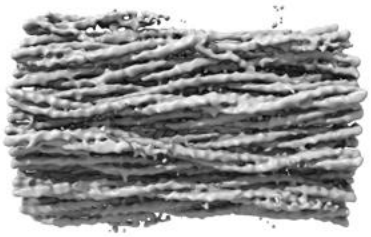
Z Index: 232

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

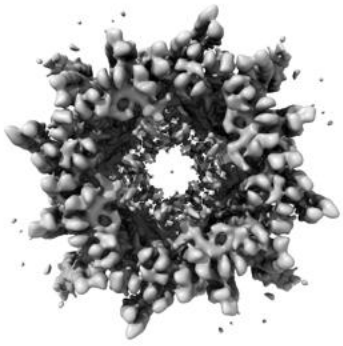
## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

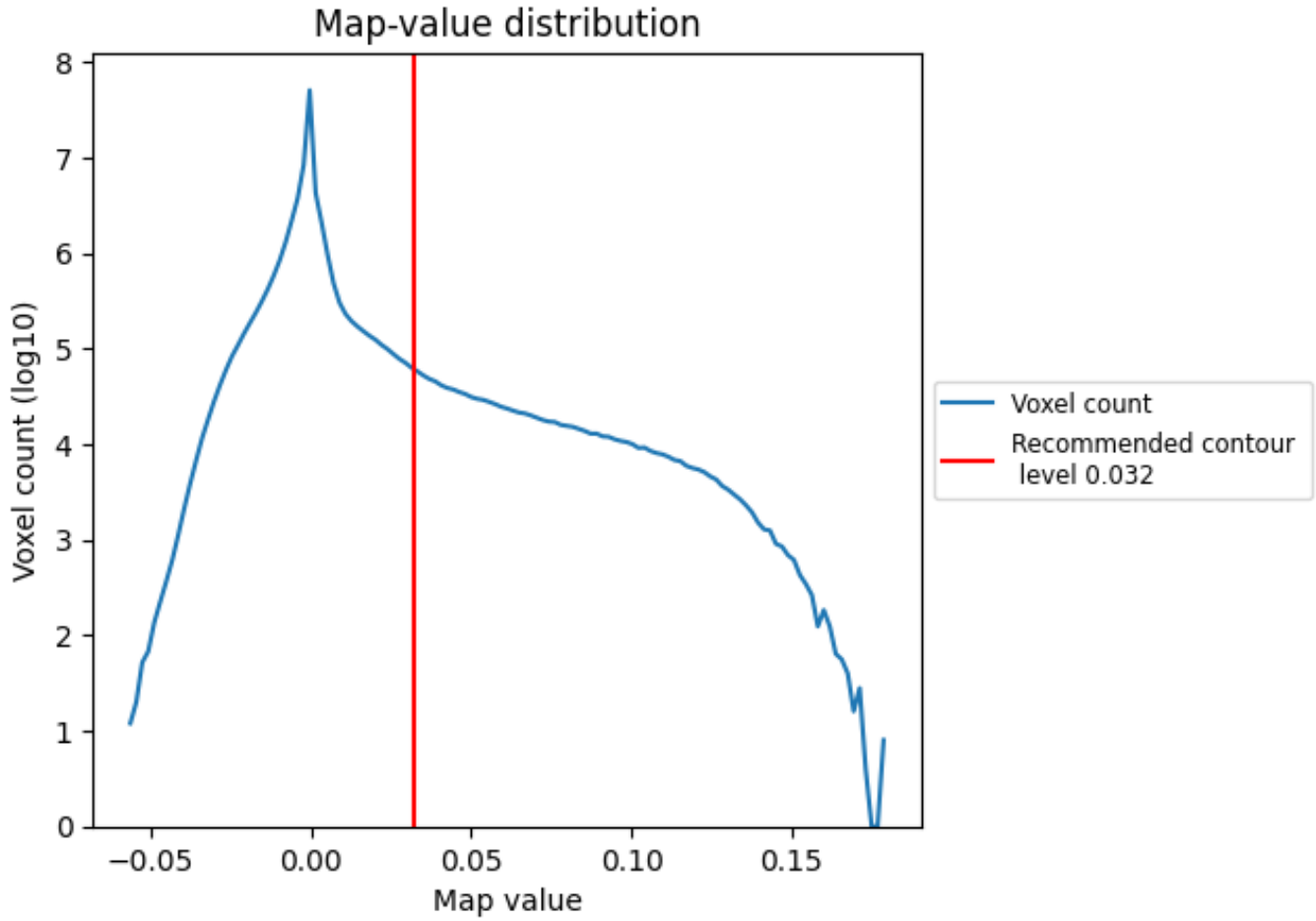
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

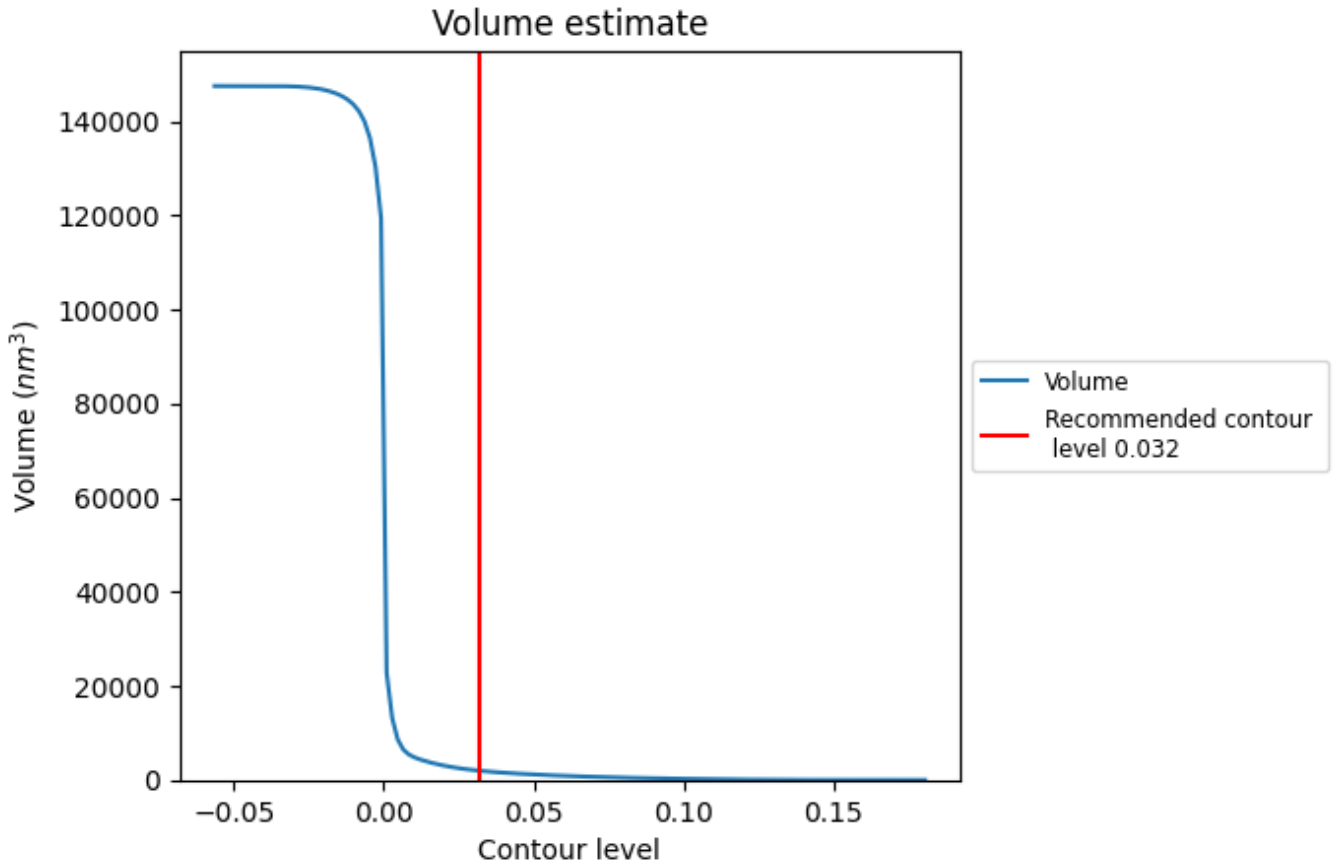
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

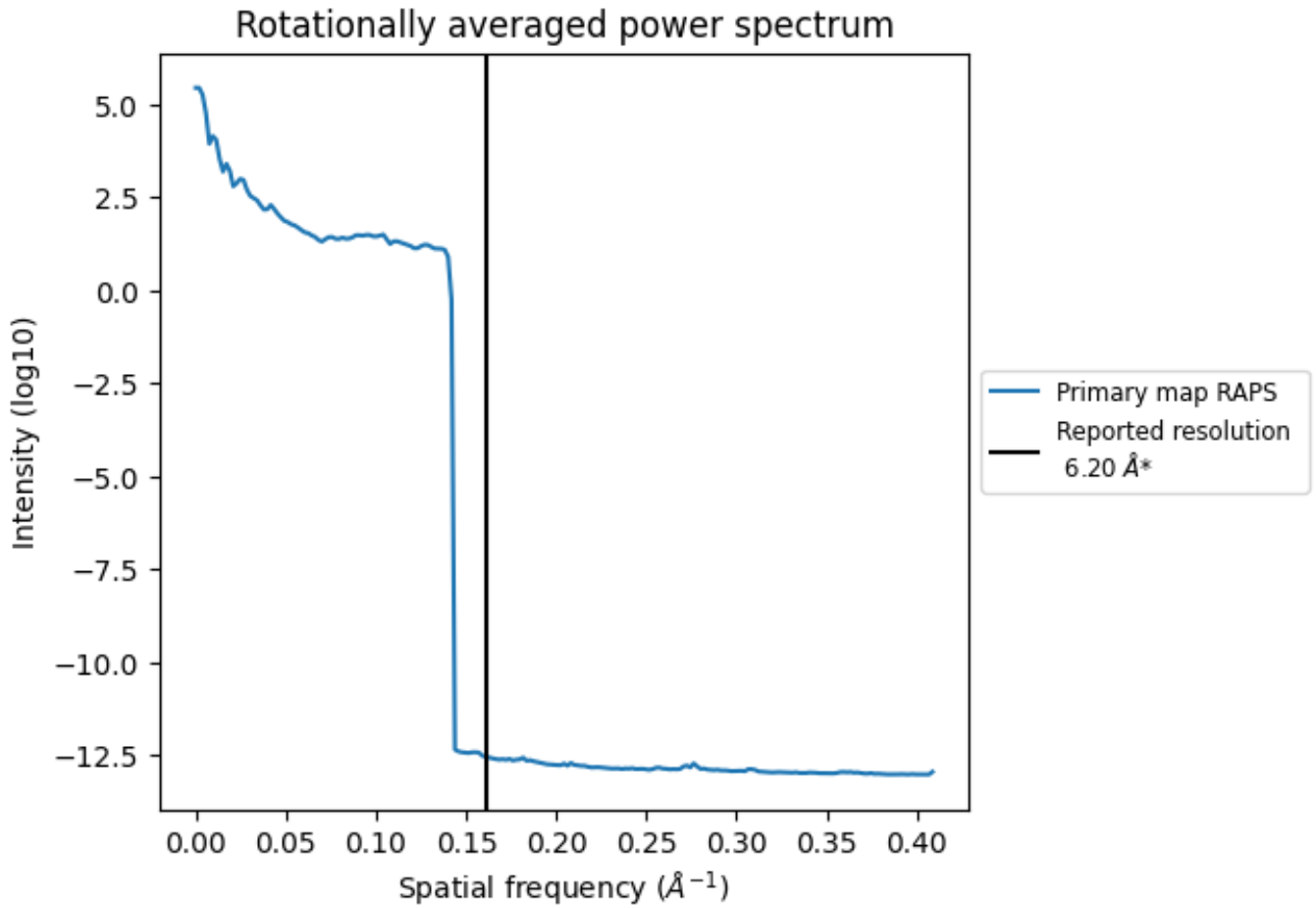
## 7.2 Volume estimate




The volume at the recommended contour level is 1954 $nm^3$; this corresponds to an approximate mass of 1765 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

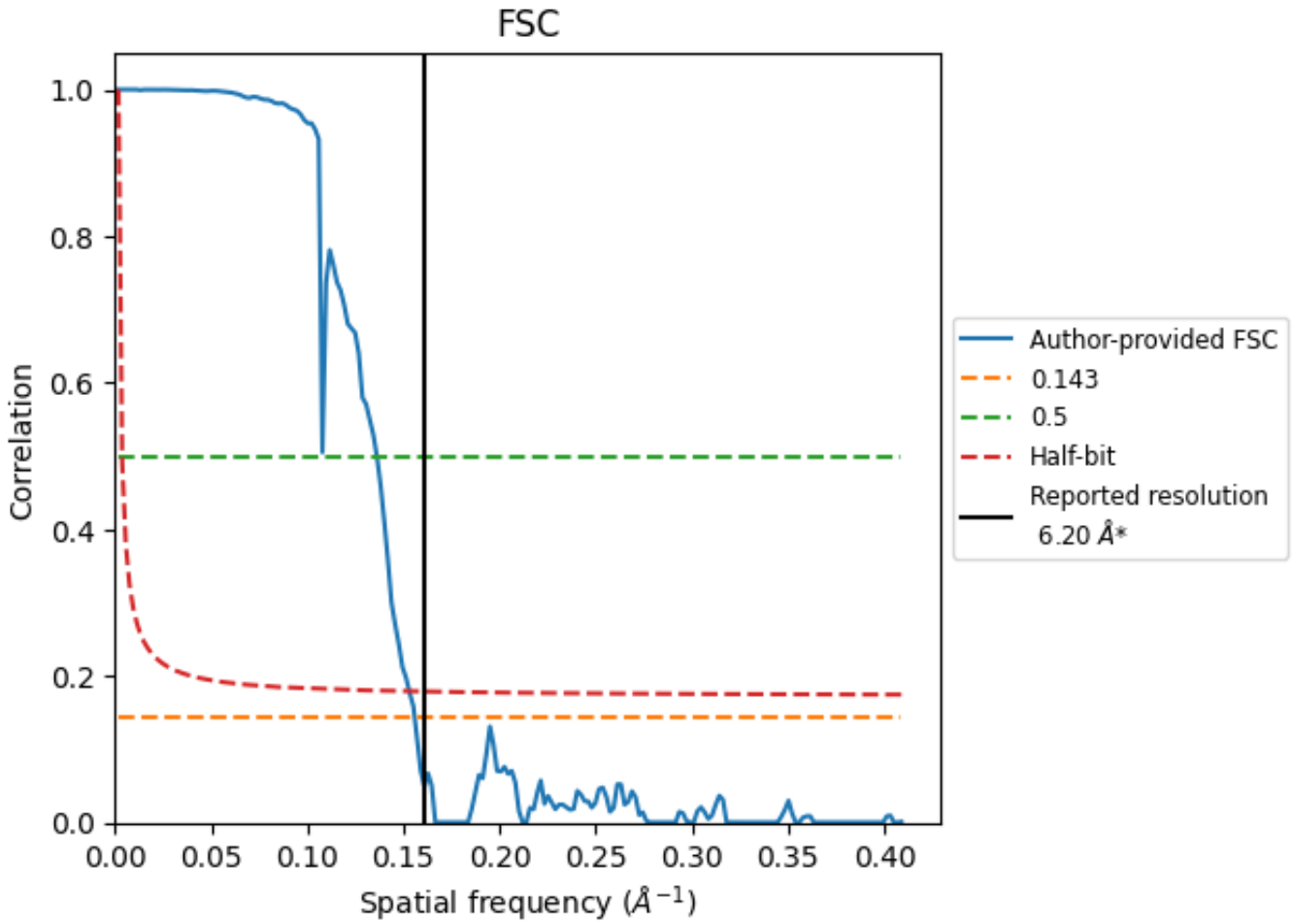



*Reported resolution corresponds to spatial frequency of 0.161 $Å^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.161 Å$^{-1}$

## 8.2 Resolution estimates (i)

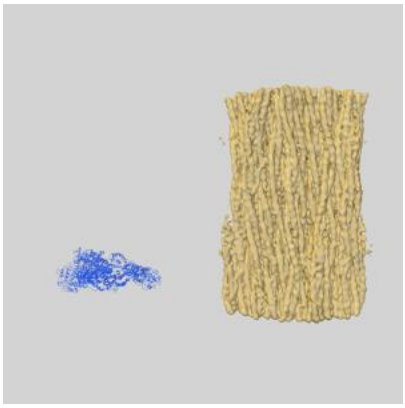
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 6.20 | - | - |
| Author-provided FSC curve | 6.41 | 7.35 | 6.53 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

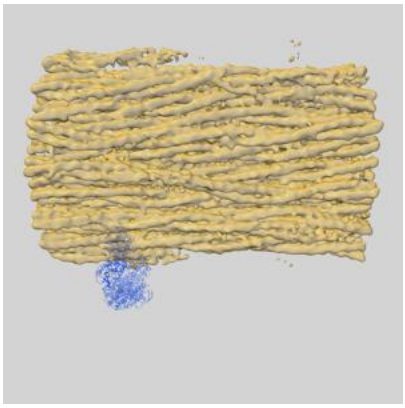
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7029 and PDB model 6SO3. Per-residue inclusion information can be found in section 3 on page 4.

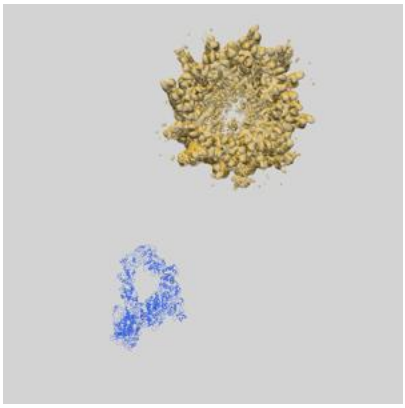
## 9.1 Map-model overlay



X



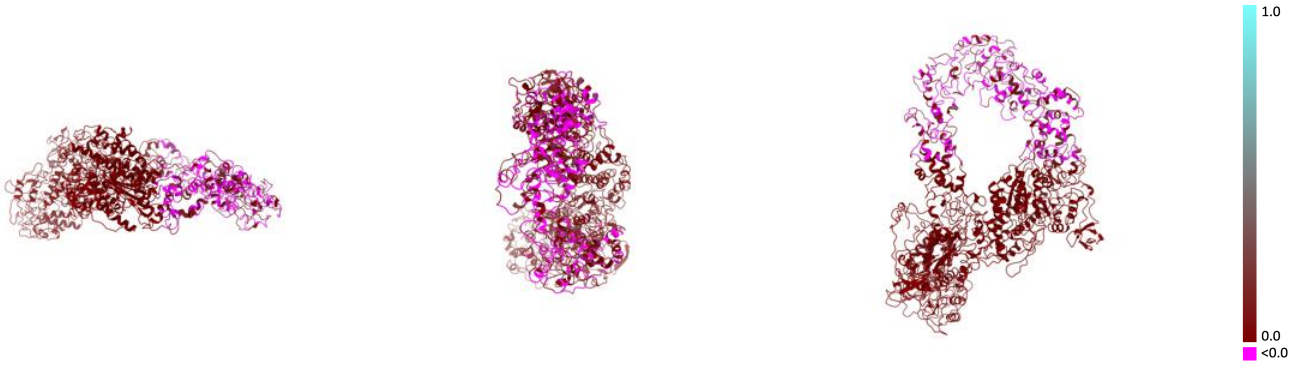
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

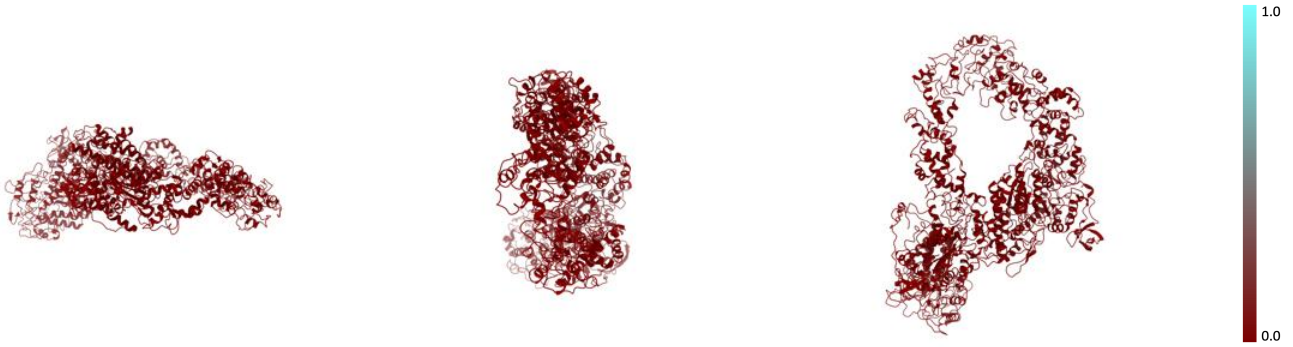
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according 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.

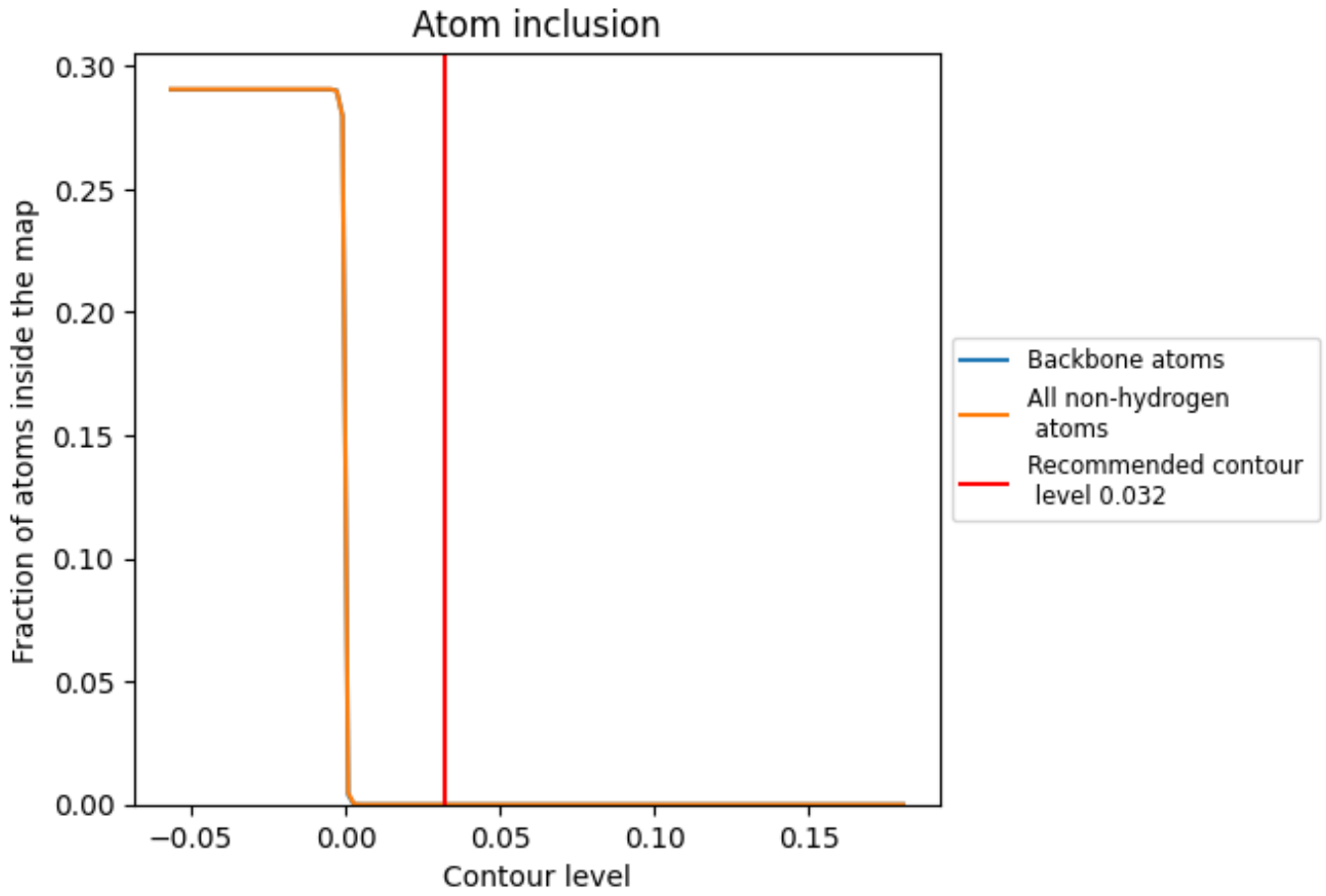
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).

## 9.4 Atom inclusion (i)




At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.0000 | 0.0000 |
| A | 0.0000 | 0.0010 |
| B | 0.0000 | 0.0010 |
| C | 0.0000 | -0.0010 |
| D | 0.0000 | -0.0070 |
| E | 0.0000 | 0.0250 |
| F | 0.0000 | -0.0260 |