



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 10:58 pm GMT

PDB ID : 5A31
EMDB ID : EMD-2925
Title : Structure of the human APC-Cdh1-Hsl1-UbcH10 complex.
Authors : Chang, L.; Zhang, Z.; Yang, J.; Mclaughlin, S.H.; Barford, D.
Deposited on : 2015-05-26
Resolution : 4.30 Å(reported)

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
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

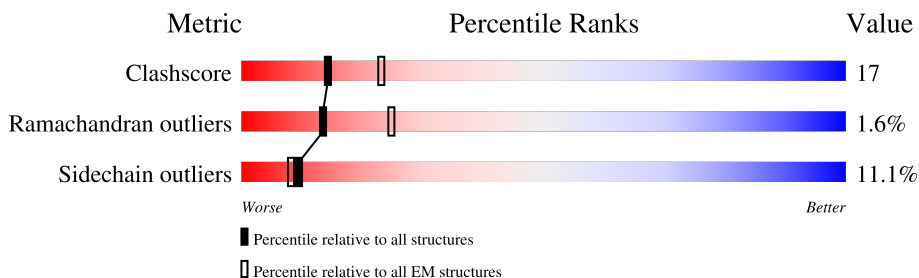
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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 | 1441 | <div style="display: flex; justify-content: space-between;"> 28% 61% 34% 5% </div> |
| 2 | B | 84 | <div style="display: flex; justify-content: space-between;"> 14% 51% 36% 8% 5% </div> |
| 3 | C | 597 | <div style="display: flex; justify-content: space-between;"> 23% 60% 23% •• 12% </div> |
| 3 | P | 597 | <div style="display: flex; justify-content: space-between;"> 11% 57% 21% • 18% </div> |
| 4 | D | 121 | <div style="display: flex; justify-content: space-between;"> 13% 32% 12% • 55% </div> |
| 5 | E | 110 | <div style="display: flex; justify-content: space-between;"> 13% 35% 15% • 49% </div> |
| 6 | F | 824 | <div style="display: flex; justify-content: space-between;"> 12% 44% 15% • 40% </div> |
| 6 | H | 824 | <div style="display: flex; justify-content: space-between;"> 13% 42% 14% • 41% </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 7 | G | 85 | |
| 7 | W | 85 | |
| 8 | I | 808 | |
| 9 | J | 620 | |
| 10 | K | 620 | |
| 11 | L | 185 | |
| 12 | M | 74 | |
| 13 | N | 703 | |
| 14 | O | 755 | |
| 15 | Q | 162 | |
| 16 | R | 386 | |
| 17 | T | 21 | |
| 18 | U | 24 | |
| 19 | V | 13 | |
| 20 | X | 599 | |
| 20 | Y | 599 | |

2 Entry composition i

There are 21 unique types of molecules in this entry. The entry contains 67685 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 ANAPHASE-PROMOTING COMPLEX SUBUNIT 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 1441 | 10950 | 7046 | 1853 | 1977 | 74 | 0 | 0 |

- Molecule 2 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | B | 84 | 650 | 418 | 117 | 98 | 17 | 1 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| B | 13 | LEU | THR | conflict | UNP Q9NYG5 |

- Molecule 3 is a protein called CELL DIVISION CYCLE PROTEIN 23 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | C | 524 | 4305 | 2774 | 726 | 781 | 24 | 0 | 0 |
| 3 | P | 491 | 4042 | 2611 | 678 | 729 | 24 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C | 161 | LEU | LYS | conflict | UNP Q9UJX2 |
| P | 161 | LEU | LYS | conflict | UNP Q9UJX2 |

- Molecule 4 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 15.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 4 | D | 55 | 437 | 277 | 73 | 87 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| D | 1 | MET | - | expression tag | UNP P60006 |
| D | 2 | SER | - | expression tag | UNP P60006 |
| D | 3 | THR | - | expression tag | UNP P60006 |
| D | 4 | LEU | - | expression tag | UNP P60006 |
| D | 5 | TYR | - | expression tag | UNP P60006 |

- Molecule 5 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | E | 56 | 450 | 290 | 74 | 85 | 1 | 0 | 0 |

- Molecule 6 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | F | 498 | 3923 | 2514 | 664 | 719 | 26 | 0 | 0 |
| 6 | H | 483 | 3853 | 2473 | 650 | 704 | 26 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| F | 475 | SER | ALA | conflict | UNP P30260 |
| F | 484 | SER | ALA | conflict | UNP P30260 |
| H | 475 | SER | ALA | conflict | UNP P30260 |
| H | 484 | SER | ALA | conflict | UNP P30260 |

- Molecule 7 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | G | 25 | 211 | 133 | 40 | 37 | 1 | 0 | 0 |
| 7 | W | 25 | 213 | 133 | 40 | 39 | 1 | 0 | 0 |

- Molecule 8 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | I | 730 | 5709 | 3660 | 950 | 1066 | 33 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| I | 430 | ASP | GLU | conflict | UNP Q9UJX5 |

- Molecule 9 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 9 | J | 504 | 4047 | 2602 | 685 | 735 | 25 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| J | 225 | ASN | ASP | conflict | UNP Q13042 |
| J | 228 | GLU | GLN | conflict | UNP Q13042 |
| J | 229 | LYS | GLU | conflict | UNP Q13042 |
| J | 347 | ALA | GLU | conflict | UNP Q13042 |
| J | 524 | ALA | GLU | conflict | UNP Q13042 |

- Molecule 10 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | K | 493 | 3988 | 2565 | 673 | 726 | 24 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| K | 228 | GLU | GLN | conflict | UNP Q13042 |
| K | 229 | LYS | GLU | conflict | UNP Q13042 |
| K | 265 | LYS | ALA | conflict | UNP Q13042 |

- Molecule 11 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 11 | L | 182 | 1435 | 898 | 263 | 268 | 6 | 0 | 0 |

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 12 | M | 59 | 493 | 310 | 79 | 102 | 2 | 0 | 0 |

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 13 | N | 703 | 5400 | 3438 | 968 | 969 | 25 | 0 | 0 |

- Molecule 14 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 14 | O | 685 | 5396 | 3439 | 939 | 991 | 27 | 0 | 0 |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| O | 42 | SER | ASN | conflict | UNP Q9UJX4 |
| O | 55 | VAL | MET | conflict | UNP Q9UJX4 |
| O | 63 | GLN | LEU | conflict | UNP Q9UJX4 |
| O | 75 | VAL | LEU | conflict | UNP Q9UJX4 |
| O | 79 | LEU | TYR | conflict | UNP Q9UJX4 |
| O | 164 | SER | ASN | conflict | UNP Q9UJX4 |
| O | 165 | ASP | GLY | conflict | UNP Q9UJX4 |
| O | 167 | ASN | LYS | conflict | UNP Q9UJX4 |

- Molecule 15 is a protein called FUSION PROTEIN - UBIQUITIN-CONJUGATING ENZYME E2 C, UBIQUITIN-CONJUGATING ENZYME E2 S.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 15 | Q | 162 | 1227 | 789 | 204 | 229 | 5 | 1 | 0 |

- Molecule 16 is a protein called THE ANAPHASE-PROMOTING COMPLEX CHAIN R.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 16 | R | 386 | 2990 | 1884 | 530 | 564 | 12 | 0 | 0 |

- Molecule 17 is a protein called THE ANAPHASE-PROMOTING COMPLEX CHAIN T.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 17 | T | 21 | 109 | 65 | 22 | 22 | 0 | 0 |

- Molecule 18 is a protein called THE ANAPHASE-PROMOTING COMPLEX CHAIN U.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 18 | U | 24 | 120 | 72 | 24 | 24 | 0 | 0 |

- Molecule 19 is a protein called THE ANAPHASE-PROMOTING COMPLEX CHAIN V.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 19 | V | 13 | 99 | 64 | 19 | 16 | 0 | 0 |

- Molecule 20 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 20 | X | 484 | 3770 | 2394 | 650 | 705 | 21 | 0 | 0 |
| 20 | Y | 496 | 3865 | 2450 | 667 | 725 | 23 | 0 | 0 |

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

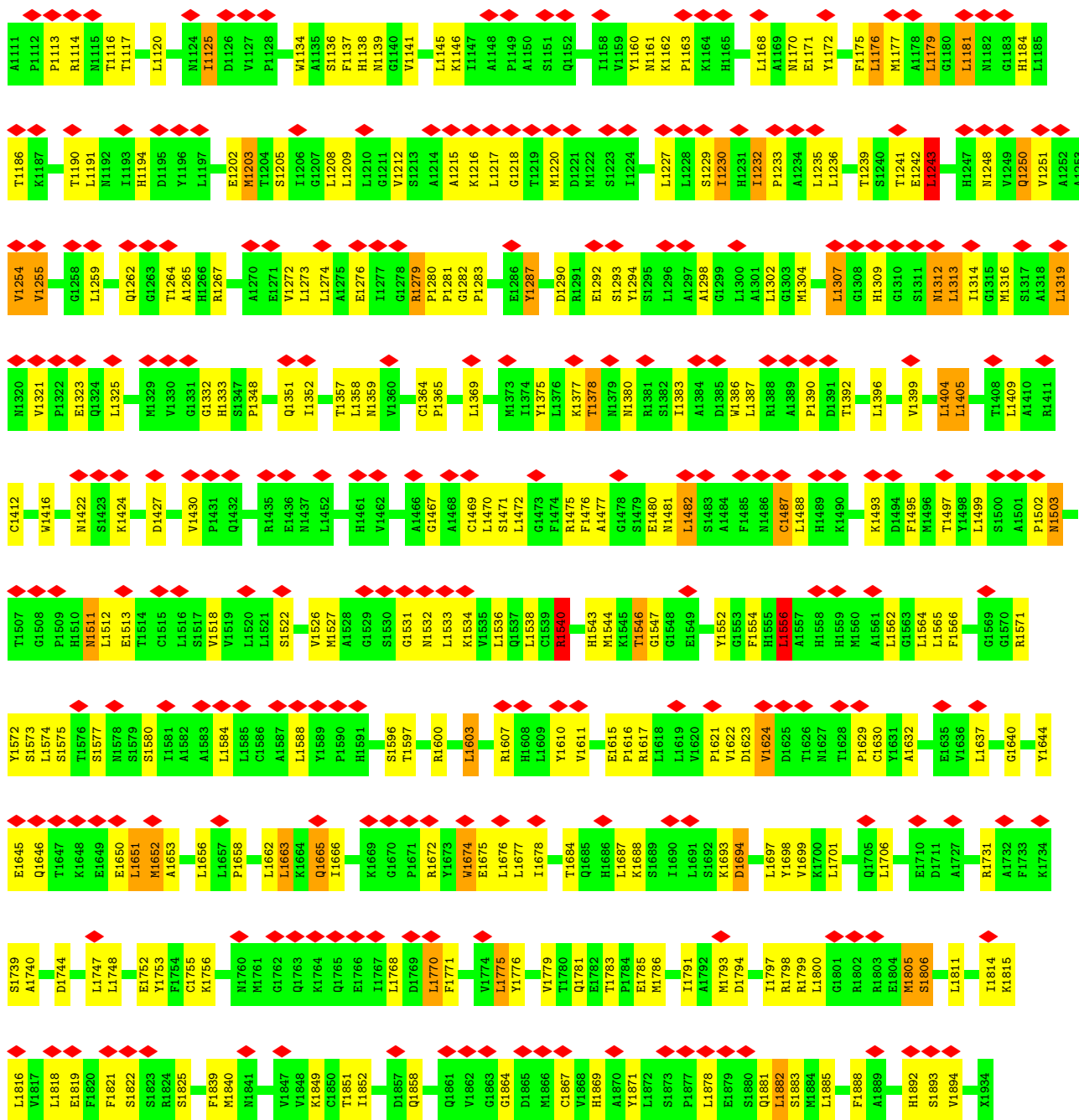
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Zn | |
| 21 | B | 3 | 3 | 3 | 0 |

3 Residue-property plots

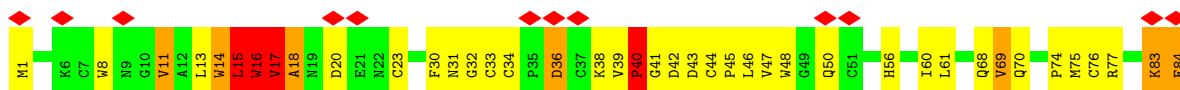
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ANAPHASE-PROMOTING COMPLEX SUBUNIT 1



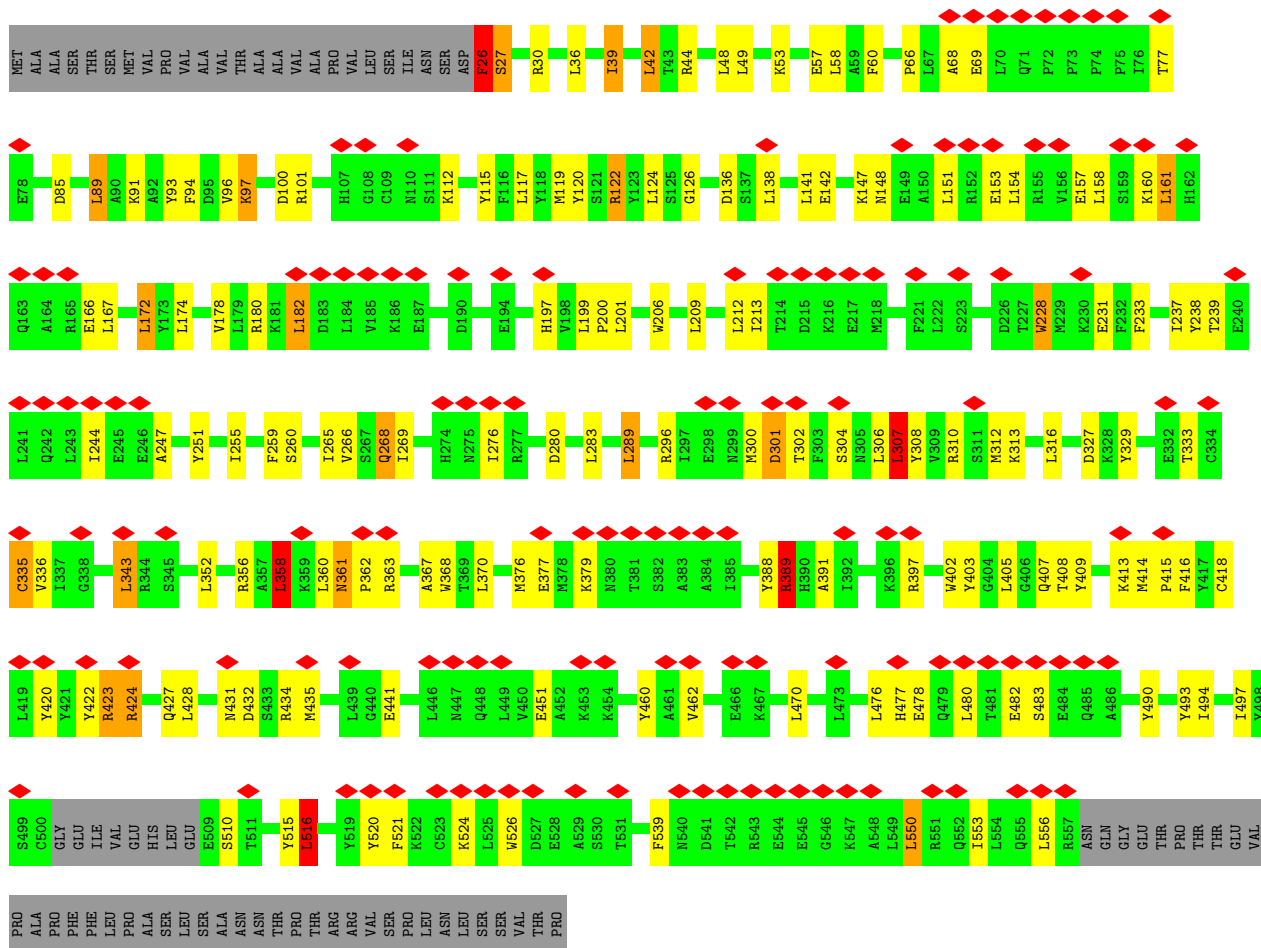


• Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

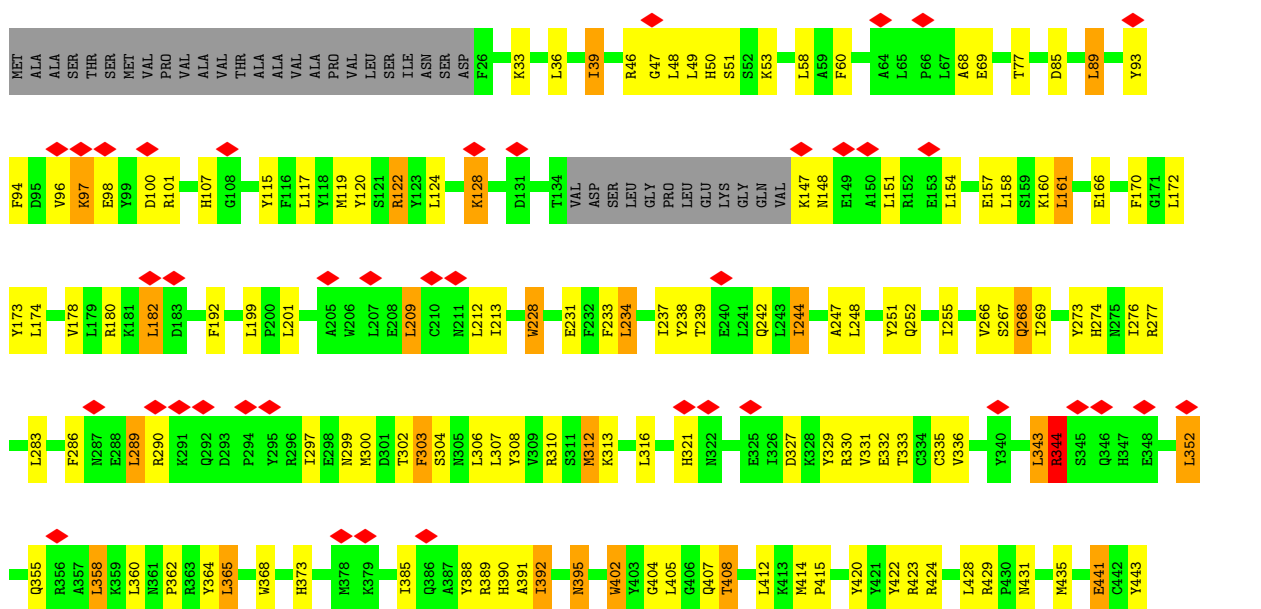


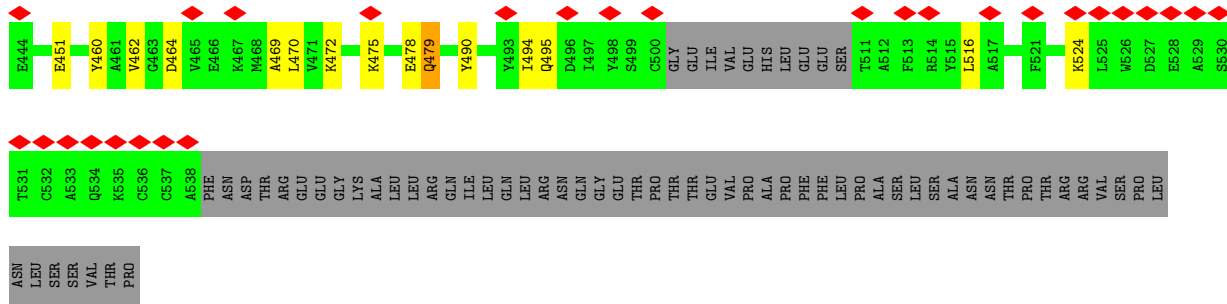
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG



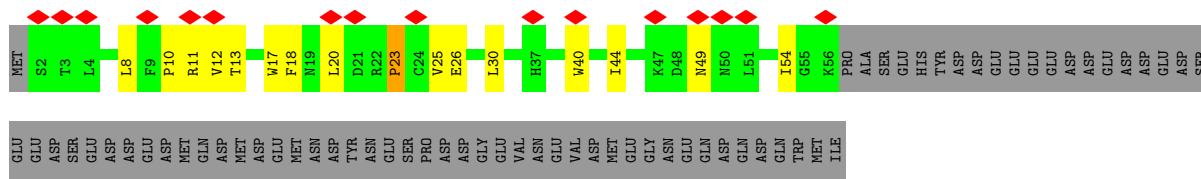
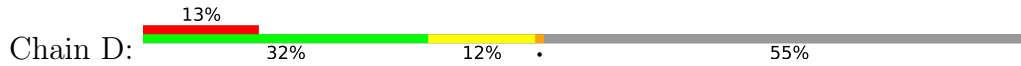


• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

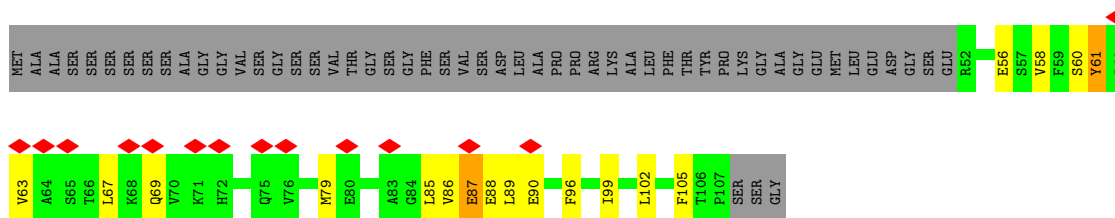
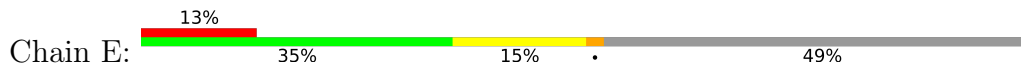




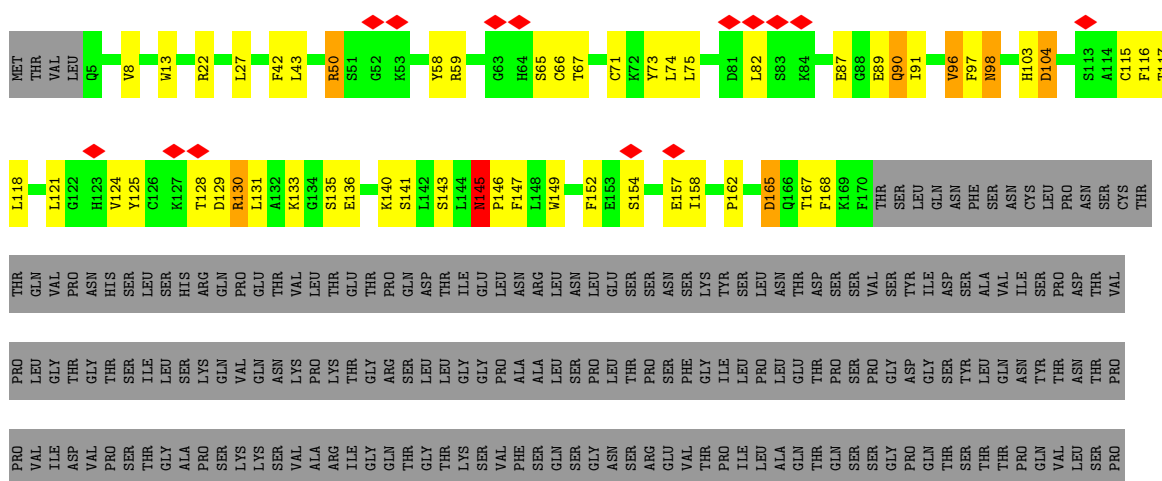
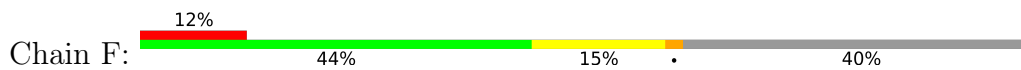
- Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

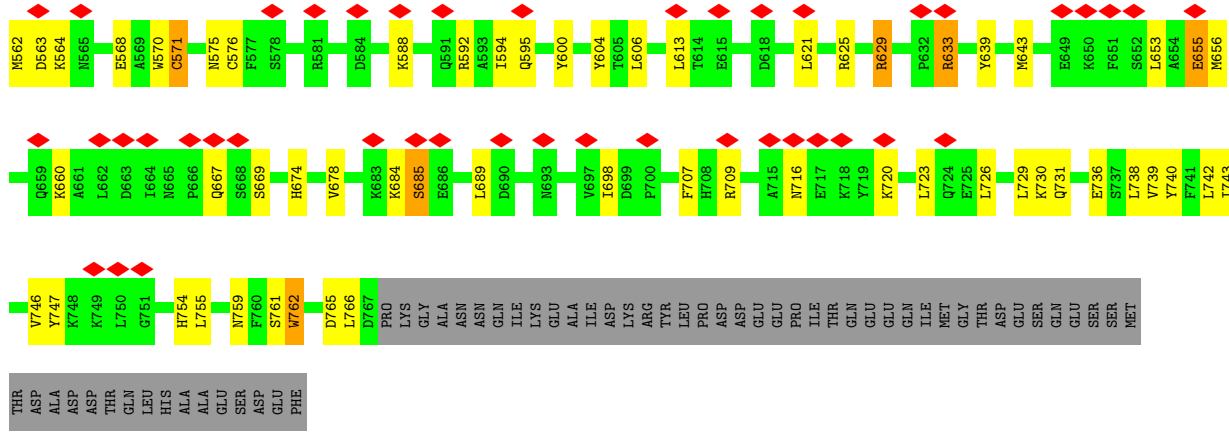


- Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

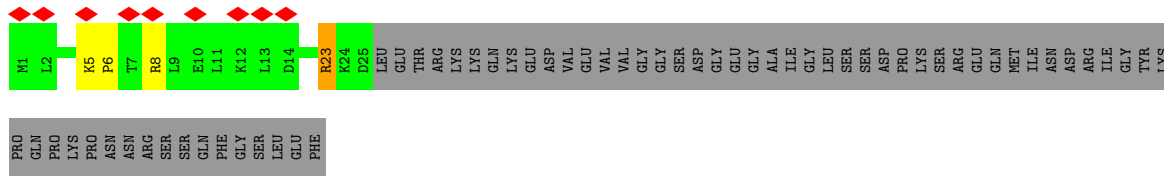


- Molecule 6: ANAPHASE-PROMOTING COMPLEX SUBUNIT 3

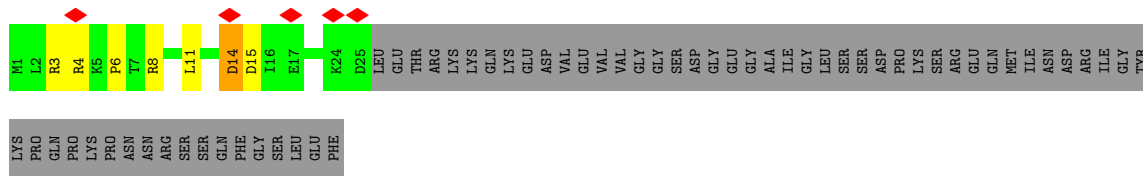




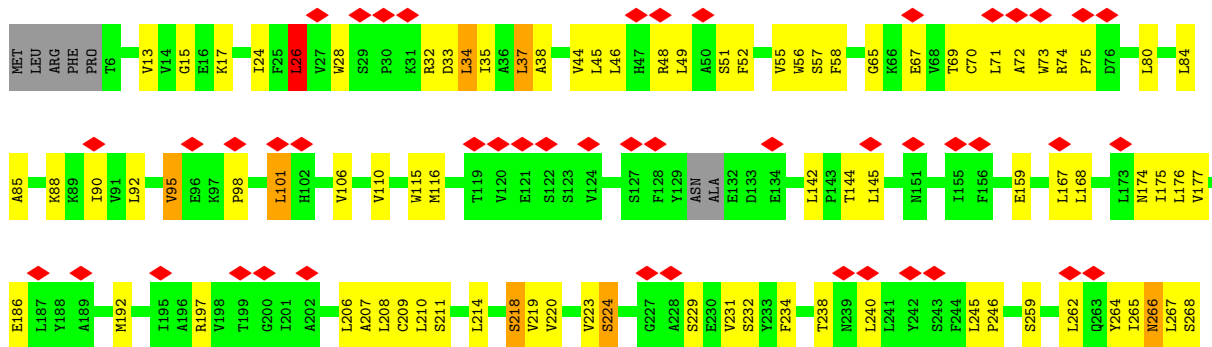
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

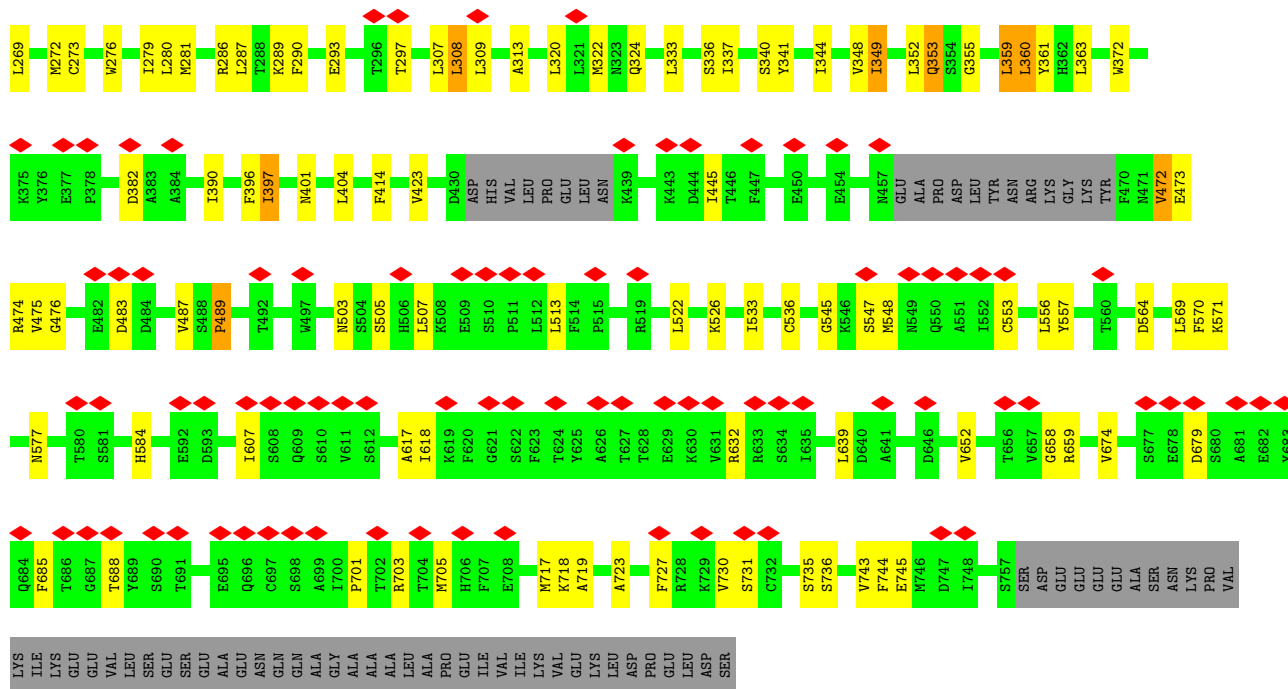


• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

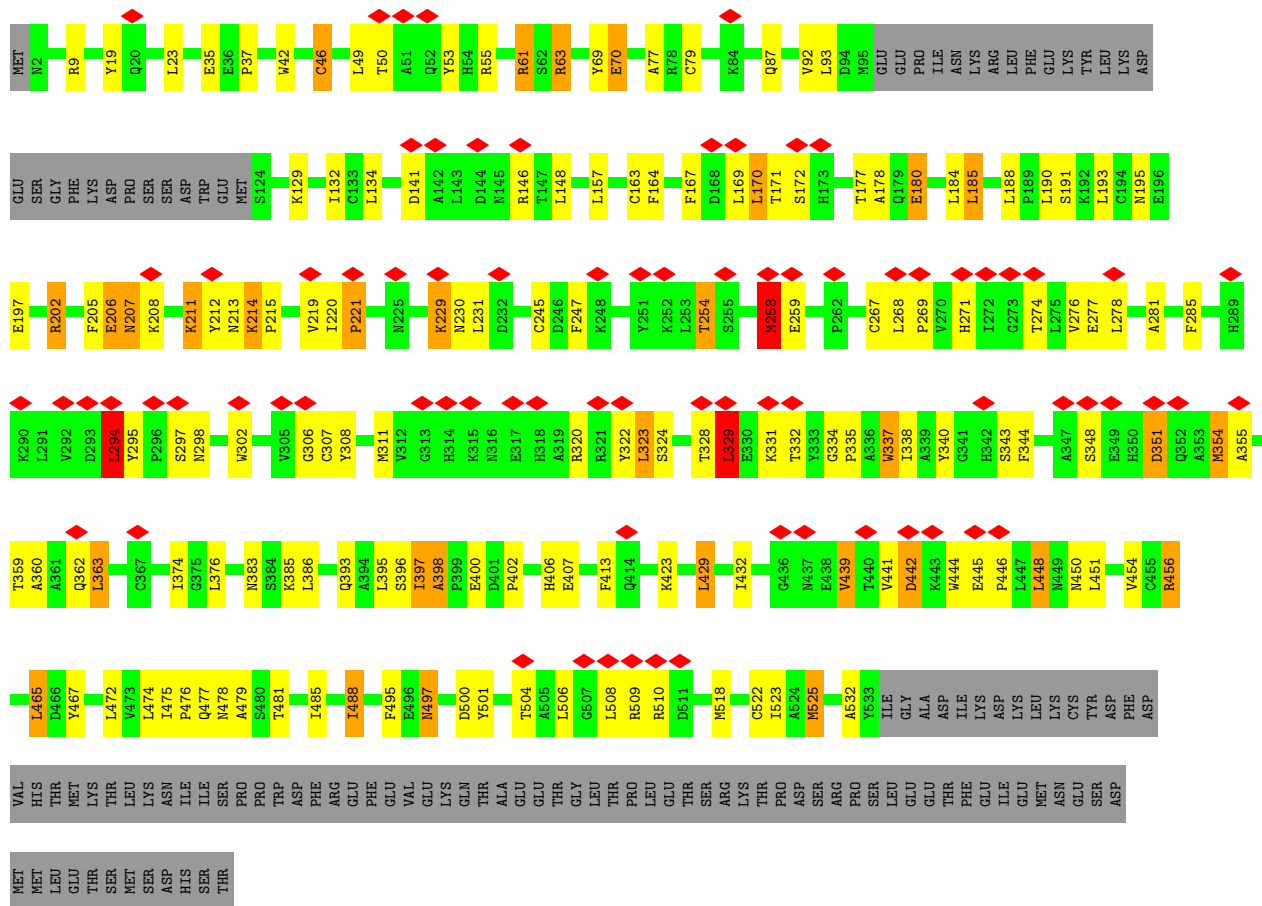


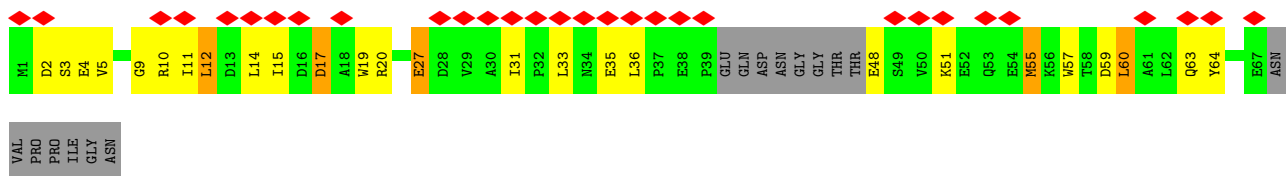
• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4



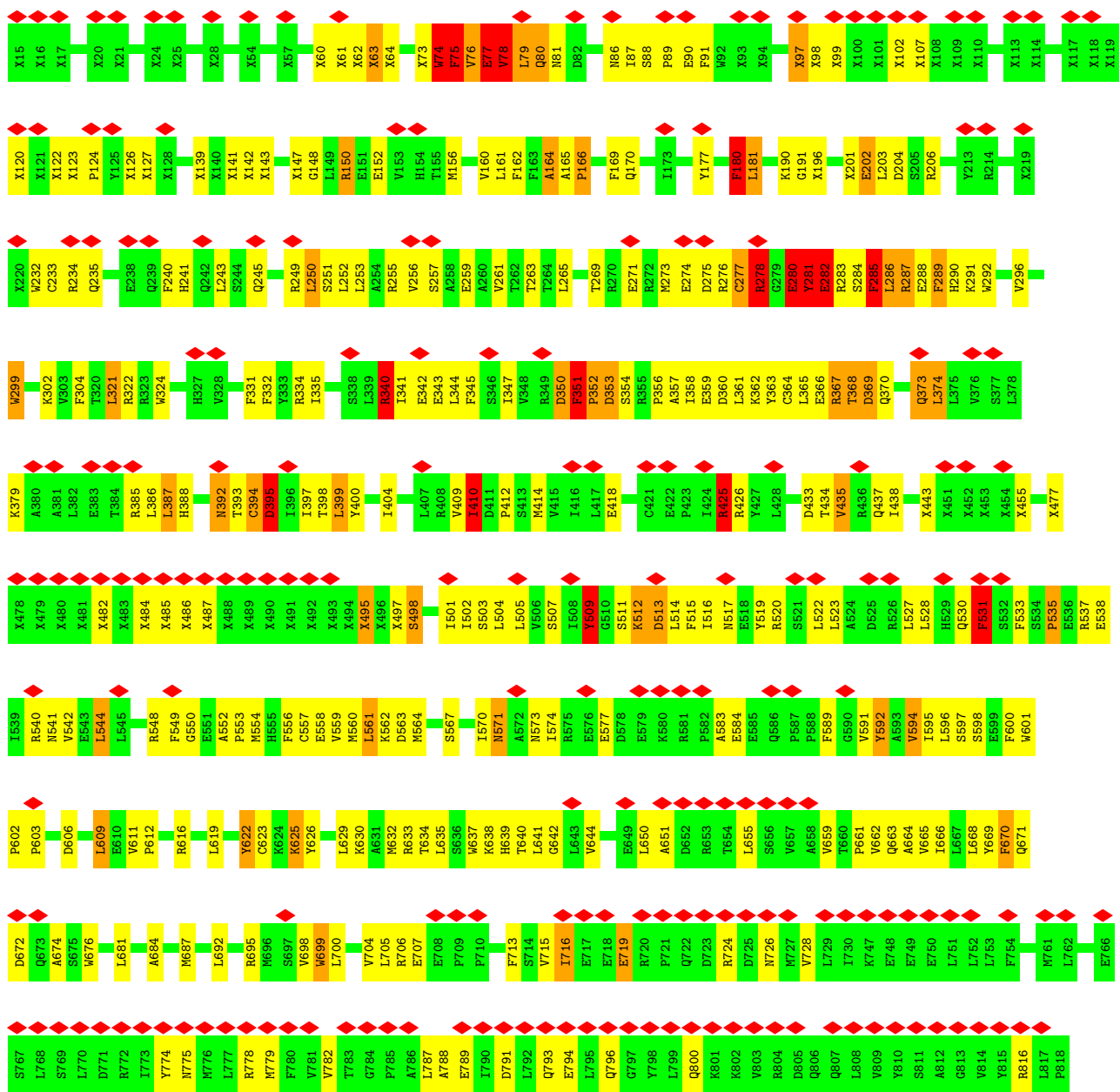


● Molecule 9: ANAPHASE-PROMOTING COMPLEX SUBUNIT 6





● Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

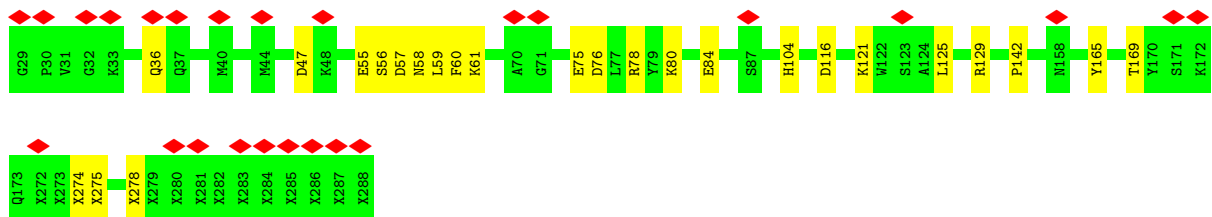
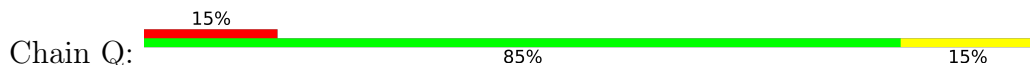


● Molecule 14: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

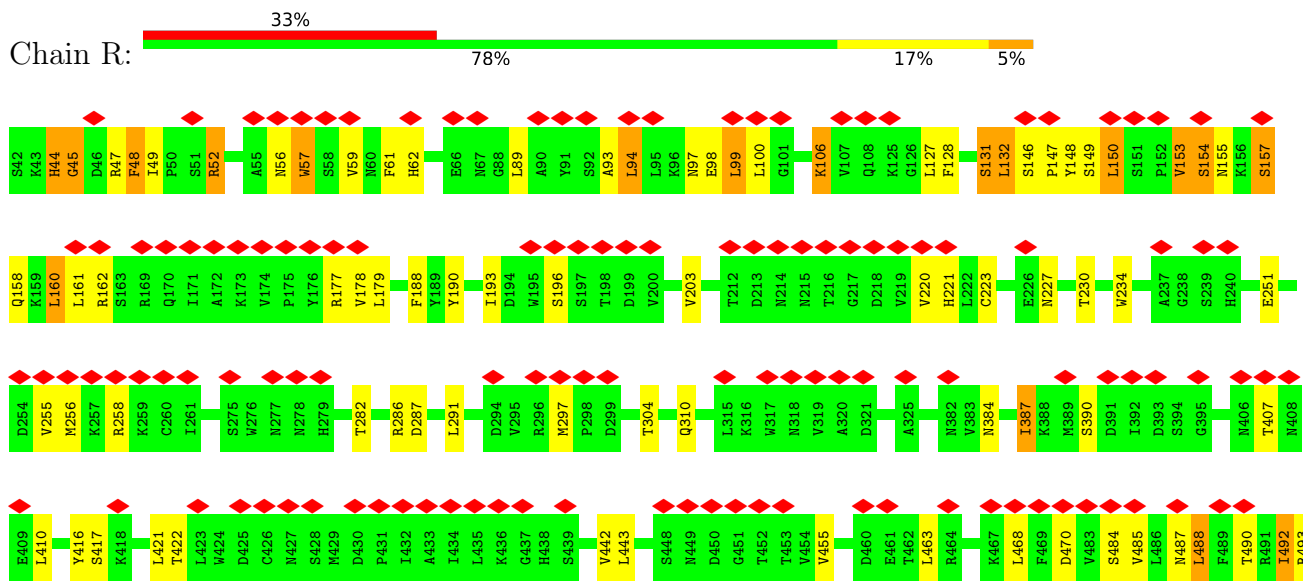




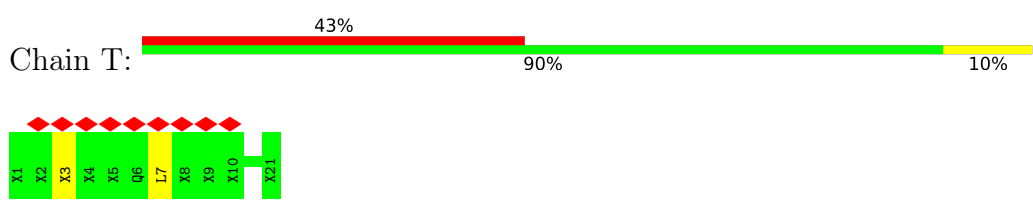
● Molecule 15: FUSION PROTEIN - UBIQUITIN-CONJUGATING ENZYME E2 C, UBIQUITIN-CONJUGATING ENZYME E2 S



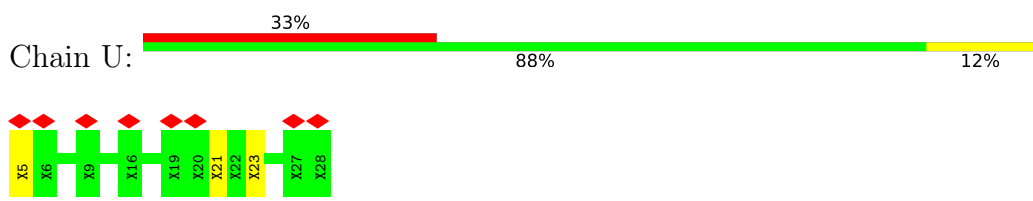
● Molecule 16: THE ANAPHASE-PROMOTING COMPLEX CHAIN R



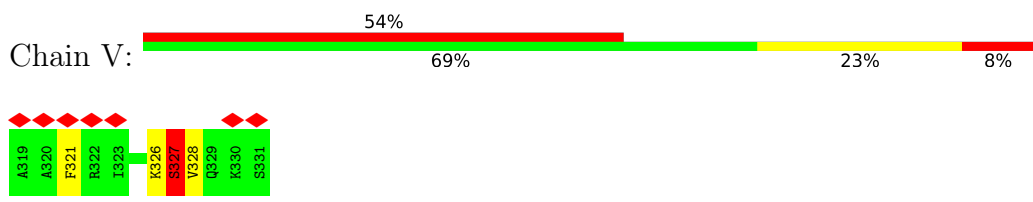
• Molecule 17: THE ANAPHASE-PROMOTING COMPLEX CHAIN T



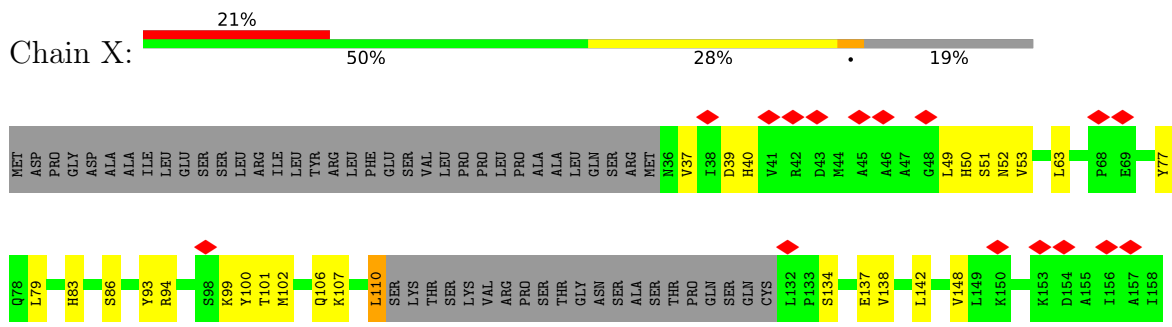
• Molecule 18: THE ANAPHASE-PROMOTING COMPLEX CHAIN U

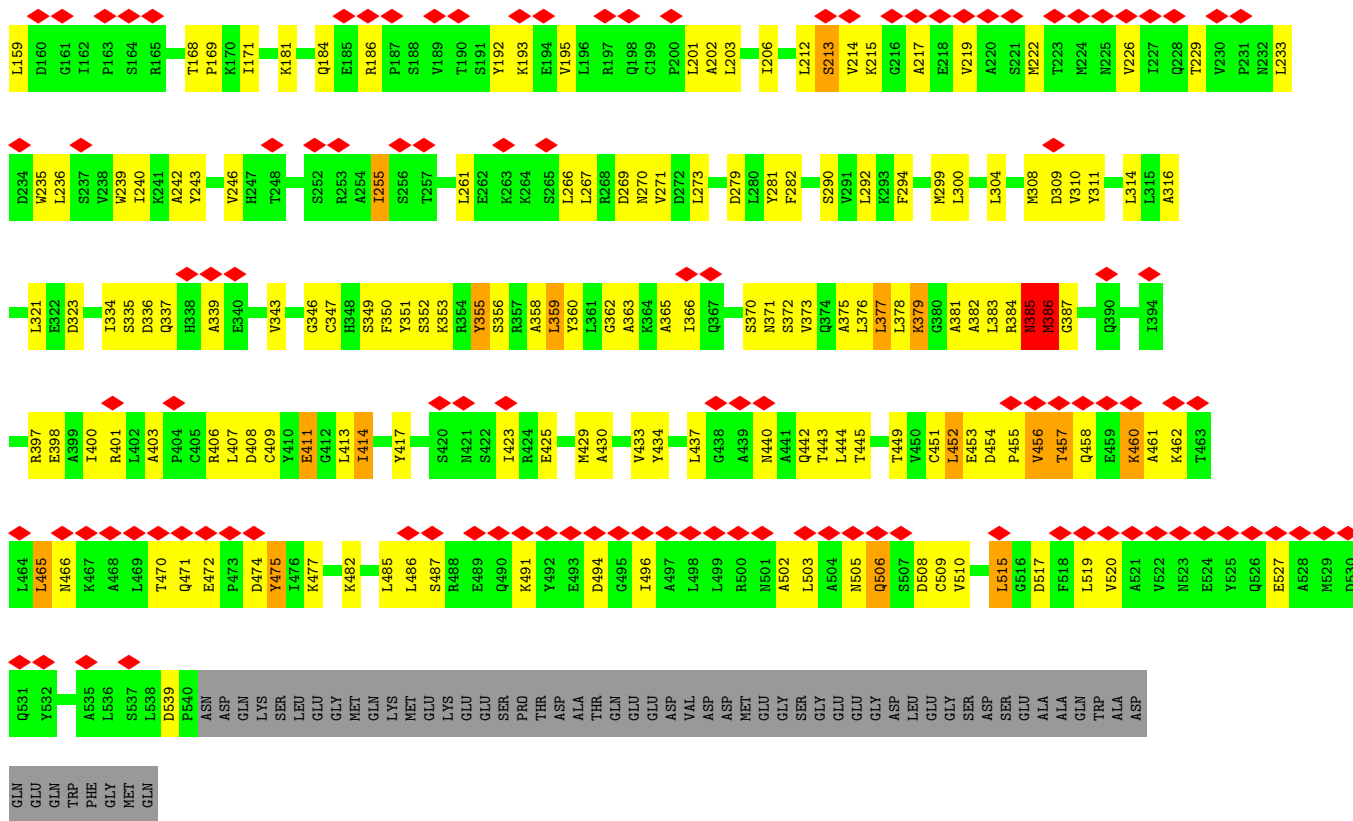


• Molecule 19: THE ANAPHASE-PROMOTING COMPLEX CHAIN V

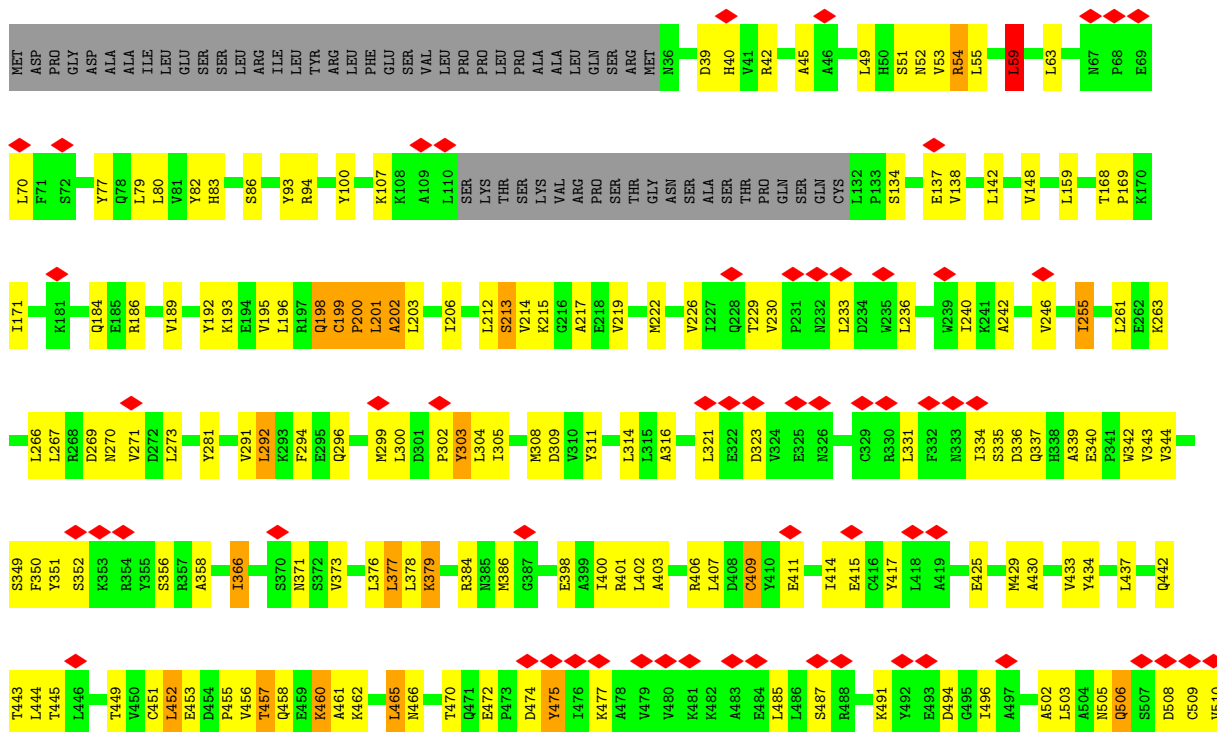


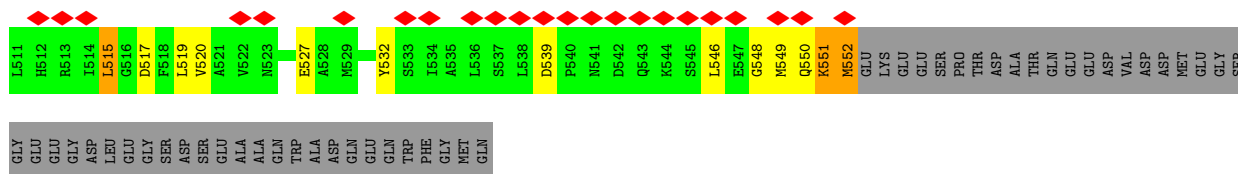
• Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7





● Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7





4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 19939 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | Not provided | |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 16 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 78000 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.397 | Depositor |
| Minimum map value | -0.133 | Depositor |
| Average map value | 0.005 | Depositor |
| Map value standard deviation | 0.023 | Depositor |
| Recommended contour level | 0.07 | Depositor |
| Map size (\AA) | 354.0, 354.0, 354.0 | wwPDB |
| Map dimensions | 200, 200, 200 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.77, 1.77, 1.77 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.75 | 0/10949 | 1.00 | 18/14903 (0.1%) |
| 2 | B | 0.52 | 0/675 | 0.85 | 1/914 (0.1%) |
| 3 | C | 0.75 | 1/4403 (0.0%) | 0.96 | 9/5945 (0.2%) |
| 3 | P | 0.70 | 2/4137 (0.0%) | 0.92 | 4/5587 (0.1%) |
| 4 | D | 0.70 | 0/447 | 0.98 | 1/612 (0.2%) |
| 5 | E | 0.66 | 0/459 | 0.86 | 0/619 |
| 6 | F | 0.70 | 3/4013 (0.1%) | 0.90 | 7/5428 (0.1%) |
| 6 | H | 0.70 | 2/3943 (0.1%) | 0.90 | 4/5329 (0.1%) |
| 7 | G | 0.63 | 0/212 | 1.03 | 1/281 (0.4%) |
| 7 | W | 0.65 | 0/214 | 1.01 | 0/284 |
| 8 | I | 0.58 | 0/5827 | 0.85 | 3/7899 (0.0%) |
| 9 | J | 0.75 | 3/4146 (0.1%) | 0.97 | 8/5615 (0.1%) |
| 10 | K | 0.89 | 3/4086 (0.1%) | 0.96 | 5/5532 (0.1%) |
| 11 | L | 0.71 | 0/1468 | 0.96 | 5/1993 (0.3%) |
| 12 | M | 0.73 | 0/502 | 1.05 | 1/680 (0.1%) |
| 13 | N | 0.60 | 1/4885 (0.0%) | 0.96 | 8/6596 (0.1%) |
| 14 | O | 0.73 | 5/5494 (0.1%) | 0.97 | 5/7425 (0.1%) |
| 15 | Q | 0.59 | 0/1174 | 0.69 | 0/1601 |
| 16 | R | 0.61 | 0/3052 | 0.85 | 2/4139 (0.0%) |
| 17 | T | 0.84 | 0/13 | 0.99 | 0/16 |
| 19 | V | 0.65 | 0/99 | 0.91 | 0/130 |
| 20 | X | 0.60 | 4/3830 (0.1%) | 0.84 | 6/5187 (0.1%) |
| 20 | Y | 0.54 | 0/3925 | 0.85 | 4/5311 (0.1%) |
| All | All | 0.70 | 24/67953 (0.0%) | 0.93 | 92/92026 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 9 |
| 8 | I | 0 | 2 |
| 9 | J | 0 | 1 |
| 13 | N | 0 | 28 |
| 16 | R | 0 | 2 |
| 17 | T | 0 | 1 |
| 20 | X | 0 | 1 |
| All | All | 0 | 44 |

The worst 5 of 24 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10 | K | 229 | LYS | CB-CG | 33.03 | 2.41 | 1.52 |
| 20 | X | 385 | ASN | N-CA | 9.74 | 1.65 | 1.46 |
| 9 | J | 302 | TRP | CB-CG | -9.04 | 1.33 | 1.50 |
| 20 | X | 355 | TYR | CE1-CZ | 8.78 | 1.50 | 1.38 |
| 9 | J | 337 | TRP | CB-CG | -8.44 | 1.35 | 1.50 |

The worst 5 of 92 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | A | 1540 | ARG | NE-CZ-NH1 | 16.30 | 128.45 | 120.30 |
| 10 | K | 229 | LYS | CA-CB-CG | -13.30 | 84.15 | 113.40 |
| 20 | X | 379 | LYS | CD-CE-NZ | 10.58 | 136.04 | 111.70 |
| 13 | N | 425 | ARG | NE-CZ-NH1 | 9.72 | 125.16 | 120.30 |
| 20 | Y | 379 | LYS | CD-CE-NZ | 9.03 | 132.47 | 111.70 |

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 11 | MET | Peptide |
| 1 | A | 124 | GLN | Peptide |
| 1 | A | 14 | ALA | Peptide |
| 1 | A | 83 | ILE | Peptide |
| 1 | A | 86 | ASP | 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 | 10950 | 0 | 10677 | 405 | 0 |
| 2 | B | 650 | 0 | 598 | 120 | 0 |
| 3 | C | 4305 | 0 | 4273 | 122 | 0 |
| 3 | P | 4042 | 0 | 3998 | 138 | 0 |
| 4 | D | 437 | 0 | 396 | 14 | 0 |
| 5 | E | 450 | 0 | 435 | 12 | 0 |
| 6 | F | 3923 | 0 | 3813 | 90 | 0 |
| 6 | H | 3853 | 0 | 3788 | 99 | 0 |
| 7 | G | 211 | 0 | 220 | 2 | 0 |
| 7 | W | 213 | 0 | 220 | 8 | 0 |
| 8 | I | 5709 | 0 | 5597 | 123 | 0 |
| 9 | J | 4047 | 0 | 3962 | 126 | 0 |
| 10 | K | 3988 | 0 | 3917 | 124 | 0 |
| 11 | L | 1435 | 0 | 1382 | 61 | 0 |
| 12 | M | 493 | 0 | 469 | 28 | 0 |
| 13 | N | 5400 | 0 | 4967 | 426 | 0 |
| 14 | O | 5396 | 0 | 5425 | 162 | 0 |
| 15 | Q | 1227 | 0 | 1128 | 27 | 0 |
| 16 | R | 2990 | 0 | 2913 | 62 | 0 |
| 17 | T | 109 | 0 | 32 | 3 | 0 |
| 18 | U | 120 | 0 | 27 | 2 | 0 |
| 19 | V | 99 | 0 | 111 | 1 | 0 |
| 20 | X | 3770 | 0 | 3829 | 254 | 0 |
| 20 | Y | 3865 | 0 | 3925 | 159 | 0 |
| 21 | B | 3 | 0 | 0 | 0 | 0 |
| All | All | 67685 | 0 | 66102 | 2317 | 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 17.

The worst 5 of 2317 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) |
|------------------|-------------------|--------------------------|-------------------|
| 13:N:435:VAL:CG1 | 13:N:515:PHE:CE2 | 1.81 | 1.63 |
| 1:A:1114:ARG:HE | 13:N:779:MET:CG | 1.13 | 1.57 |
| 2:B:14:TRP:CH2 | 2:B:41:GLY:N | 1.73 | 1.54 |
| 13:N:502:ILE:CG1 | 13:N:548:ARG:HH12 | 1.21 | 1.50 |
| 1:A:1116:THR:CG2 | 13:N:779:MET:CE | 1.87 | 1.49 |

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 | 1354/1441 (94%) | 1217 (90%) | 106 (8%) | 31 (2%) | 6 | 37 |
| 2 | B | 83/84 (99%) | 69 (83%) | 8 (10%) | 6 (7%) | 1 | 16 |
| 3 | C | 520/597 (87%) | 495 (95%) | 23 (4%) | 2 (0%) | 34 | 72 |
| 3 | P | 485/597 (81%) | 459 (95%) | 25 (5%) | 1 (0%) | 47 | 81 |
| 4 | D | 53/121 (44%) | 46 (87%) | 6 (11%) | 1 (2%) | 8 | 41 |
| 5 | E | 54/110 (49%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 6 | F | 494/824 (60%) | 477 (97%) | 11 (2%) | 6 (1%) | 13 | 50 |
| 6 | H | 479/824 (58%) | 462 (96%) | 12 (2%) | 5 (1%) | 15 | 54 |
| 7 | G | 23/85 (27%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 7 | W | 23/85 (27%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 8 | I | 722/808 (89%) | 690 (96%) | 28 (4%) | 4 (1%) | 25 | 65 |
| 9 | J | 500/620 (81%) | 467 (93%) | 28 (6%) | 5 (1%) | 15 | 54 |
| 10 | K | 489/620 (79%) | 458 (94%) | 26 (5%) | 5 (1%) | 15 | 54 |
| 11 | L | 180/185 (97%) | 169 (94%) | 9 (5%) | 2 (1%) | 14 | 52 |
| 12 | M | 55/74 (74%) | 46 (84%) | 9 (16%) | 0 | 100 | 100 |
| 13 | N | 572/703 (81%) | 501 (88%) | 33 (6%) | 38 (7%) | 1 | 18 |
| 14 | O | 677/755 (90%) | 645 (95%) | 24 (4%) | 8 (1%) | 13 | 50 |
| 15 | Q | 144/162 (89%) | 139 (96%) | 5 (4%) | 0 | 100 | 100 |
| 16 | R | 374/386 (97%) | 334 (89%) | 35 (9%) | 5 (1%) | 12 | 48 |
| 17 | T | 2/21 (10%) | 2 (100%) | 0 | 0 | 100 | 100 |
| 19 | V | 11/13 (85%) | 8 (73%) | 1 (9%) | 2 (18%) | 0 | 2 |
| 20 | X | 480/599 (80%) | 462 (96%) | 15 (3%) | 3 (1%) | 25 | 65 |
| 20 | Y | 492/599 (82%) | 471 (96%) | 16 (3%) | 5 (1%) | 15 | 54 |
| All | All | 8266/10313 (80%) | 7717 (93%) | 420 (5%) | 129 (2%) | 13 | 45 |

5 of 129 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 274 | VAL |
| 1 | A | 630 | PRO |
| 1 | A | 857 | ALA |
| 1 | A | 860 | TYR |
| 1 | A | 1125 | ILE |

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 | 1150/1206 (95%) | 988 (86%) | 162 (14%) | 3 | 19 |
| 2 | B | 65/75 (87%) | 54 (83%) | 11 (17%) | 2 | 13 |
| 3 | C | 452/520 (87%) | 399 (88%) | 53 (12%) | 5 | 23 |
| 3 | P | 422/520 (81%) | 373 (88%) | 49 (12%) | 5 | 24 |
| 4 | D | 46/115 (40%) | 41 (89%) | 5 (11%) | 6 | 26 |
| 5 | E | 47/89 (53%) | 37 (79%) | 10 (21%) | 1 | 7 |
| 6 | F | 407/729 (56%) | 367 (90%) | 40 (10%) | 8 | 29 |
| 6 | H | 408/729 (56%) | 372 (91%) | 36 (9%) | 10 | 34 |
| 7 | G | 22/77 (29%) | 20 (91%) | 2 (9%) | 9 | 32 |
| 7 | W | 23/77 (30%) | 22 (96%) | 1 (4%) | 29 | 55 |
| 8 | I | 620/730 (85%) | 572 (92%) | 48 (8%) | 13 | 39 |
| 9 | J | 424/546 (78%) | 368 (87%) | 56 (13%) | 4 | 20 |
| 10 | K | 423/549 (77%) | 380 (90%) | 43 (10%) | 7 | 28 |
| 11 | L | 155/170 (91%) | 140 (90%) | 15 (10%) | 8 | 29 |
| 12 | M | 55/67 (82%) | 44 (80%) | 11 (20%) | 1 | 8 |
| 13 | N | 516/526 (98%) | 459 (89%) | 57 (11%) | 6 | 25 |
| 14 | O | 578/651 (89%) | 491 (85%) | 87 (15%) | 3 | 17 |
| 15 | Q | 122/127 (96%) | 122 (100%) | 0 | 100 | 100 |
| 16 | R | 326/334 (98%) | 295 (90%) | 31 (10%) | 8 | 30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 17 | T | 1/2 (50%) | 1 (100%) | 0 | 100 | 100 |
| 19 | V | 10/10 (100%) | 7 (70%) | 3 (30%) | 0 | 2 |
| 20 | X | 407/513 (79%) | 378 (93%) | 29 (7%) | 14 | 41 |
| 20 | Y | 418/513 (82%) | 382 (91%) | 36 (9%) | 10 | 35 |
| All | All | 7097/8875 (80%) | 6312 (89%) | 785 (11%) | 9 | 25 |

5 of 785 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | K | 510 | ARG |
| 14 | O | 280 | ARG |
| 11 | L | 113 | LEU |
| 10 | K | 497 | ASN |
| 13 | N | 379 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | P | 236 | HIS |
| 3 | P | 305 | ASN |
| 20 | X | 371 | ASN |
| 6 | H | 545 | HIS |
| 6 | H | 480 | ASN |

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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 | A | 20 |
| 13 | N | 10 |
| 16 | R | 5 |
| 15 | Q | 1 |

The worst 5 of 36 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | Q | 173:GLN | C | 272:UNK | N | 71.87 |
| 1 | A | 986:ALA | C | 1013:ASP | N | 34.04 |
| 1 | N | 730:ILE | C | 747:LYS | N | 25.53 |
| 1 | N | 458:UNK | C | 476:UNK | N | 22.96 |
| 1 | R | 132:LEU | C | 146:SER | N | 22.90 |

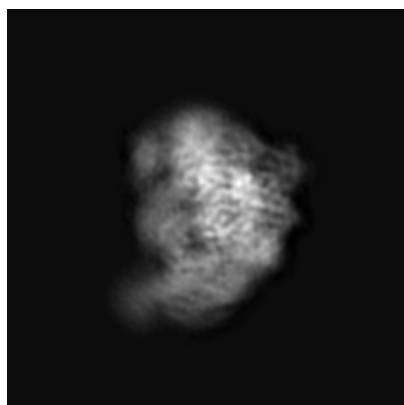
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2925. These allow visual inspection of the internal detail of the map and identification of artifacts.

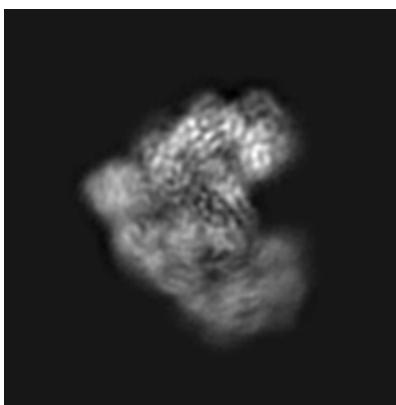
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

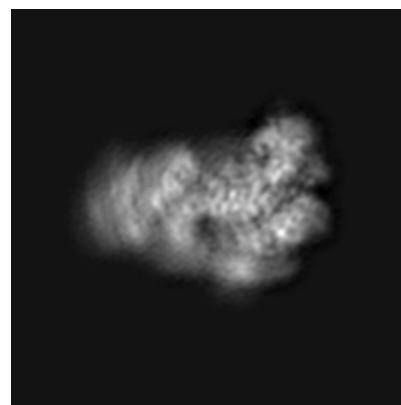
6.1.1 Primary map



X



Y



Z

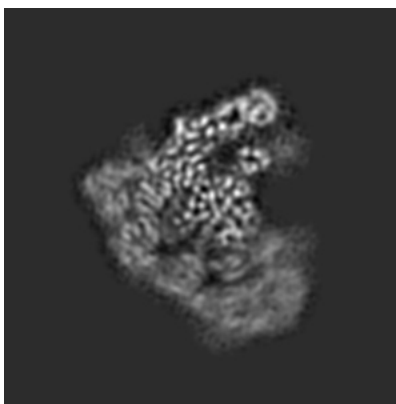
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

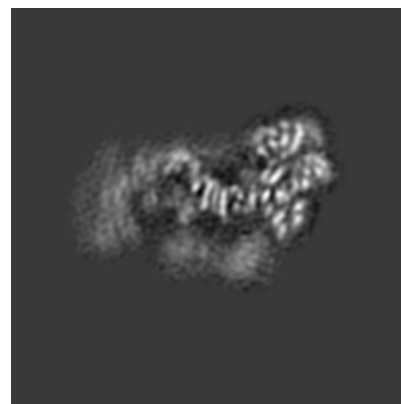
6.2.1 Primary map



X Index: 100



Y Index: 100

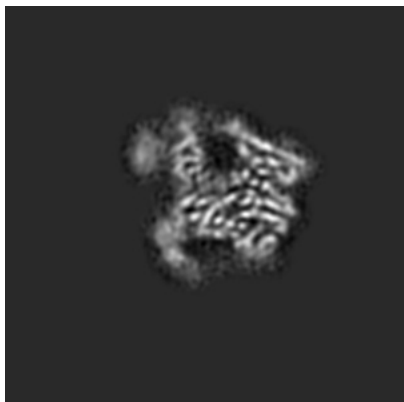


Z Index: 100

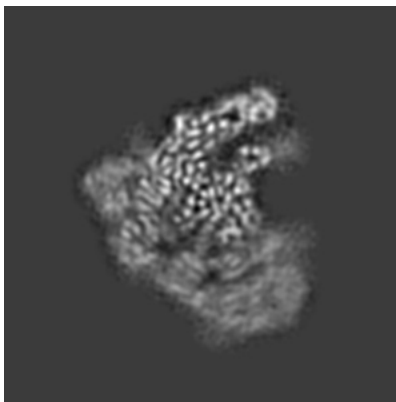
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

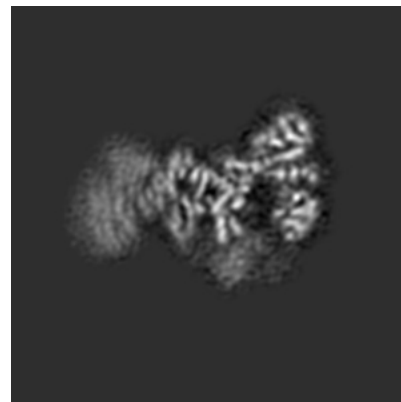
6.3.1 Primary map



X Index: 136



Y Index: 101



Z Index: 112

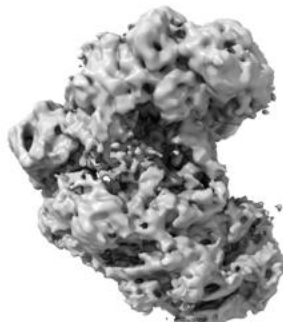
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

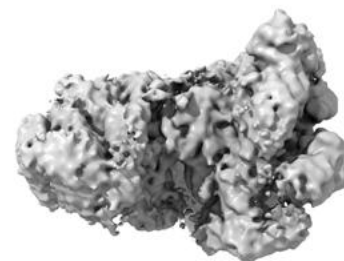
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

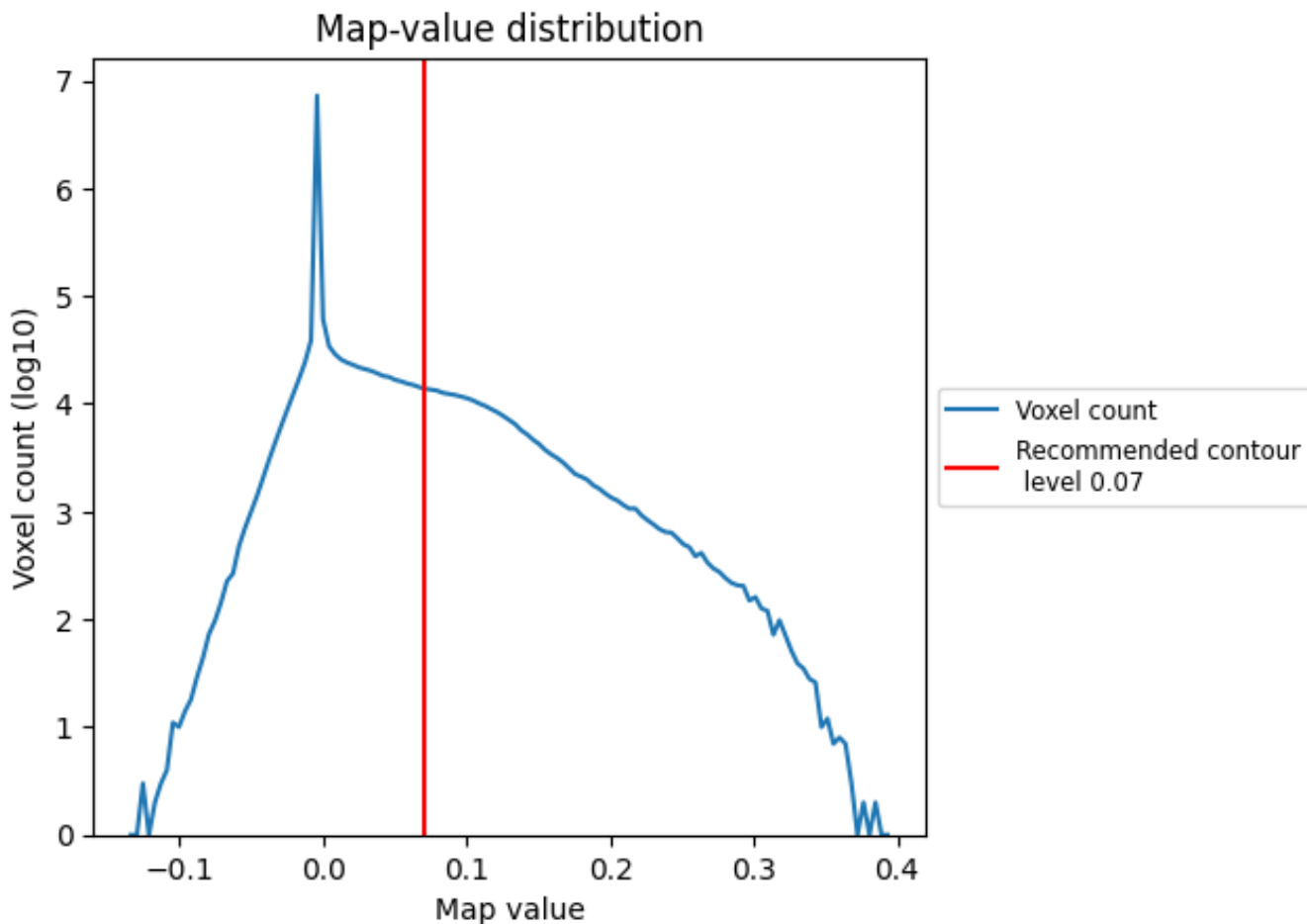
6.5 Mask visualisation

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

7 Map analysis [i](#)

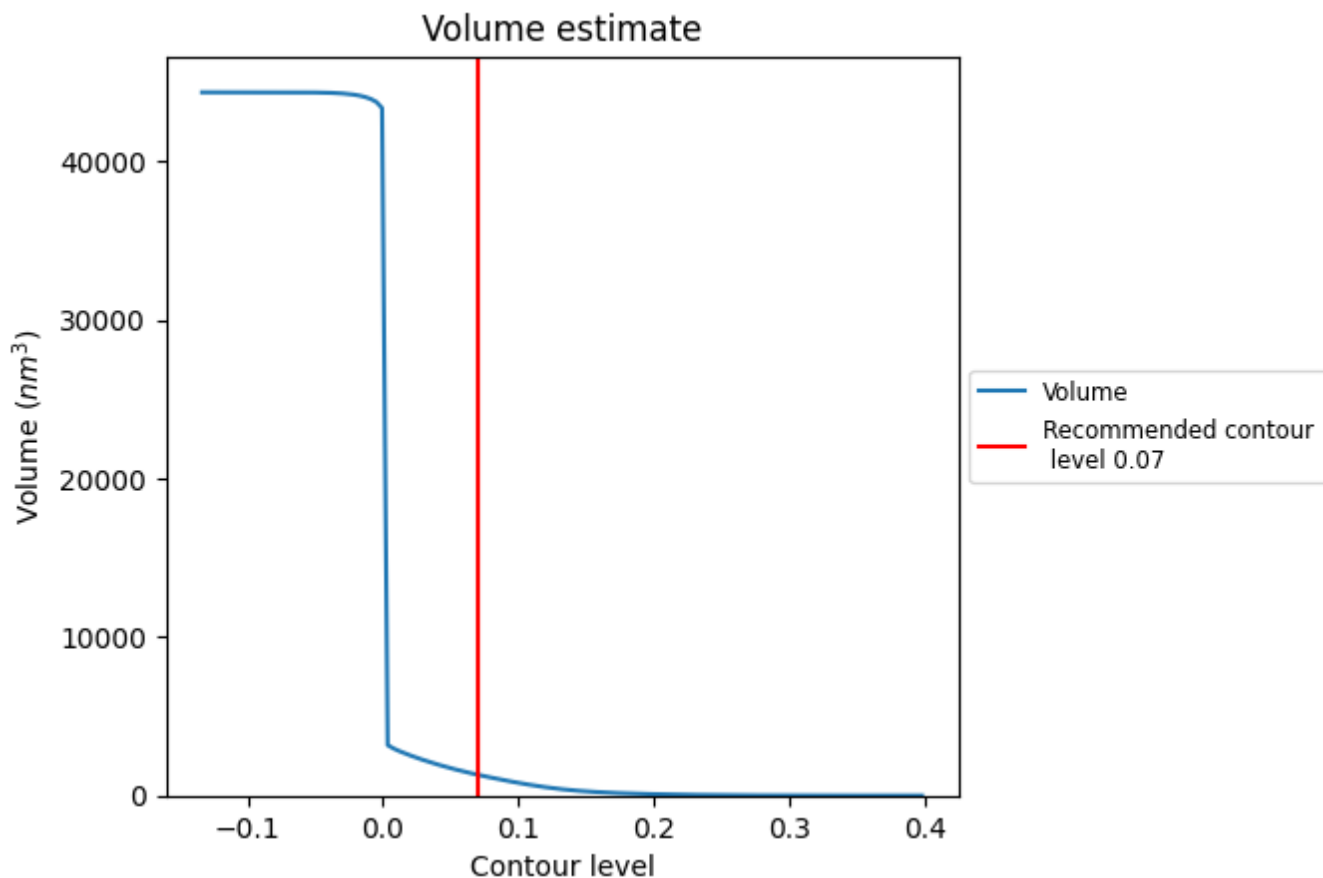
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

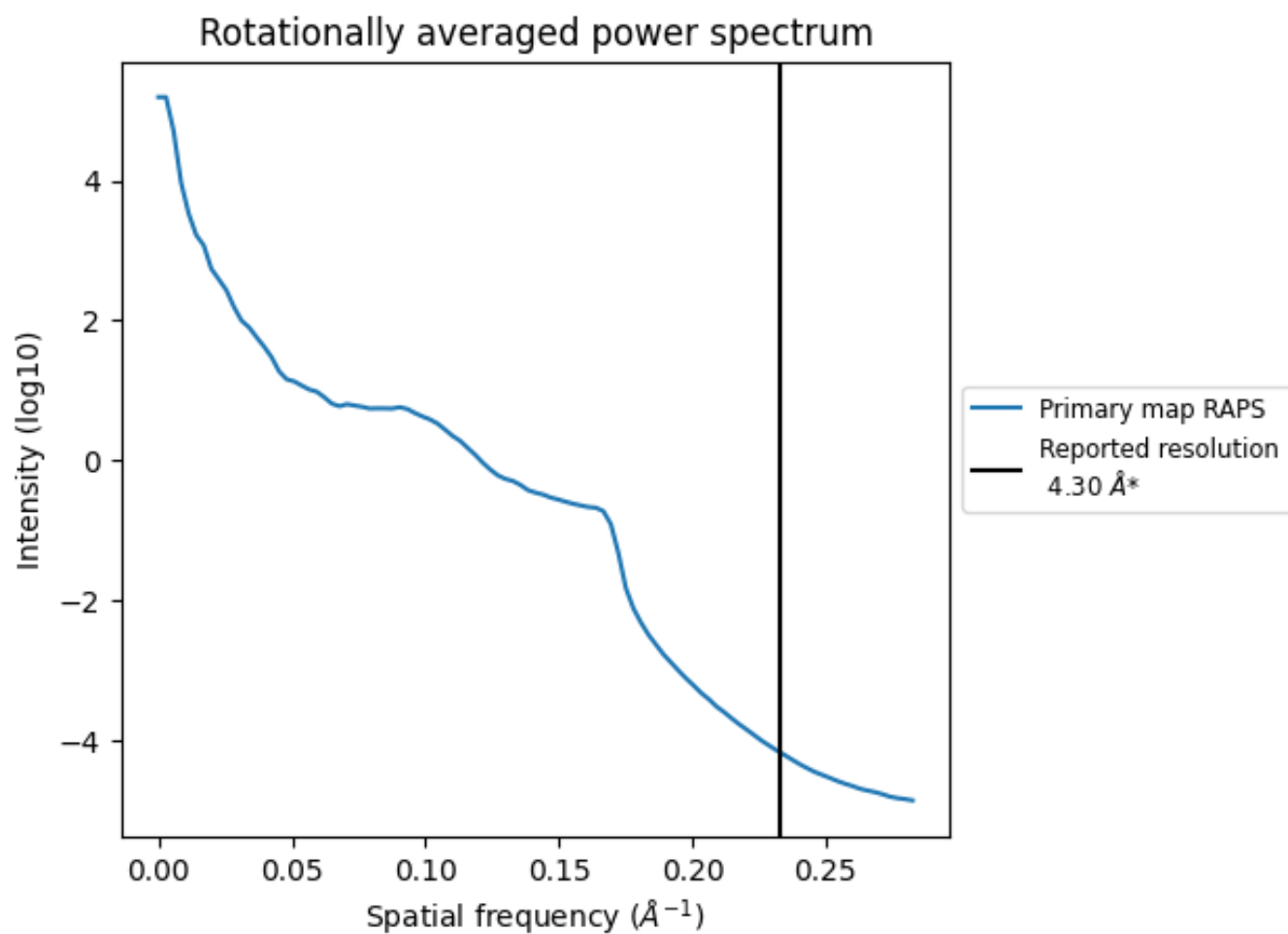
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1309 nm³; this corresponds to an approximate mass of 1182 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 0.233 Å⁻¹

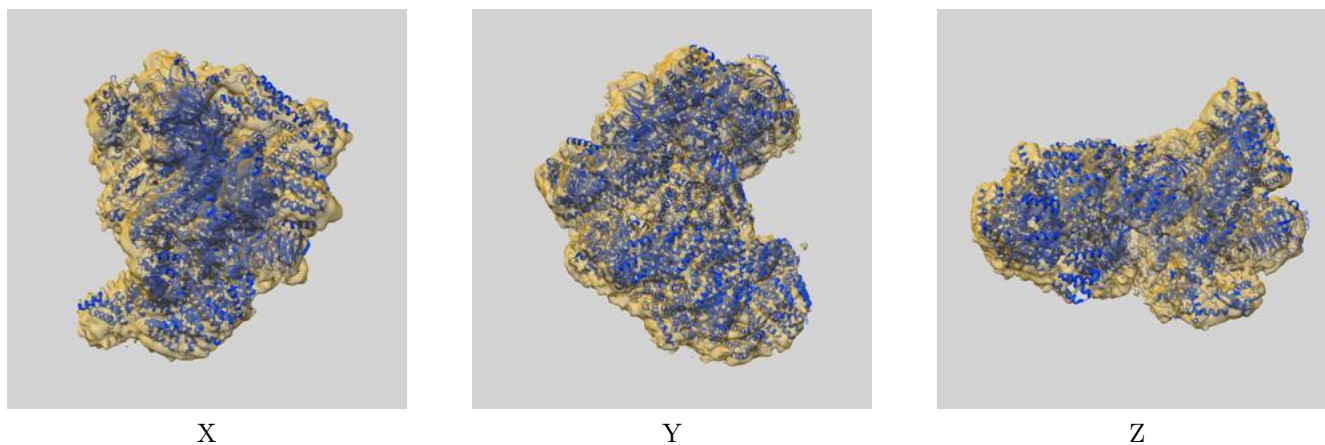
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

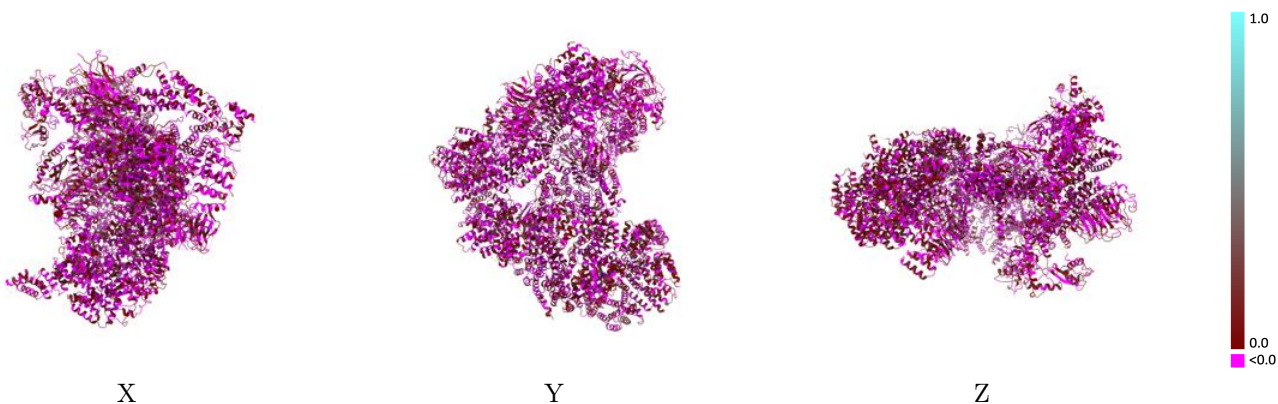
This section contains information regarding the fit between EMDB map EMD-2925 and PDB model 5A31. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



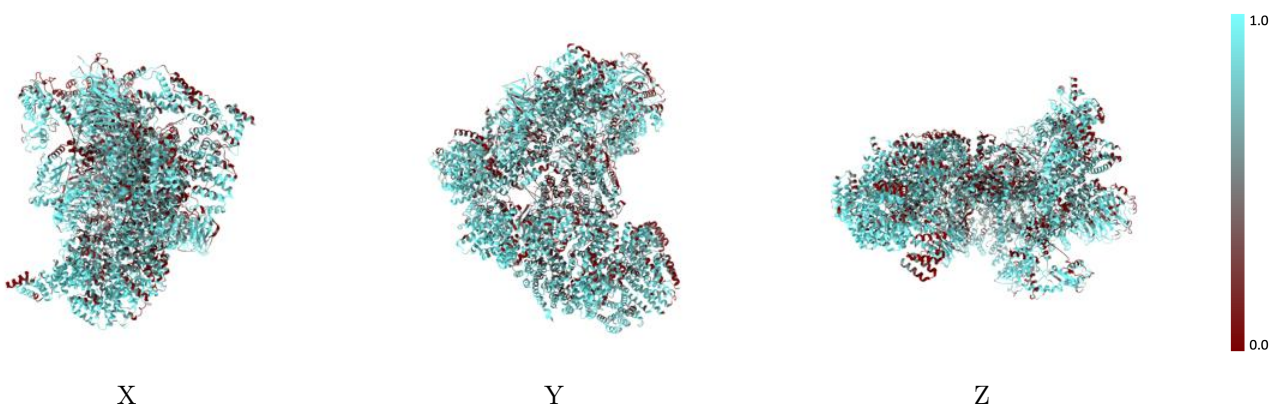
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



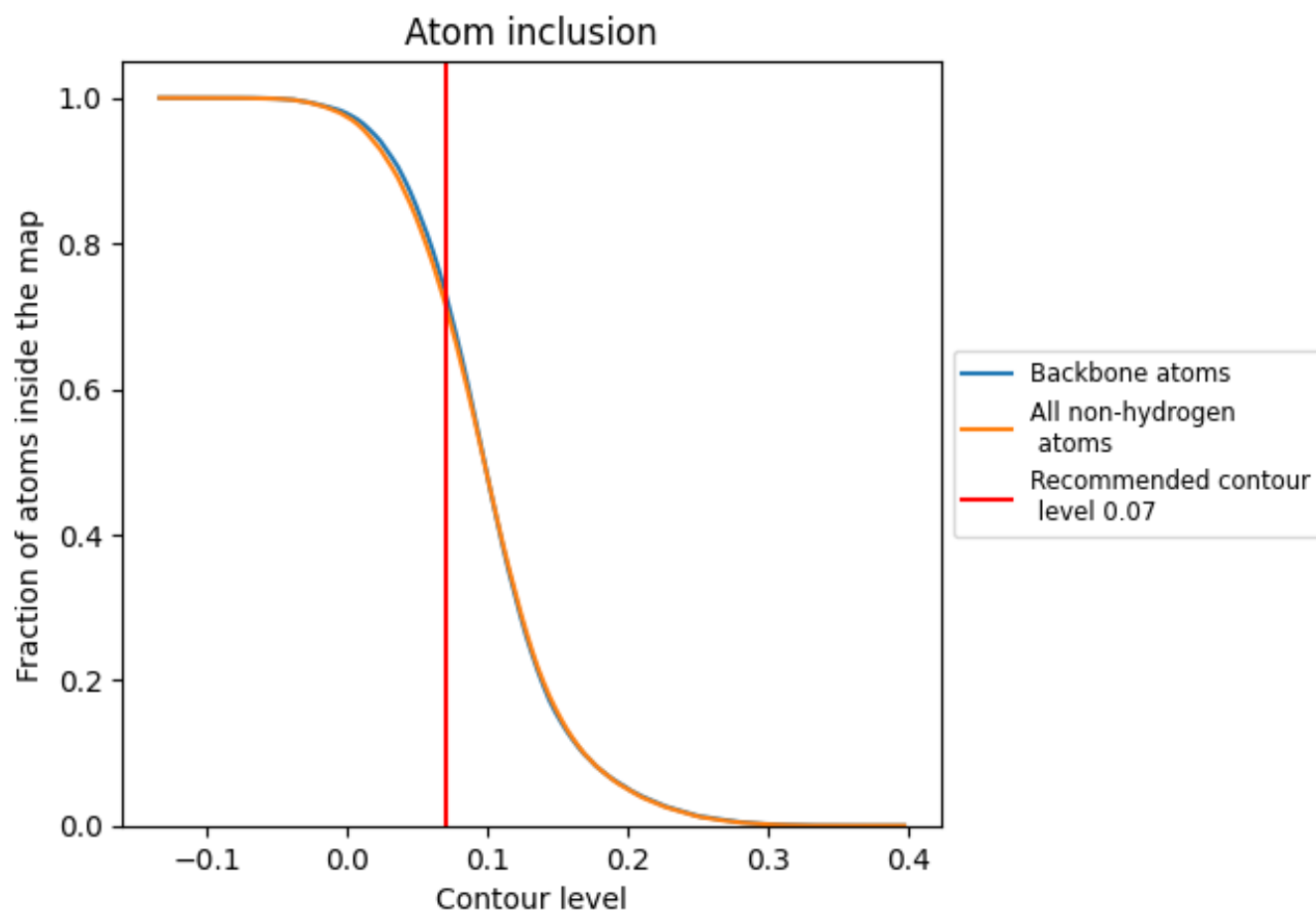
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.07).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% 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 (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|---|
| All |  0.7182 |  0.0070 |
| A |  0.6672 |  -0.0150 |
| B |  0.8150 |  0.0470 |
| C |  0.6676 |  -0.0110 |
| D |  0.6019 |  0.0420 |
| E |  0.6104 |  0.0040 |
| F |  0.7774 |  -0.0020 |
| G |  0.5665 |  -0.0150 |
| H |  0.7160 |  0.0300 |
| I |  0.7467 |  0.0370 |
| J |  0.7996 |  -0.0120 |
| K |  0.7544 |  0.0240 |
| L |  0.6690 |  0.0160 |
| M |  0.4555 |  -0.0260 |
| N |  0.6779 |  -0.0050 |
| O |  0.7117 |  0.0230 |
| P |  0.8138 |  -0.0260 |
| Q |  0.8292 |  0.0480 |
| R |  0.6395 |  -0.0080 |
| T |  0.5321 |  -0.0430 |
| U |  0.6500 |  -0.0220 |
| V |  0.5052 |  0.0200 |
| W |  0.7707 |  0.0460 |
| X |  0.6952 |  0.0350 |
| Y |  0.7888 |  0.0250 |

