# wwPDB EM Validation Summary Report (i)

May 1, 2024 – 02:20 am BST

| | | |
|---|---|---|
| PDB ID | : | 4UI9 |
| EMDB ID | : | EMD-2924 |
| Title | : | Atomic structure of the human Anaphase-Promoting Complex |
| Authors | : | Chang, L.; Zhang, Z.; Yang, J.; McLaughlin, S.H.; Barford, D. |
| Deposited on | : | 2015-03-27 |
| Resolution | : | 3.60 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 (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:

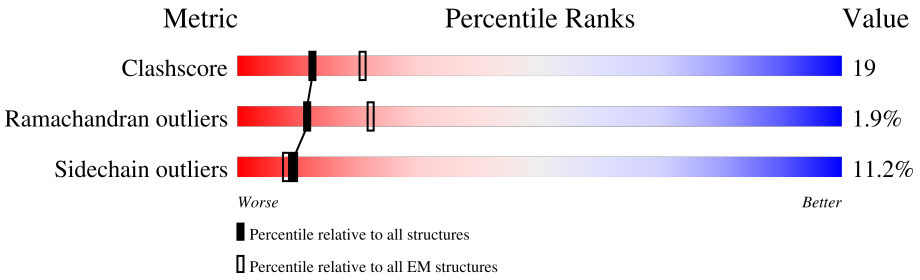
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 3.60 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%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1944 | 45% 25% • 26% |
| 2 | B | 84 | 64% 25% 8% • |
| 3 | C | 591 | 61% 24% • • 11% |
| 3 | P | 591 | 58% 21% • 17% |
| 4 | D | 121 | 33% 12% • 55% |
| 5 | E | 110 | 35% 15% • 49% |
| 6 | F | 824 | 43% 15% • 40% |
| 6 | H | 824 | 42% 14% • 41% |
| 7 | G | 85 | 25% • • 71% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | I | 808 | 67% 21% 10% |
| 9 | J | 620 | 55% 21% 5% 19% |
| 10 | K | 620 | 54% 22% 20% |
| 11 | L | 183 | 62% 32% 5% |
| 12 | M | 74 | 45% 28% 7% 20% |
| 13 | N | 822 | 40% 28% 7% 23% |
| 14 | O | 756 | 60% 25% 6% 9% |
| 15 | R | 493 | 37% 32% 8% 22% |
| 16 | S | 447 | 14% 6% 79% |
| 17 | T | 21 | 71% 19% 10% |
| 18 | U | 24 | 75% 25% |
| 19 | W | 85 | 21% 7% 71% |
| 20 | X | 565 | 53% 29% 14% |
| 20 | Y | 565 | 56% 27% 12% |

# 2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 66453 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 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1441 | Total | C | N | O | S | 0 | 0 |
| | | | 10947 | 7043 | 1853 | 1977 | 74 | | |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 291 | PHE | THR | conflict | UNP Q9H1A4 |
| A | 940 | ILE | THR | conflict | UNP Q9H1A4 |
| A | 1059 | GLU | ASP | conflict | UNP Q9H1A4 |
| A | 1358 | LEU | ILE | conflict | UNP Q9H1A4 |
| A | 1637 | LEU | THR | conflict | UNP Q9H1A4 |
| A | 1880 | PRO | LEU | conflict | UNP Q9H1A4 |
| A | 1881 | LEU | GLU | conflict | UNP Q9H1A4 |

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

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

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 |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 524 | Total | C | N | O | S | 0 | 0 |
| | | | 4305 | 2774 | 726 | 781 | 24 | | |
| 3 | P | 491 | Total | C | N | O | S | 0 | 0 |
| | | | 4042 | 2611 | 678 | 729 | 24 | | |

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 |
|---|---|---|---|---|---|---|---|---|
| 4 | D | 55 | Total | C | N | O | 0 | 0 |
| | | | 437 | 277 | 73 | 87 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 5 | TYR | PHE | conflict | UNP P60006 |

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

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

- Molecule 6 is a protein called CELL DIVISION CYCLE PROTEIN 27 HOMOLOG.

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

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 403 | GLU | LYS | conflict | UNP P30260 |
| F | 475 | SER | ALA | conflict | UNP P30260 |
| F | 484 | SER | ALA | conflict | UNP P30260 |
| H | 403 | GLU | LYS | 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 |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 214 | 134 | 40 | 39 | 1 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 14 | GLU | ASP | conflict | UNP Q8NHZ8 |

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

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

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 CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

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

There are 3 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 |

- Molecule 10 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

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

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| K | 228 | GLU | GLN | conflict | UNP Q13042 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 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 |
|---|---|---|---|---|---|---|---|---|---|
| 11 | L | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1435 | 898 | 263 | 268 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| L | ? | - | GLU | deletion | UNP Q9UM13 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | N | 631 | Total | C | N | O | S | 0 | 0 |
| | | | 4831 | 3064 | 877 | 868 | 22 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| N | 410 | ILE | LEU | conflict | UNP Q9UJX6 |

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

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

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| O | 42 | SER | ASN | conflict | UNP Q9UJX4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 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 | - | insertion | UNP Q9UJX4 |

- Molecule 15 is a protein called FIZZY-RELATED PROTEIN HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | R | 387 | Total | C | N | O | S | 0 | 0 |
| | | | 3003 | 1895 | 541 | 557 | 10 | | |

- Molecule 16 is a protein called F-BOX ONLY PROTEIN 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | S | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 648 | 396 | 119 | 124 | 9 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| S | 323 | ILE | THR | conflict | UNP Q9UKT4 |
| S | 326 | LYS | ALA | conflict | UNP Q9UKT4 |

- Molecule 17 is a protein called PEPTIDE.

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

- Molecule 18 is a protein called PEPTIDE.

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

- Molecule 19 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | W | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 213 | 133 | 40 | 39 | 1 | | |

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

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

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| X | 63 | LEU | MET | conflict | UNP Q9UJX3 |
| X | 142 | LEU | MET | conflict | UNP Q9UJX3 |
| X | 148 | VAL | MET | conflict | UNP Q9UJX3 |
| X | 466 | ASN | ASP | conflict | UNP Q9UJX3 |
| X | 472 | GLU | ARG | conflict | UNP Q9UJX3 |
| Y | 63 | LEU | MET | conflict | UNP Q9UJX3 |
| Y | 142 | LEU | MET | conflict | UNP Q9UJX3 |
| Y | 148 | VAL | MET | conflict | UNP Q9UJX3 |
| Y | 466 | ASN | ASP | conflict | UNP Q9UJX3 |
| Y | 472 | GLU | ARG | conflict | UNP Q9UJX3 |

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

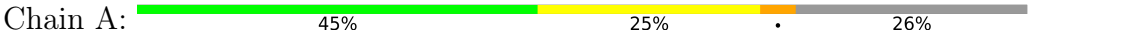
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 21 | B | 3 | Total | Zn | 0 |
| | | | 3 | 3 | |
| 21 | S | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |

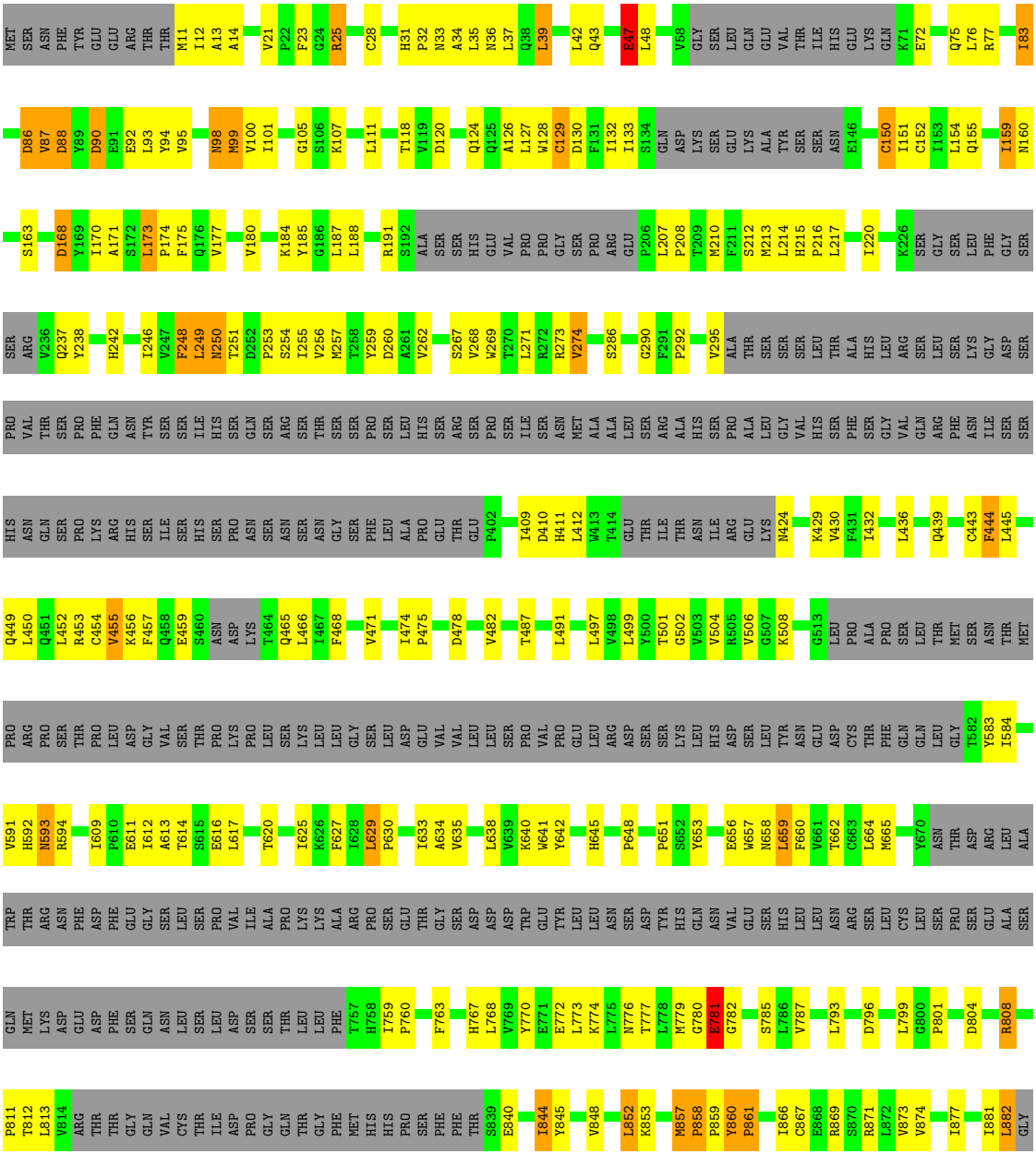
# 3 Residue-property plots (i)

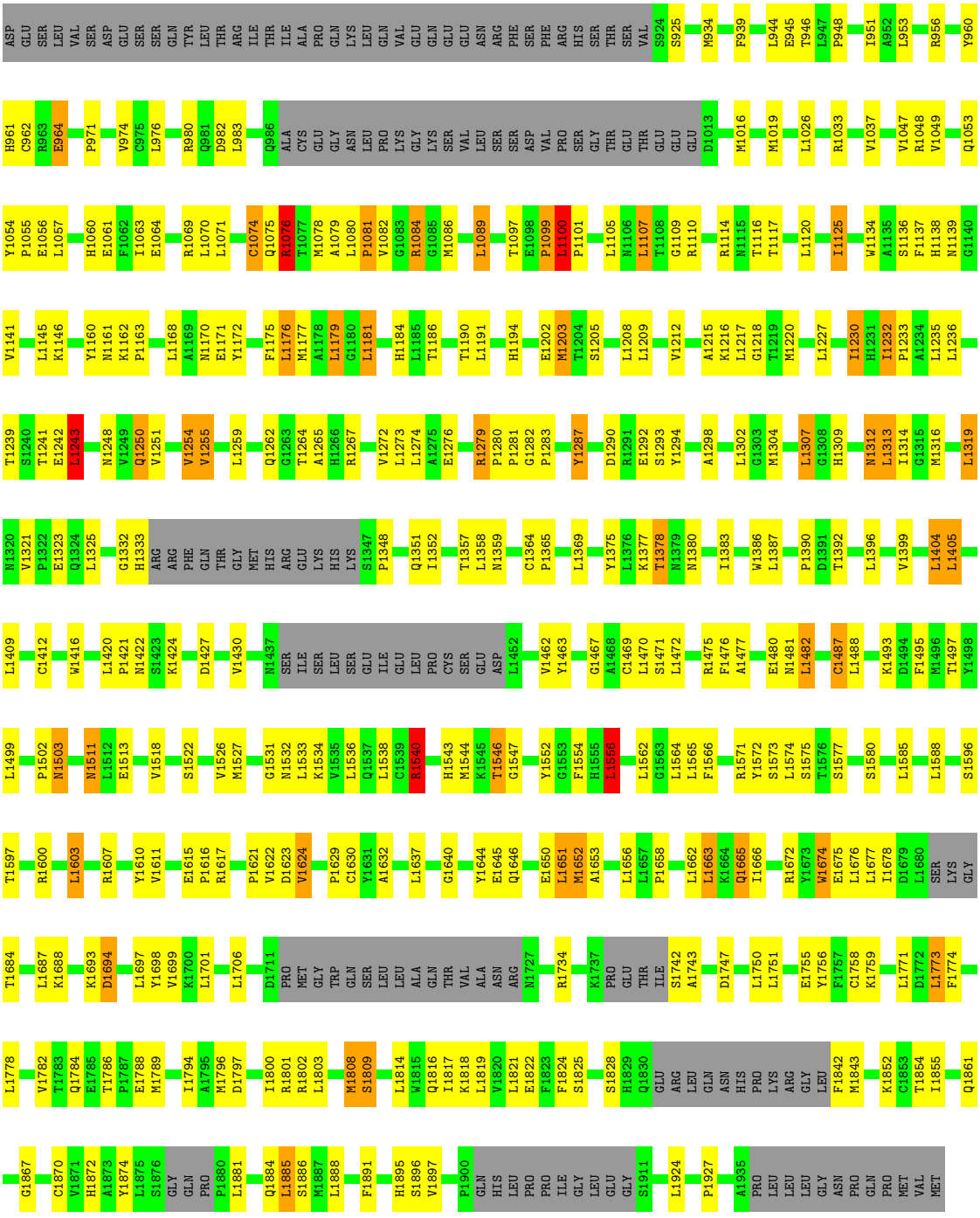
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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

Chain A:



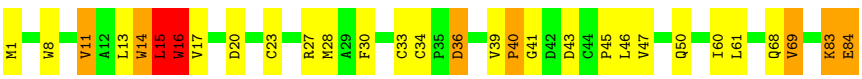





• Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

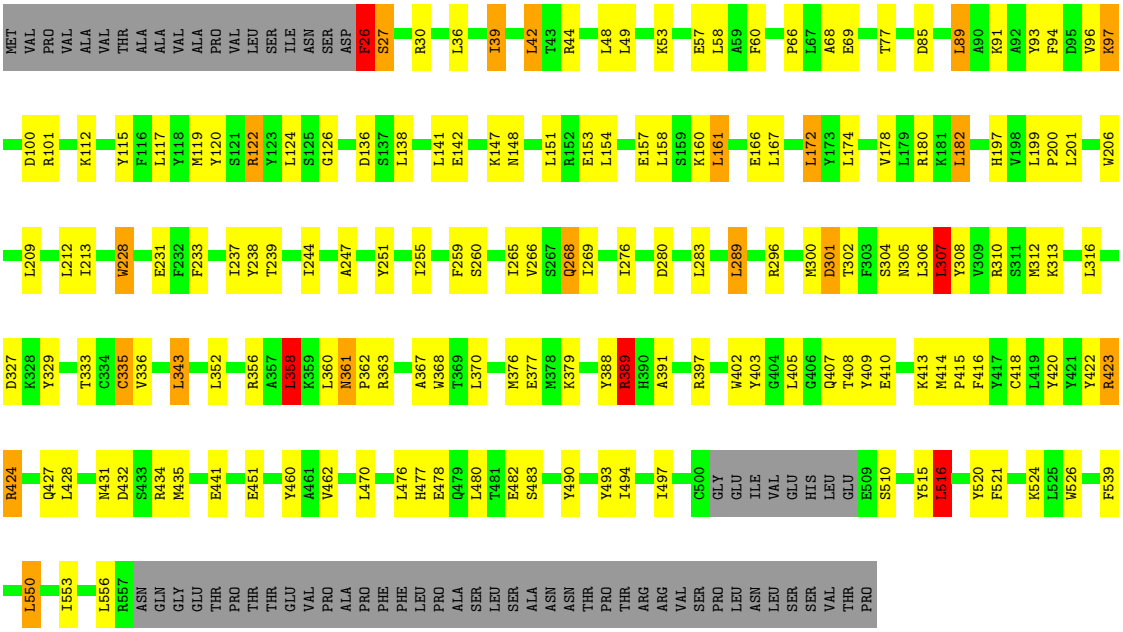
Chain B:



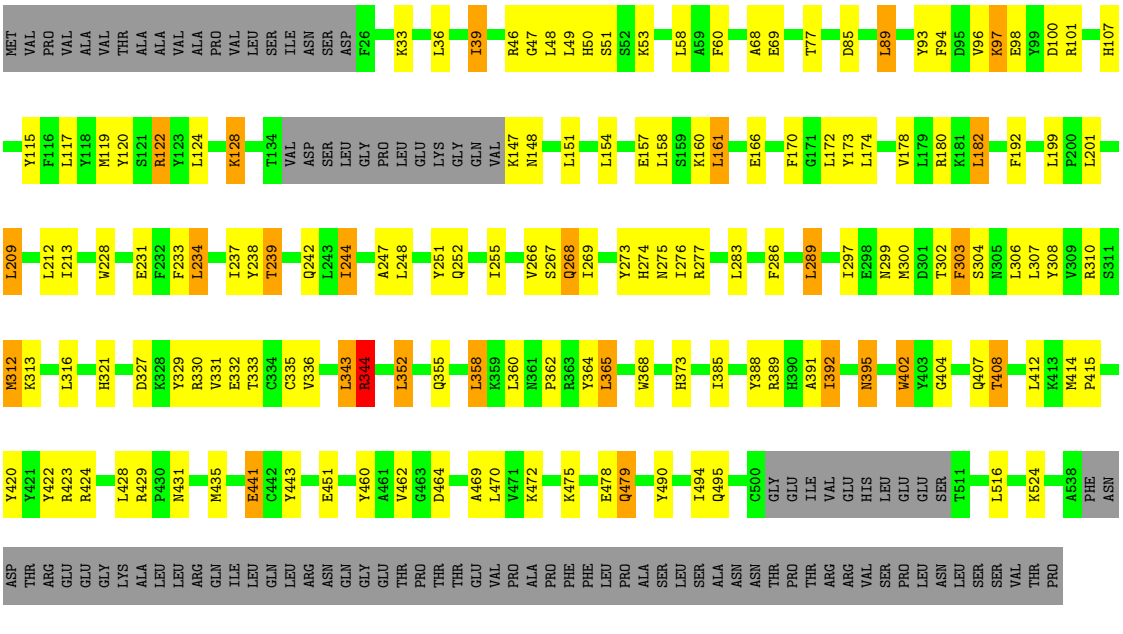
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

Chain C:



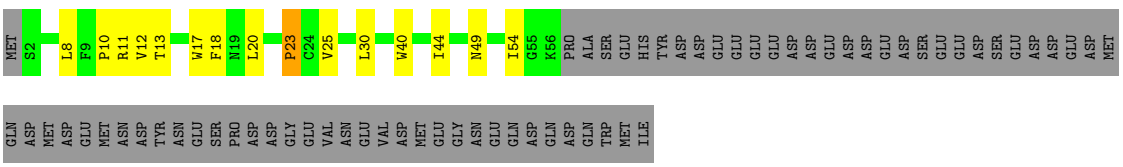
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

Chain P:

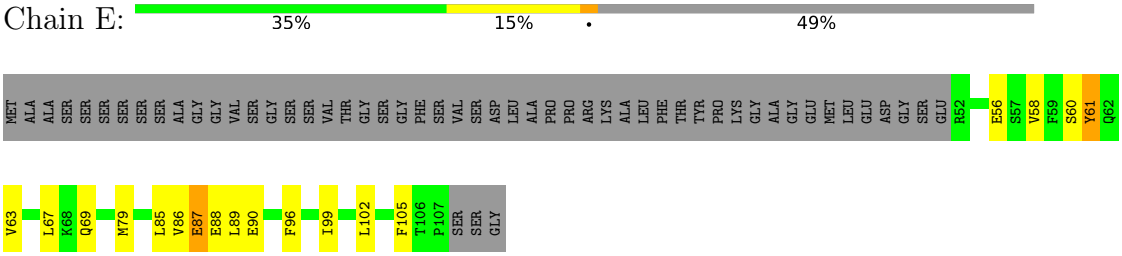
• Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

Chain D:

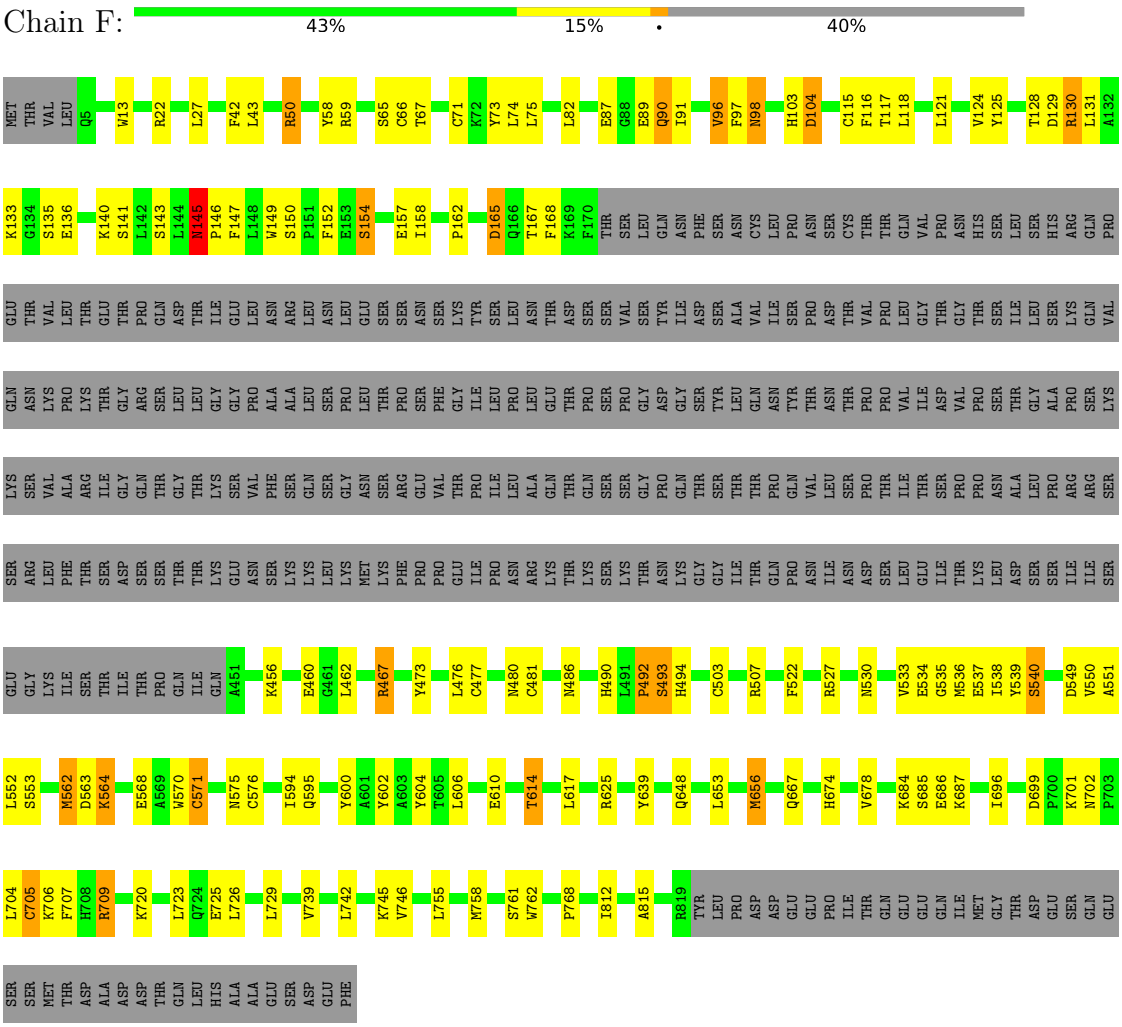
• Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

Chain E:



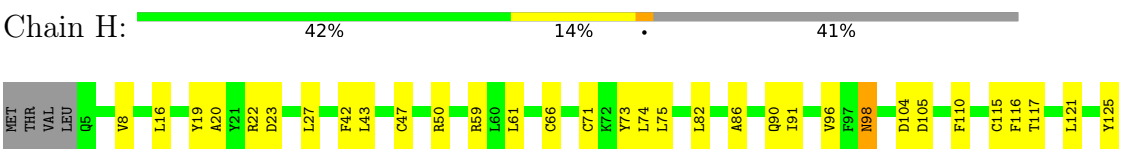

• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

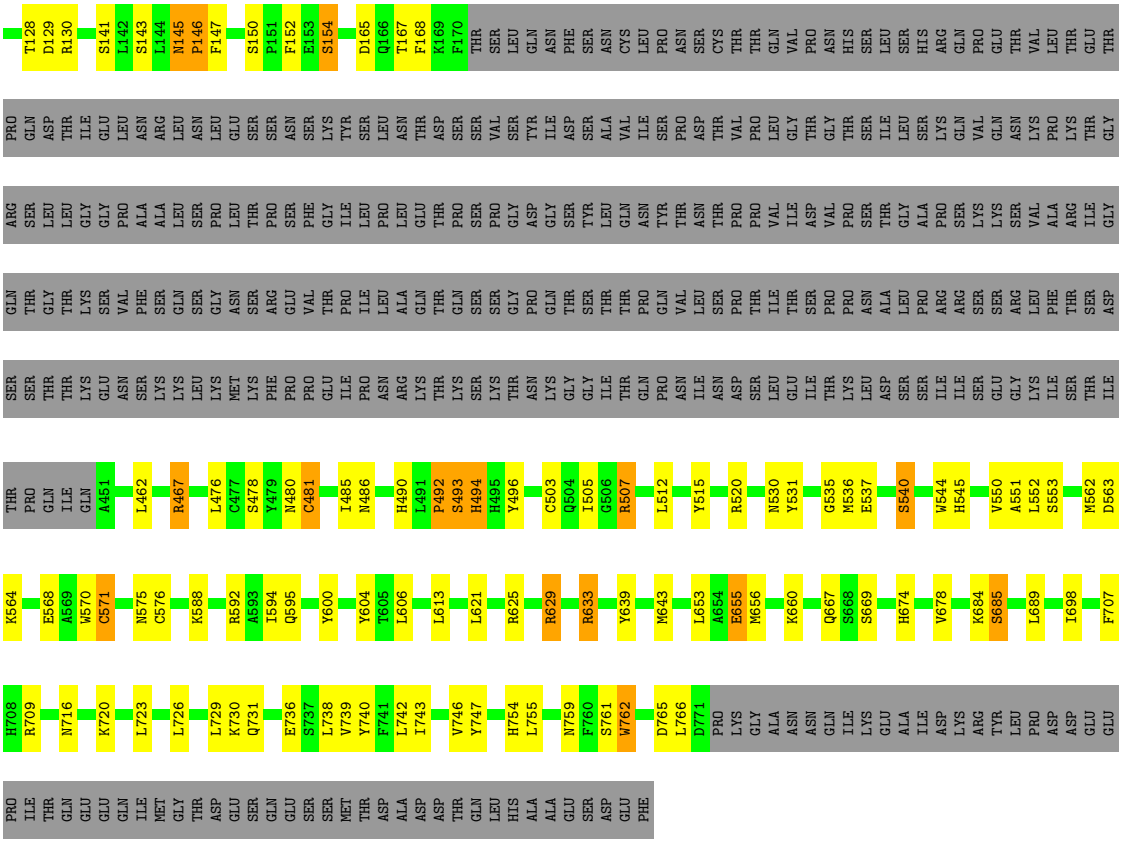
Chain F:




• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

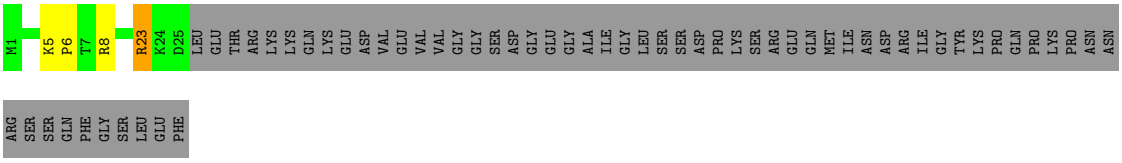
Chain H:





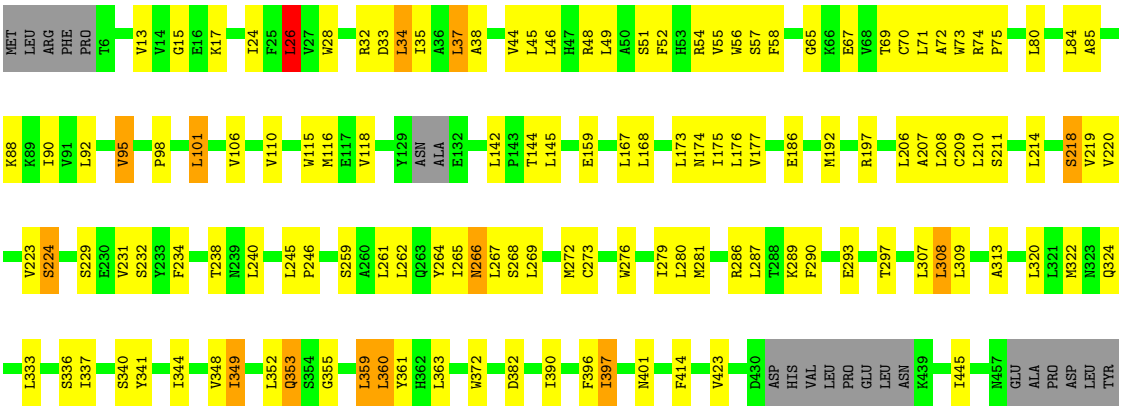
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

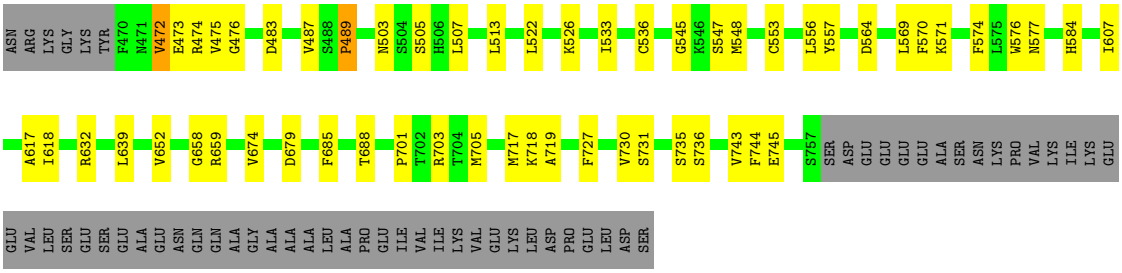
Chain G:

• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

Chain I:

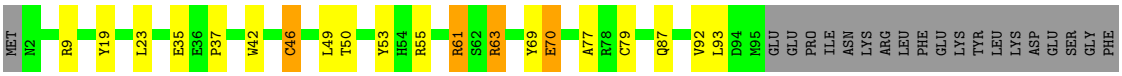


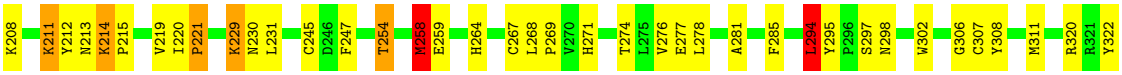


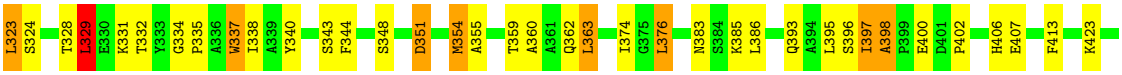


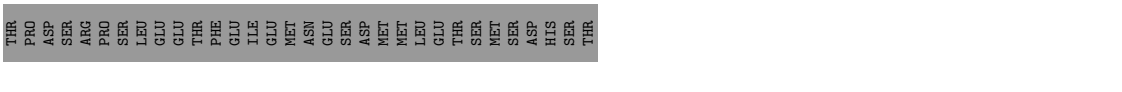
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

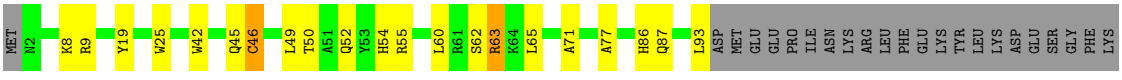
Chain J:

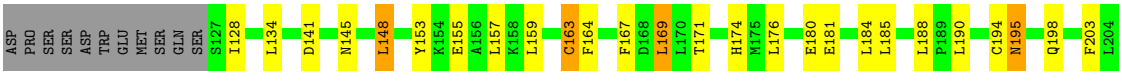



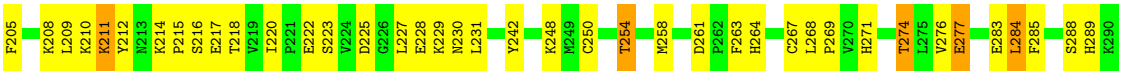


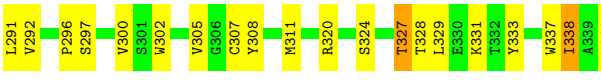






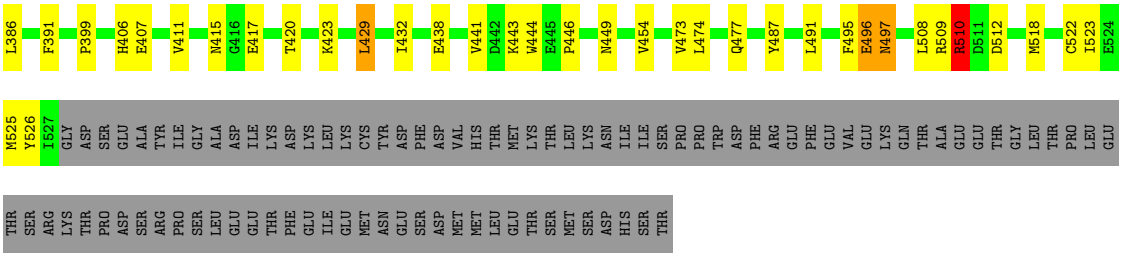






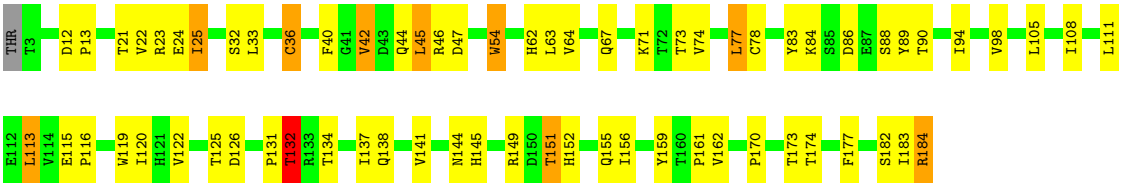
• Molecule 10: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain K:



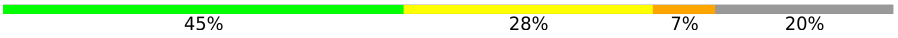
• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

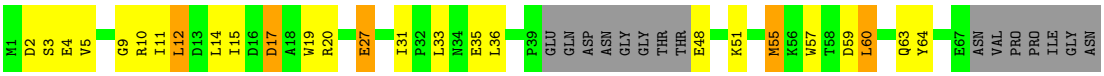
Chain L:

• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13

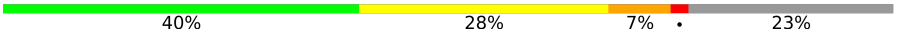
Chain M:

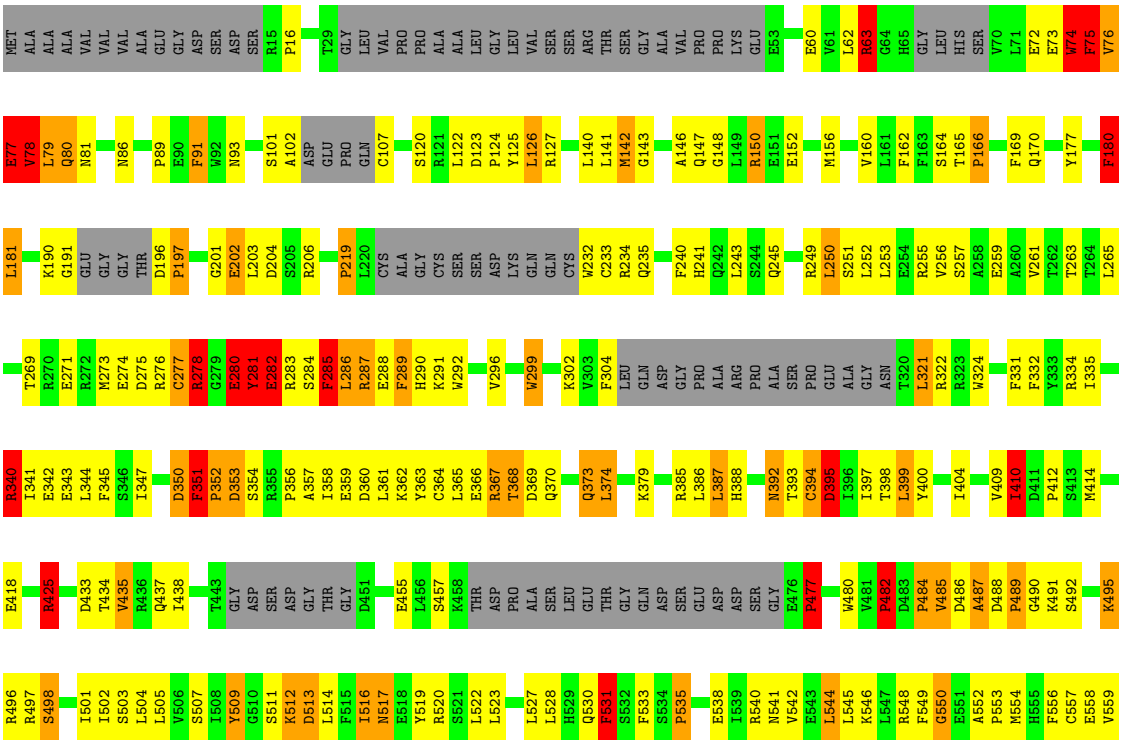


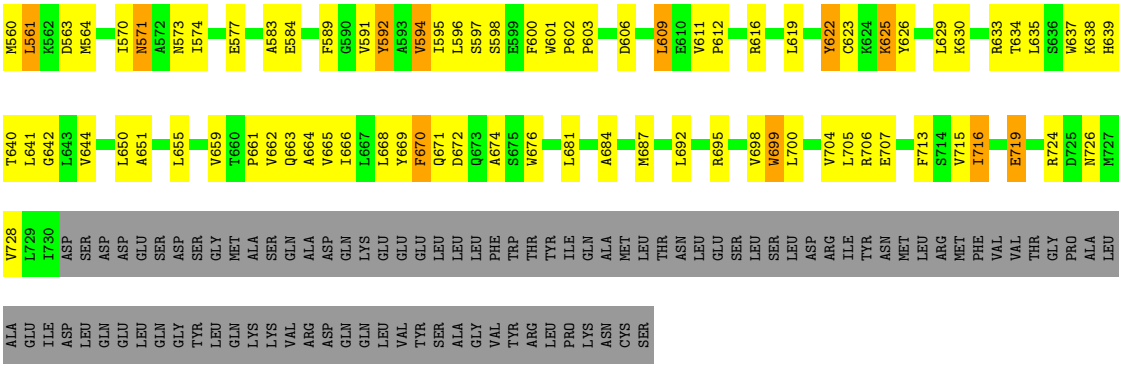



• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

Chain N:

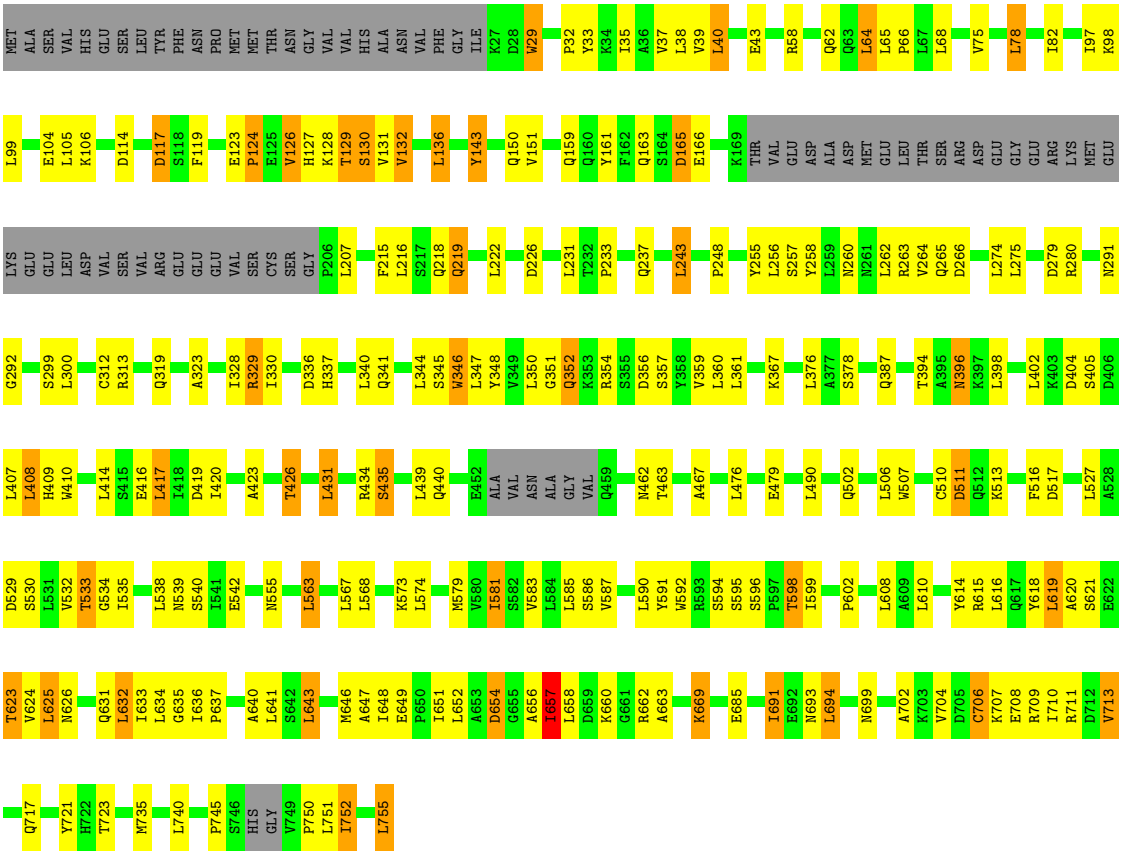




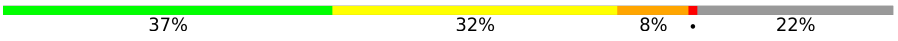
• Molecule 14: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

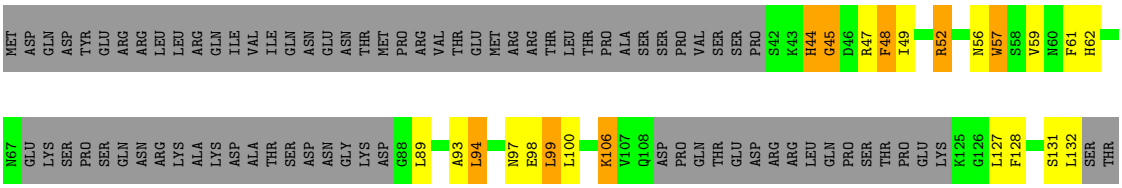
Chain O:

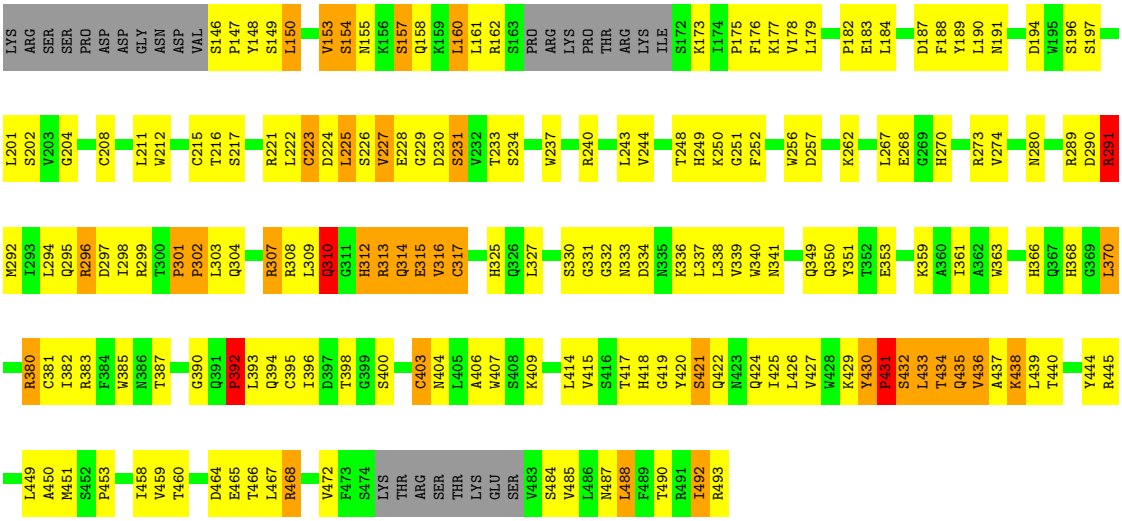



• Molecule 15: FIZZY-RELATED PROTEIN HOMOLOG

Chain R:

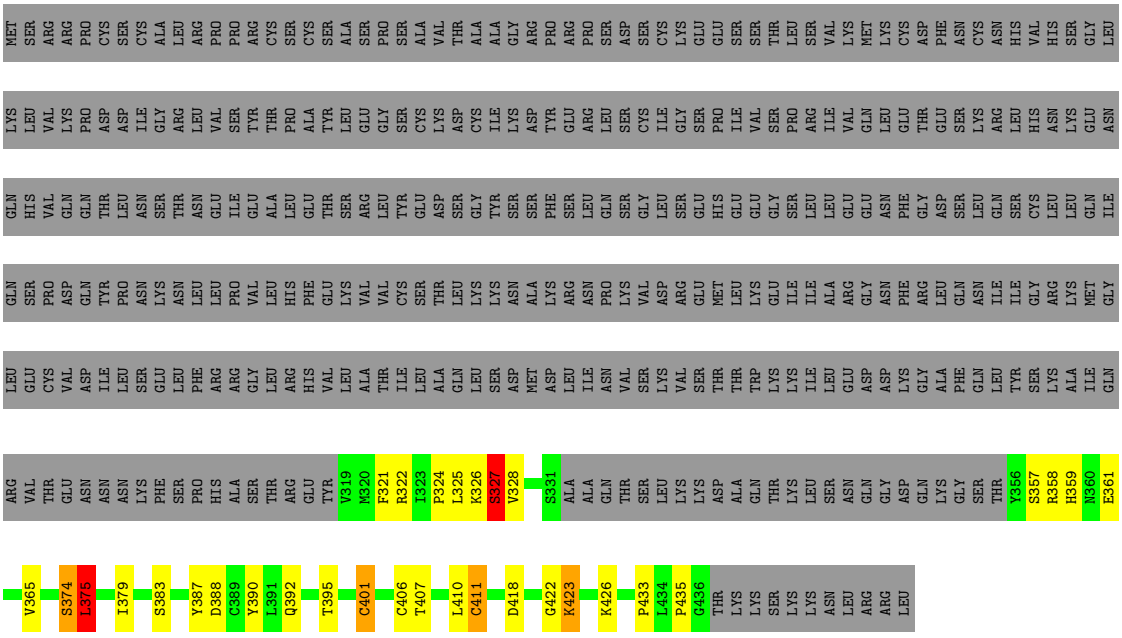




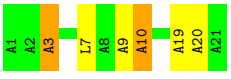
• Molecule 16: F-BOX ONLY PROTEIN 5

Chain S:

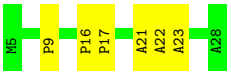
• Molecule 17: PEPTIDE

Chain T:

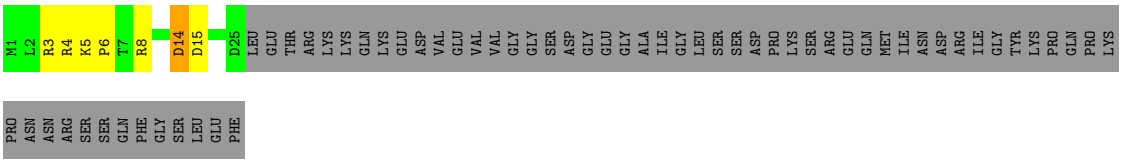
• Molecule 18: PEPTIDE

Chain U:



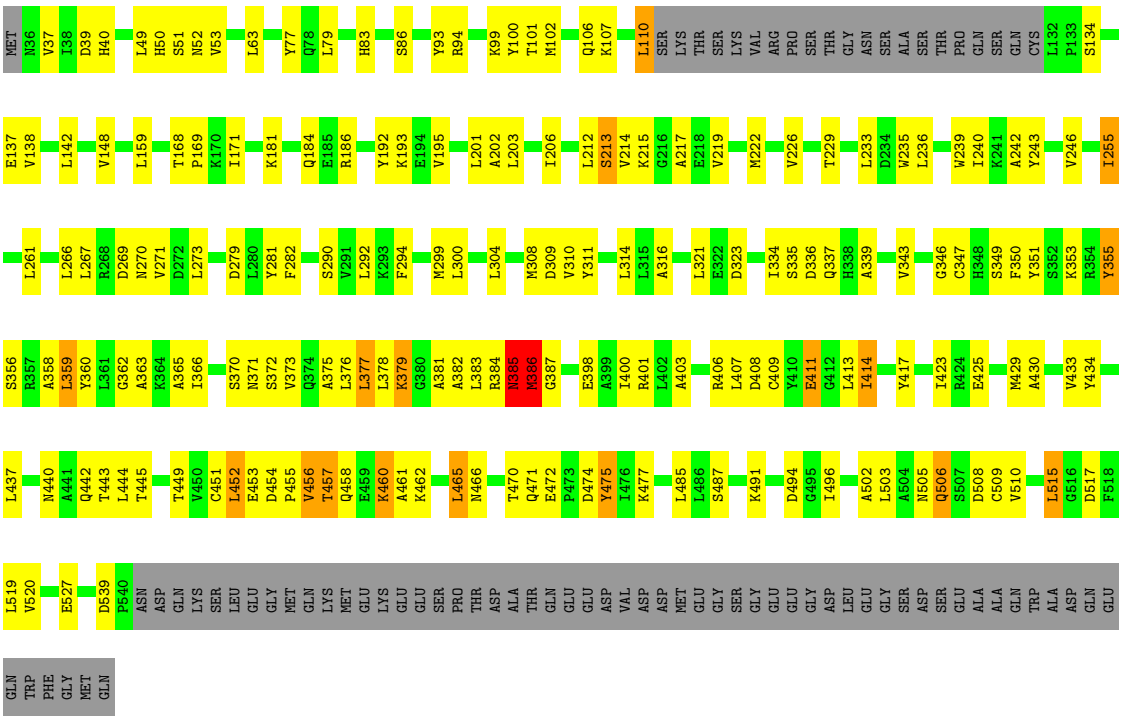

• Molecule 19: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain W:

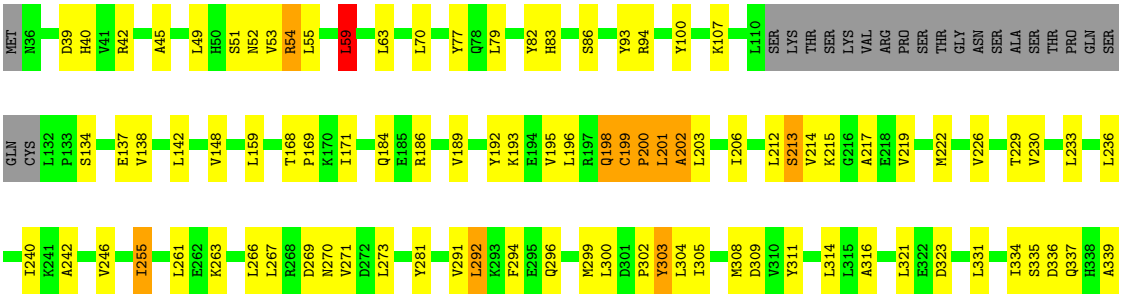

• Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

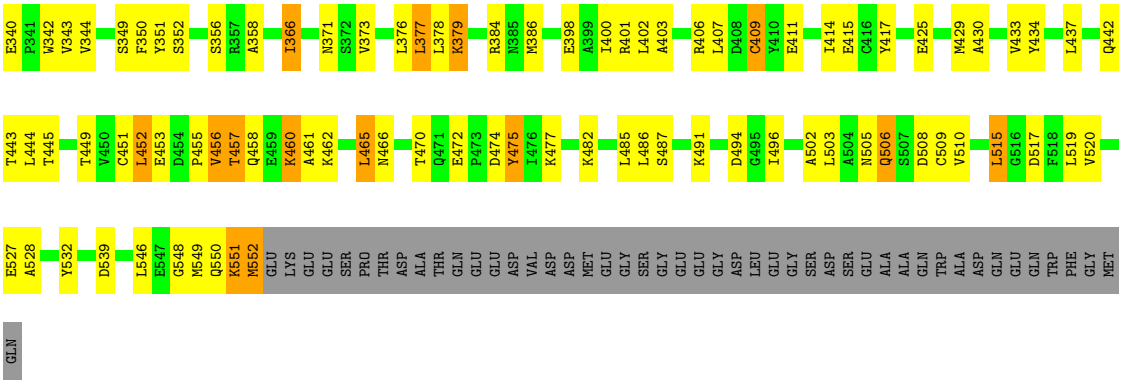
Chain X:


• Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y:


E340 P341 W342 V343 V344 S349 F350 Y351 S352 S356 R357 A358 I366 N371 S372 V373 L376 L377 L378 K379 R384 N385 M386 E398 A399 I400 R401 L402 A403 R406 L407 D408 C409 Y410 E411 I414 E415 C416 Y417 E425 M429 A430 V433 Y434 L437 Q442
T443 L444 T445 T449 V450 C451 L452 E453 D454 P455 V456 T457 Q458 E459 K460 A461 K462 L465 N466 T470 Q471 E472 P473 D474 Y475 I476 K477 K482 L485 L486 S487 K491 D494 Q495 I496 A502 L503 A504 N505 Q506 S507 D508 C509 V510 L515 G516 D517 F518 L519 V520
E527 A528 Y532 D539 L546 E547 G548 M549 Q550 K551 M552 GLU LYS GLU GLU SER PRO THR ASP ALA THR GLN GLU GLU ASP VAL ASP ASP MET GLU GLY SER GLY GLU GLU GLY ASP LEU GLU GLY SER ASP SER GLU ALA ALA GLN TRP ALA ASP GLN GLU GLN TRP PHE GLY MET
GLN

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 202084 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | Not provided | |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 27 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 78000 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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 | 0/11190 | 0.99 | 21/15238 (0.1%) |
| 2 | B | 0.52 | 0/675 | 0.86 | 1/914 (0.1%) |
| 3 | C | 0.75 | 1/4403 (0.0%) | 0.95 | 9/5945 (0.2%) |
| 3 | P | 0.70 | 1/4137 (0.0%) | 0.92 | 3/5587 (0.1%) |
| 4 | D | 0.71 | 0/447 | 0.98 | 1/612 (0.2%) |
| 5 | E | 0.65 | 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 | 0.62 | 0/215 | 1.03 | 1/285 (0.4%) |
| 8 | I | 0.58 | 0/5827 | 0.85 | 3/7899 (0.0%) |
| 9 | J | 0.75 | 3/4146 (0.1%) | 0.97 | 9/5615 (0.2%) |
| 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 | 0.63 | 1/4913 (0.0%) | 1.01 | 18/6650 (0.3%) |
| 14 | O | 0.73 | 5/5494 (0.1%) | 0.96 | 5/7425 (0.1%) |
| 15 | R | 2.23 | 11/3068 (0.4%) | 2.62 | 75/4162 (1.8%) |
| 16 | S | 0.54 | 0/654 | 0.81 | 3/880 (0.3%) |
| 17 | T | 1.02 | 0/108 | 1.11 | 0/149 |
| 18 | U | 0.91 | 0/119 | 1.10 | 3/165 (1.8%) |
| 19 | W | 0.64 | 0/214 | 1.02 | 0/284 |
| 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 | 0.83 | 34/67836 (0.1%) | 1.07 | 184/91889 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 9 |
| 8 | I | 0 | 2 |
| 9 | J | 0 | 1 |
| 13 | N | 0 | 26 |
| 15 | R | 0 | 5 |
| 17 | T | 0 | 1 |
| 20 | X | 0 | 1 |
| All | All | 0 | 45 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | R | 431 | PRO | N-CD | 53.78 | 2.23 | 1.47 |
| 15 | R | 392 | PRO | N-CD | 50.89 | 2.19 | 1.47 |
| 15 | R | 302 | PRO | N-CD | 48.99 | 2.16 | 1.47 |
| 15 | R | 301 | PRO | N-CD | 47.51 | 2.14 | 1.47 |
| 10 | K | 229 | LYS | CB-CG | 33.09 | 2.42 | 1.52 |

The worst 5 of 184 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | R | 431 | PRO | O-C-N | -52.04 | 39.44 | 122.70 |
| 15 | R | 310 | GLN | O-C-N | -29.51 | 73.03 | 123.20 |
| 15 | R | 240 | ARG | NE-CZ-NH2 | -25.22 | 107.69 | 120.30 |
| 15 | R | 307 | ARG | NE-CZ-NH2 | -25.20 | 107.70 | 120.30 |
| 15 | R | 313 | ARG | NE-CZ-NH2 | -25.18 | 107.71 | 120.30 |

There are no chirality outliers.

5 of 45 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 | 10947 | 0 | 10690 | 367 | 0 |
| 2 | B | 650 | 0 | 600 | 33 | 0 |
| 3 | C | 4305 | 0 | 4273 | 121 | 0 |
| 3 | P | 4042 | 0 | 3998 | 137 | 0 |
| 4 | D | 437 | 0 | 396 | 14 | 0 |
| 5 | E | 450 | 0 | 435 | 12 | 0 |
| 6 | F | 3923 | 0 | 3813 | 95 | 0 |
| 6 | H | 3853 | 0 | 3788 | 95 | 0 |
| 7 | G | 214 | 0 | 222 | 2 | 0 |
| 8 | I | 5709 | 0 | 5597 | 124 | 0 |
| 9 | J | 4047 | 0 | 3956 | 138 | 0 |
| 10 | K | 3988 | 0 | 3917 | 126 | 0 |
| 11 | L | 1435 | 0 | 1382 | 69 | 0 |
| 12 | M | 493 | 0 | 469 | 28 | 0 |
| 13 | N | 4831 | 0 | 4527 | 292 | 0 |
| 14 | O | 5396 | 0 | 5425 | 160 | 0 |
| 15 | R | 3003 | 0 | 2951 | 432 | 0 |
| 16 | S | 648 | 0 | 543 | 31 | 0 |
| 17 | T | 109 | 0 | 107 | 9 | 0 |
| 18 | U | 120 | 0 | 80 | 1 | 0 |
| 19 | W | 213 | 0 | 220 | 8 | 0 |
| 20 | X | 3770 | 0 | 3829 | 254 | 0 |
| 20 | Y | 3865 | 0 | 3925 | 168 | 0 |
| 21 | B | 3 | 0 | 0 | 0 | 0 |
| 21 | S | 2 | 0 | 0 | 0 | 0 |
| All | All | 66453 | 0 | 65143 | 2494 | 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 19.

The worst 5 of 2494 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) |
|---|---|---|---|
| 15:R:404:ASN:CB | 15:R:449:LEU:HD21 | 1.22 | 1.60 |
| 15:R:404:ASN:HB2 | 15:R:449:LEU:CD2 | 1.35 | 1.53 |
| 15:R:292:MET:CE | 15:R:309:LEU:HD21 | 1.42 | 1.47 |
| 20:X:358:ALA:HB3 | 20:X:382:ALA:CB | 1.43 | 1.46 |
| 20:X:355:TYR:CD2 | 20:X:386:MET:N | 1.83 | 1.46 |

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 | 1399/1944 (72%) | 1260 (90%) | 107 (8%) | 32 (2%) | 6 38 |
| 2 | B | 83/84 (99%) | 72 (87%) | 7 (8%) | 4 (5%) | 2 22 |
| 3 | C | 520/591 (88%) | 495 (95%) | 23 (4%) | 2 (0%) | 34 71 |
| 3 | P | 485/591 (82%) | 460 (95%) | 24 (5%) | 1 (0%) | 47 79 |
| 4 | D | 53/121 (44%) | 46 (87%) | 6 (11%) | 1 (2%) | 8 42 |
| 5 | E | 54/110 (49%) | 54 (100%) | 0 | 0 | 100 100 |
| 6 | F | 494/824 (60%) | 477 (97%) | 11 (2%) | 6 (1%) | 13 51 |
| 6 | H | 479/824 (58%) | 462 (96%) | 12 (2%) | 5 (1%) | 15 55 |
| 7 | G | 23/85 (27%) | 23 (100%) | 0 | 0 | 100 100 |
| 8 | I | 722/808 (89%) | 690 (96%) | 28 (4%) | 4 (1%) | 25 64 |
| 9 | J | 500/620 (81%) | 467 (93%) | 28 (6%) | 5 (1%) | 15 55 |
| 10 | K | 489/620 (79%) | 458 (94%) | 26 (5%) | 5 (1%) | 15 55 |
| 11 | L | 180/183 (98%) | 170 (94%) | 8 (4%) | 2 (1%) | 14 53 |
| 12 | M | 55/74 (74%) | 46 (84%) | 9 (16%) | 0 | 100 100 |
| 13 | N | 609/822 (74%) | 501 (82%) | 50 (8%) | 58 (10%) | 0 8 |
| 14 | O | 677/756 (90%) | 644 (95%) | 25 (4%) | 8 (1%) | 13 51 |
| 15 | R | 375/493 (76%) | 343 (92%) | 25 (7%) | 7 (2%) | 8 42 |
| 16 | S | 88/447 (20%) | 68 (77%) | 15 (17%) | 5 (6%) | 1 18 |
| 17 | T | 19/21 (90%) | 14 (74%) | 3 (16%) | 2 (10%) | 0 7 |
| 18 | U | 22/24 (92%) | 19 (86%) | 2 (9%) | 1 (4%) | 2 23 |
| 19 | W | 23/85 (27%) | 23 (100%) | 0 | 0 | 100 100 |
| 20 | X | 480/565 (85%) | 462 (96%) | 15 (3%) | 3 (1%) | 25 64 |
| 20 | Y | 492/565 (87%) | 471 (96%) | 16 (3%) | 5 (1%) | 15 55 |
| All | All | 8321/11257 (74%) | 7725 (93%) | 440 (5%) | 156 (2%) | 11 42 |

5 of 156 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 274 | VAL |
| 1 | A | 630 | PRO |
| 1 | A | 857 | MET |
| 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 | 1150/1720 (67%) | 988 (86%) | 162 (14%) | 3 21 |
| 2 | B | 65/75 (87%) | 55 (85%) | 10 (15%) | 2 18 |
| 3 | C | 452/516 (88%) | 399 (88%) | 53 (12%) | 5 29 |
| 3 | P | 422/516 (82%) | 373 (88%) | 49 (12%) | 5 29 |
| 4 | D | 46/115 (40%) | 42 (91%) | 4 (9%) | 10 41 |
| 5 | E | 47/89 (53%) | 37 (79%) | 10 (21%) | 1 7 |
| 6 | F | 407/729 (56%) | 367 (90%) | 40 (10%) | 8 36 |
| 6 | H | 408/729 (56%) | 372 (91%) | 36 (9%) | 10 40 |
| 7 | G | 23/77 (30%) | 21 (91%) | 2 (9%) | 10 41 |
| 8 | I | 620/730 (85%) | 572 (92%) | 48 (8%) | 13 45 |
| 9 | J | 424/548 (77%) | 368 (87%) | 56 (13%) | 4 23 |
| 10 | K | 423/549 (77%) | 381 (90%) | 42 (10%) | 8 35 |
| 11 | L | 155/168 (92%) | 140 (90%) | 15 (10%) | 8 36 |
| 12 | M | 55/67 (82%) | 44 (80%) | 11 (20%) | 1 8 |
| 13 | N | 459/724 (63%) | 403 (88%) | 56 (12%) | 5 26 |
| 14 | O | 578/652 (89%) | 491 (85%) | 87 (15%) | 3 19 |
| 15 | R | 324/428 (76%) | 306 (94%) | 18 (6%) | 21 56 |
| 16 | S | 56/404 (14%) | 43 (77%) | 13 (23%) | 1 5 |
| 17 | T | 1/2 (50%) | 1 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 19 | W | 23/77 (30%) | 22 (96%) | 1 (4%) | 29 63 |
| 20 | X | 407/484 (84%) | 378 (93%) | 29 (7%) | 14 48 |
| 20 | Y | 418/484 (86%) | 382 (91%) | 36 (9%) | 10 41 |
| All | All | 6963/9883 (70%) | 6185 (89%) | 778 (11%) | 9 30 |

5 of 778 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | L | 12 | ASP |
| 14 | O | 328 | ILE |
| 11 | L | 177 | PHE |
| 10 | K | 522 | CYS |
| 13 | N | 410 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | P | 71 | GLN |
| 3 | P | 299 | ASN |
| 20 | X | 106 | GLN |
| 6 | H | 595 | GLN |
| 6 | H | 545 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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 |
|---|---|---|
| 13 | N | 2 |
| 16 | S | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | S | 419:CYS | C | 420:SER | N | 27.15 |
| 1 | N | 92:TRP | C | 93:ASN | N | 3.02 |
| 1 | N | 563:ASP | C | 564:MET | N | 2.52 |

# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2924. 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

This section was not generated.

## 6.2 Central slices

This section was not generated.

## 6.3 Largest variance slices

This section was not generated.

## 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

## 6.5 Orthogonal surface views

This section was not generated.

## 6.6 Mask visualisation

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

This section was not generated.

## 7.2 Volume estimate versus contour level

This section was not generated.

## 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

# 8 Fourier-Shell correlation

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

# 9 Map-model fit

This section was not generated.