



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 21, 2016 – 05:11 PM EST

PDB ID : 5T0H
EMDB ID: : EMD-8335
Title : Structural basis for dynamic regulation of the human 26S proteasome
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.;
Kirschner, M.W.; Mao, Y.
Deposited on : 2016-08-16
Resolution : 6.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

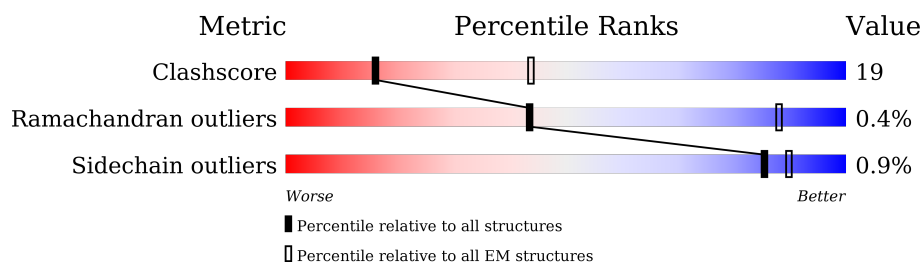
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 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.















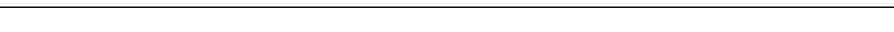



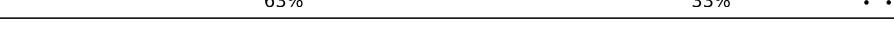

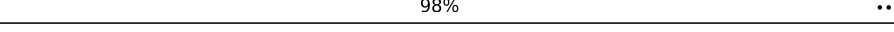




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 433 | <div> <div>34%</div> <div>48%</div> <div>17%</div> </div> |
| 2 | B | 440 | <div> <div>35%</div> <div>41%</div> <div>23%</div> </div> |
| 3 | C | 398 | <div> <div>41%</div> <div>53%</div> <div>6%</div> </div> |
| 4 | D | 418 | <div> <div>38%</div> <div>52%</div> <div>9%</div> </div> |
| 5 | E | 403 | <div> <div>43%</div> <div>43%</div> <div>12%</div> </div> |
| 6 | F | 439 | <div> <div>37%</div> <div>45%</div> <div>17%</div> </div> |
| 7 | G | 245 | <div> <div>64%</div> <div>34%</div> <div>2%</div> </div> |
| 8 | H | 233 | <div> <div>73%</div> <div>26%</div> <div>1%</div> </div> |
| 9 | I | 260 | <div> <div>72%</div> <div>25%</div> <div>3%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 10 | J | 247 |  |
| 11 | K | 240 |  |
| 12 | L | 268 |  |
| 13 | M | 254 |  |
| 14 | N | 238 |  |
| 15 | O | 276 |  |
| 16 | P | 204 |  |
| 17 | Q | 201 |  |
| 18 | R | 262 |  |
| 19 | S | 240 |  |
| 20 | T | 263 |  |
| 21 | U | 953 |  |
| 22 | V | 533 |  |
| 23 | W | 456 |  |
| 24 | X | 422 |  |
| 25 | Y | 389 |  |
| 26 | Z | 324 |  |
| 27 | a | 376 |  |
| 28 | b | 377 |  |
| 29 | c | 309 |  |
| 30 | d | 349 |  |
| 31 | e | 70 |  |
| 32 | f | 749 |  |

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 73509 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 26S protease regulatory subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 361 | Total | C | N | O | S | 0 | 0 |
| | | | 2835 | 1788 | 501 | 528 | 18 | | |

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | B | 341 | Total | C | N | O | S | 0 | 0 |
| | | | 2662 | 1671 | 453 | 526 | 12 | | |

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | C | 384 | Total | C | N | O | S | 0 | 0 |
| | | | 3015 | 1894 | 540 | 564 | 17 | | |

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | D | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3040 | 1923 | 524 | 580 | 13 | | |

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | E | 353 | Total | C | N | O | S | 0 | 0 |
| | | | 2790 | 1755 | 494 | 525 | 16 | | |

- Molecule 6 is a protein called 26S protease regulatory subunit 6A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | F | 366 | Total | C | N | O | S | 0 | 0 |
| | | | 2863 | 1802 | 496 | 549 | 16 | | |

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | G | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1826 | 1160 | 305 | 348 | 13 | | |

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8 | H | 232 | Total | C | N | O | S | 0 | 0 |
| | | | 1708 | 1081 | 289 | 333 | 5 | | |

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9 | I | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1912 | 1204 | 329 | 371 | 8 | | |

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10 | J | 239 | Total | C | N | O | S | 0 | 0 |
| | | | 1704 | 1056 | 308 | 335 | 5 | | |

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11 | K | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1722 | 1080 | 284 | 348 | 10 | | |

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | L | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1850 | 1159 | 334 | 346 | 11 | | |

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13 | M | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1856 | 1178 | 314 | 353 | 11 | | |

- Molecule 14 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14 | N | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1430 | 893 | 245 | 280 | 12 | | |

- Molecule 15 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15 | O | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1033 | 280 | 318 | 12 | | |

- Molecule 16 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16 | P | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1585 | 1010 | 262 | 294 | 19 | | |

- Molecule 17 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17 | Q | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1570 | 1006 | 265 | 290 | 9 | | |

- Molecule 18 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | R | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1548 | 974 | 273 | 292 | 9 | | |

- Molecule 19 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19 | S | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1641 | 1036 | 282 | 313 | 10 | | |

- Molecule 20 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20 | T | 215 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1052 | 285 | 318 | 12 | | |

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 21 | U | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6287 | 3990 | 1075 | 1178 | 44 | | |

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22 | V | 480 | Total | C | N | O | S | 0 | 0 |
| | | | 3852 | 2444 | 684 | 710 | 14 | | |

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23 | W | 236 | Total | C | N | O | S | 0 | 0 |
| | | | 1940 | 1237 | 331 | 361 | 11 | | |

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | X | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 414 | 107 | 124 | 2 | | |

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25 | Y | 378 | Total | C | N | O | S | 0 | 0 |
| | | | 3115 | 1987 | 533 | 578 | 17 | | |

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26 | Z | 286 | Total | C | N | O | S | 0 | 0 |
| | | | 2281 | 1457 | 392 | 427 | 5 | | |

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27 | a | 373 | Total | C | N | O | S | 0 | 0 |
| | | | 2995 | 1911 | 510 | 559 | 15 | | |

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | b | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1458 | 910 | 261 | 279 | 8 | | |

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29 | c | 287 | Total | C | N | O | S | 0 | 0 |
| | | | 2260 | 1430 | 389 | 422 | 19 | | |

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30 | d | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2116 | 1371 | 346 | 390 | 9 | | |

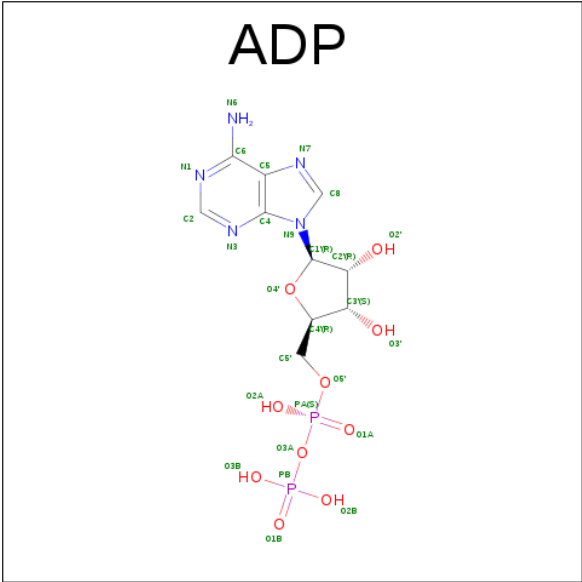
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31 | e | 24 | Total | C | N | O | S | 0 | 0 |
| | | | 197 | 121 | 34 | 40 | 2 | | |

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 32 | f | 694 | Total | C | N | O | S | 0 | 0 |
| | | | 5331 | 3364 | 899 | 1027 | 41 | | |

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 33 | A | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 33 | B | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 33 | C | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 33 | D | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 33 | E | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 33 | F | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

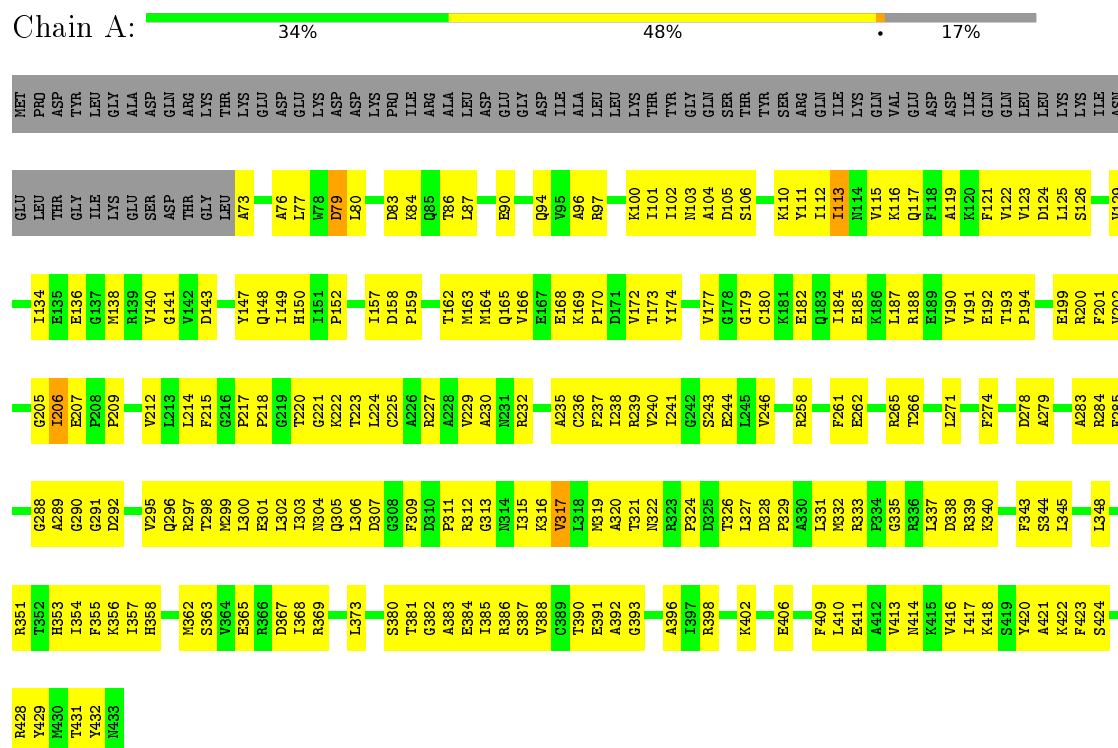
- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 34 | c | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

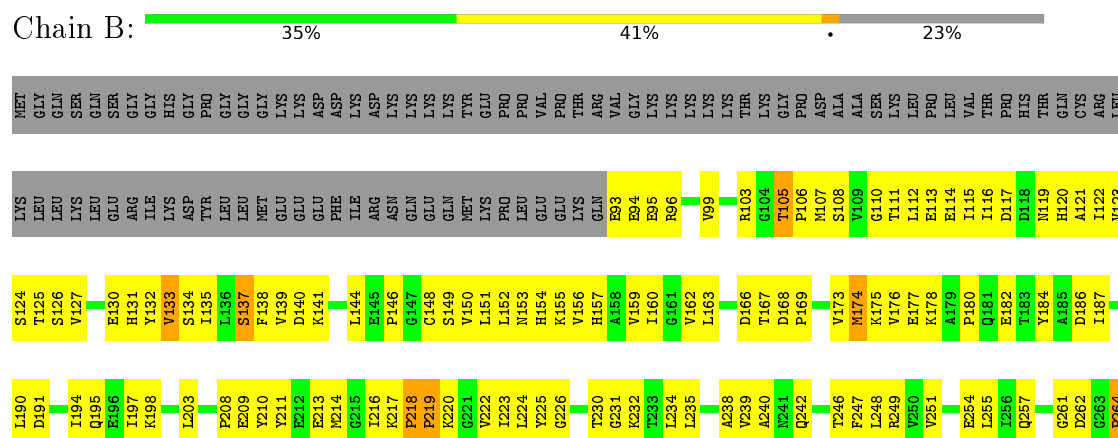
3 Residue-property plots

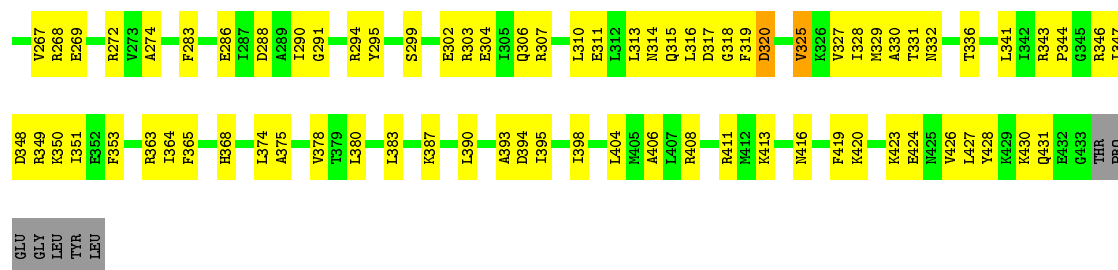
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: 26S protease regulatory subunit 7

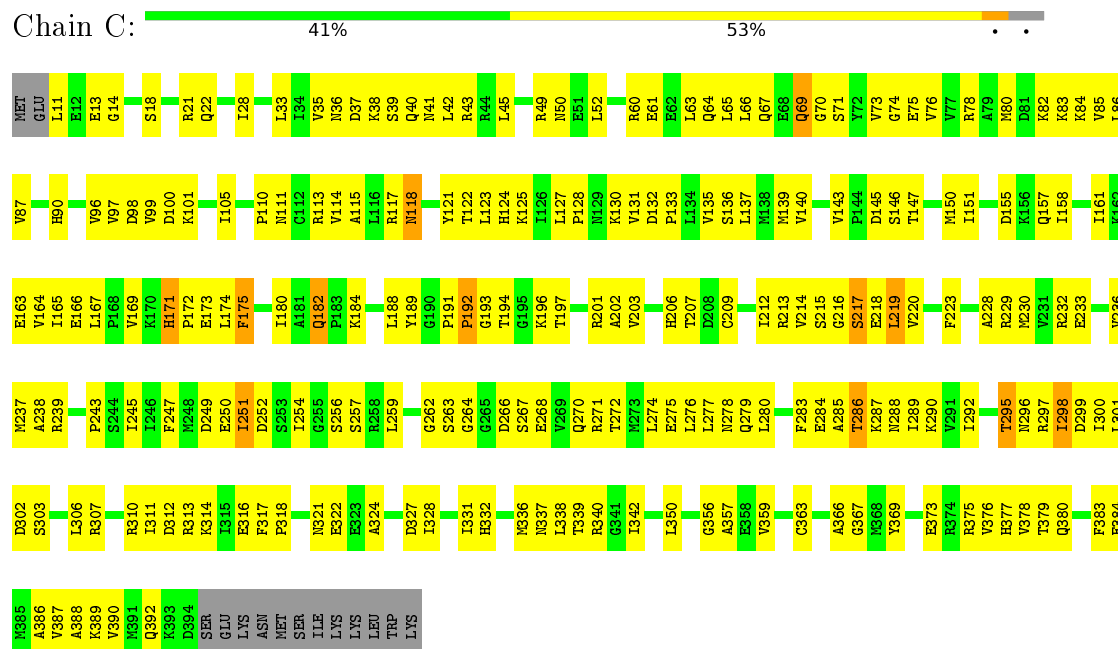


- Molecule 2: 26S protease regulatory subunit 4

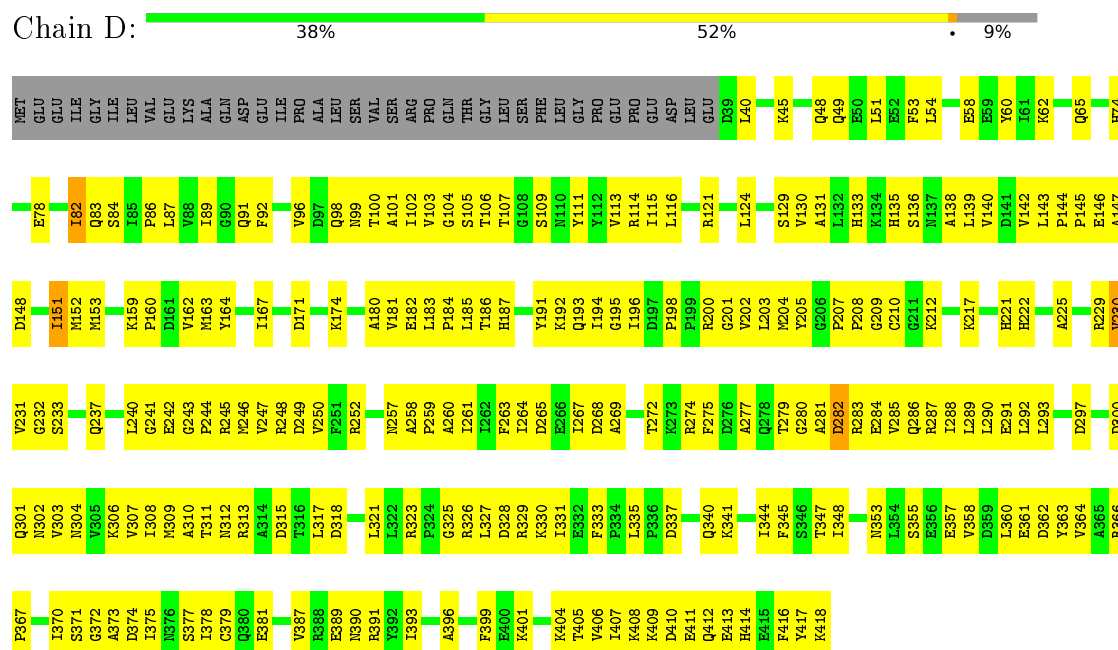




• Molecule 3: 26S protease regulatory subunit 8

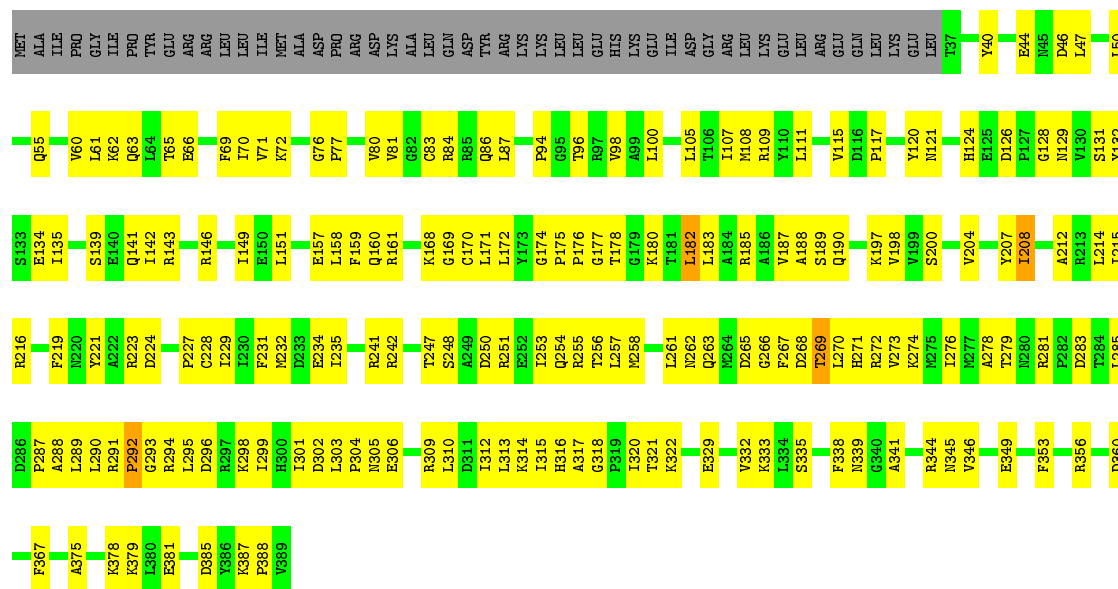


• Molecule 4: 26S protease regulatory subunit 6B



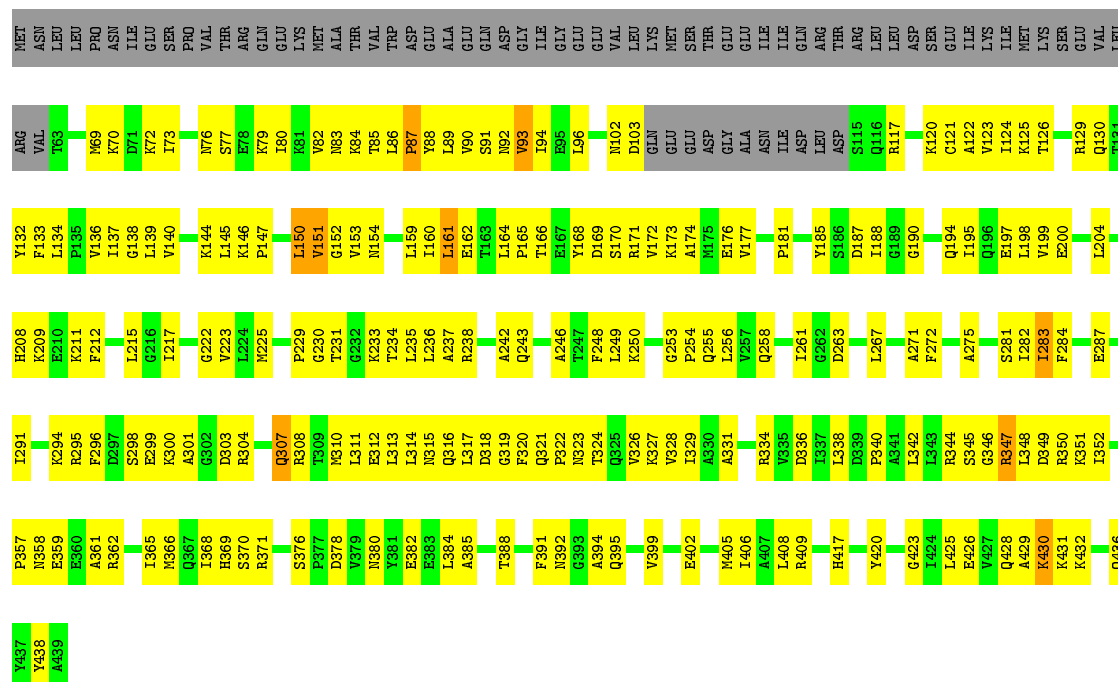
- Molecule 5: 26S protease regulatory subunit 10B

Chain E:  43% 43% 12%



- Molecule 6: 26S protease regulatory subunit 6A

Chain F:  37% 45% 17%

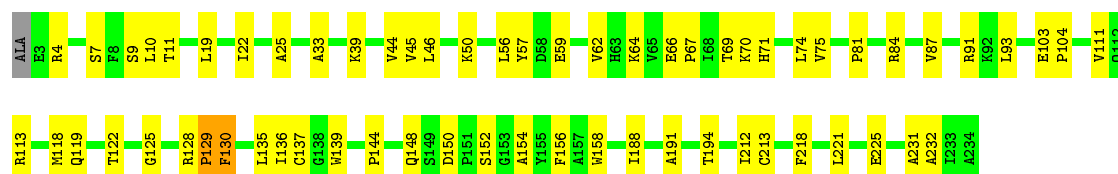


- Molecule 7: Proteasome subunit alpha type-6

Chain G:  64% 34% 2%

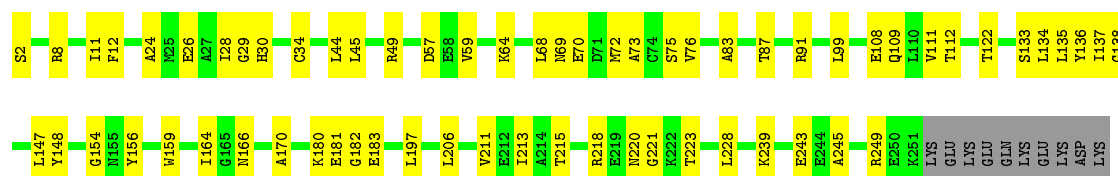
- Molecule 8: Proteasome subunit alpha type-2

Chain H:  73% 26%



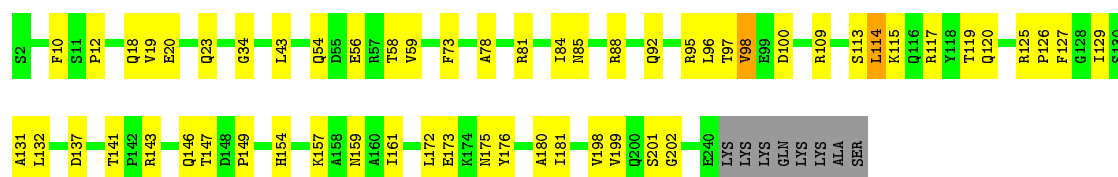
- Molecule 9: Proteasome subunit alpha type-4

Chain I:  72% 25% .



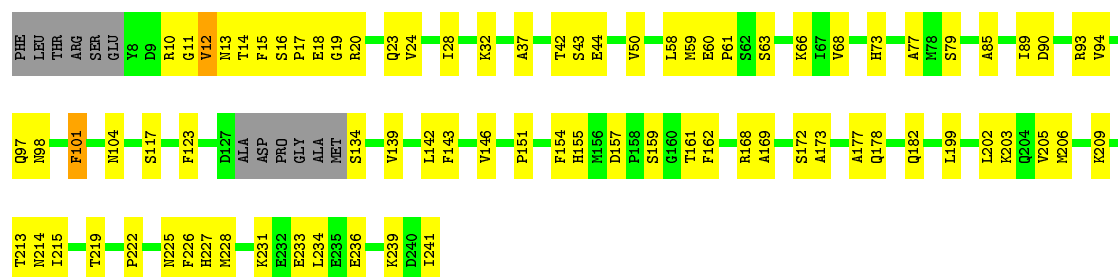
- Molecule 10: Proteasome subunit alpha type-7

Chain J: 74% 22% ..

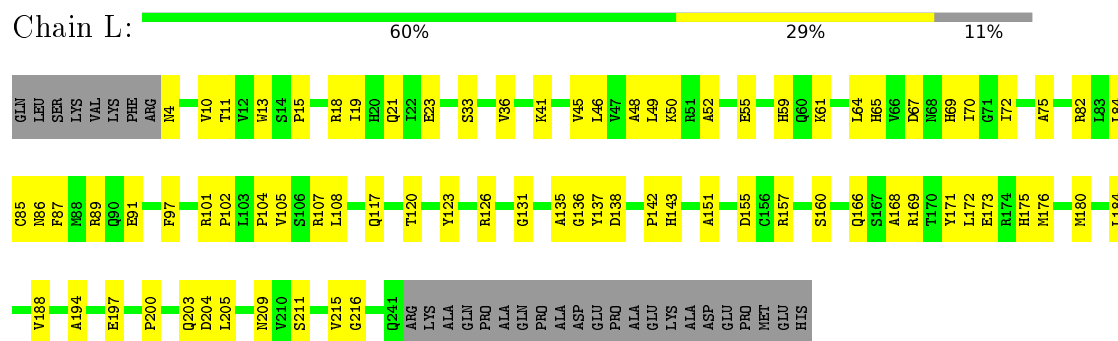


- Molecule 11: Proteasome subunit alpha type-5

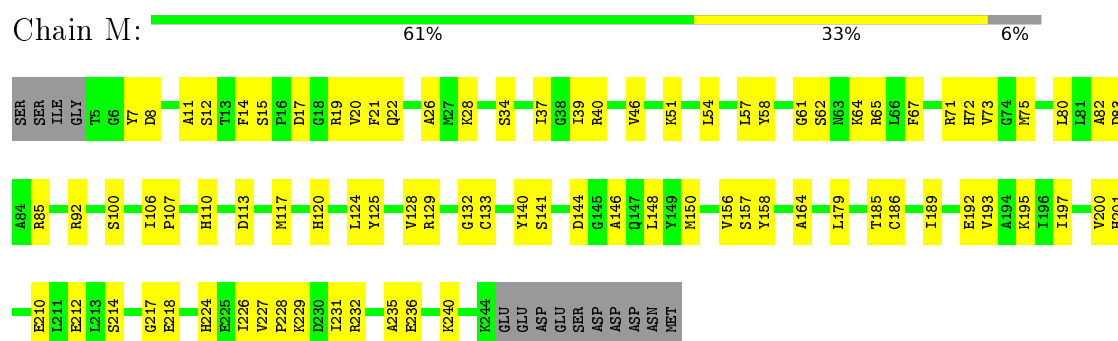
Chain K: 61% 33% 5%



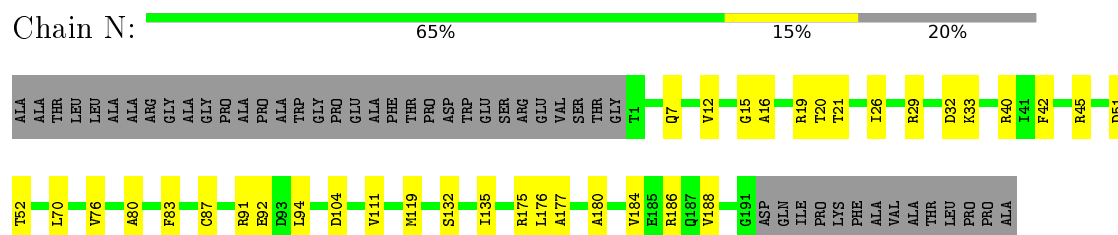
- Molecule 12: Proteasome subunit alpha type-1



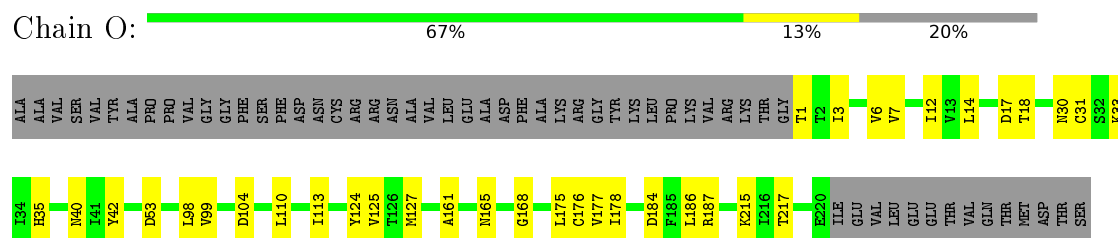
- Molecule 13: Proteasome subunit alpha type-3



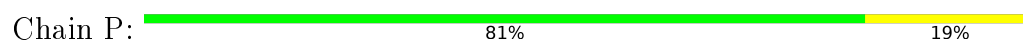
- Molecule 14: Proteasome subunit beta type-6

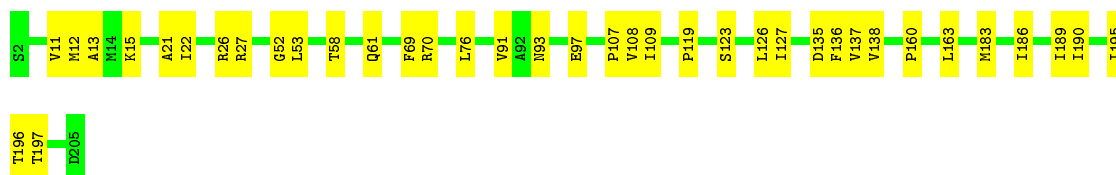


- Molecule 15: Proteasome subunit beta type-7



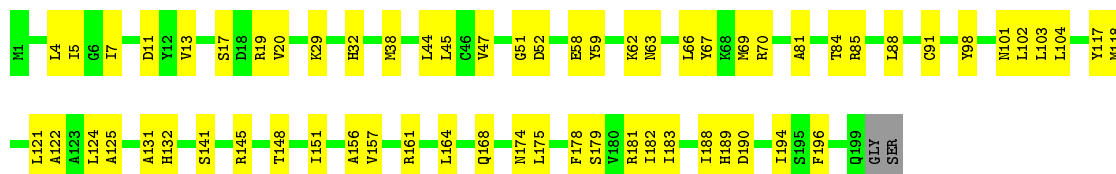
- Molecule 16: Proteasome subunit beta type-3





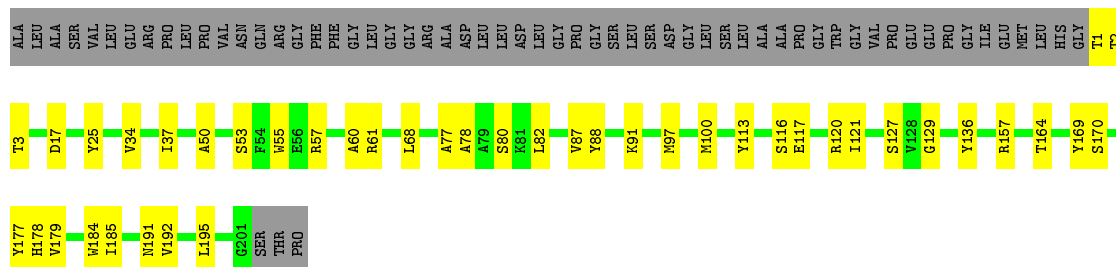
- Molecule 17: Proteasome subunit beta type-2

Chain Q: 68% 31%



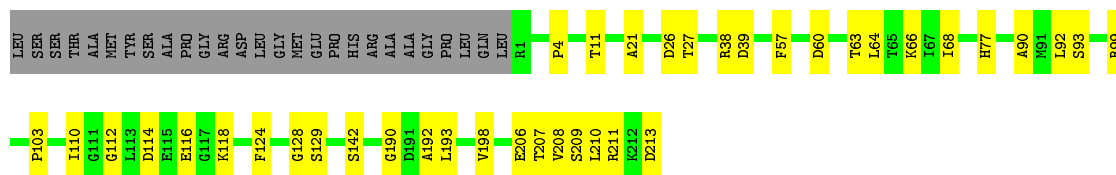
- Molecule 18: Proteasome subunit beta type-5

Chain R: 60% 16% 23%



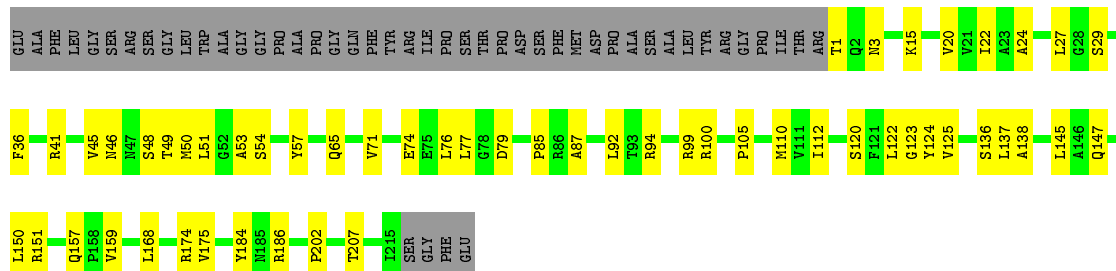
- Molecule 19: Proteasome subunit beta type-1

Chain S: 73% 16% 11%

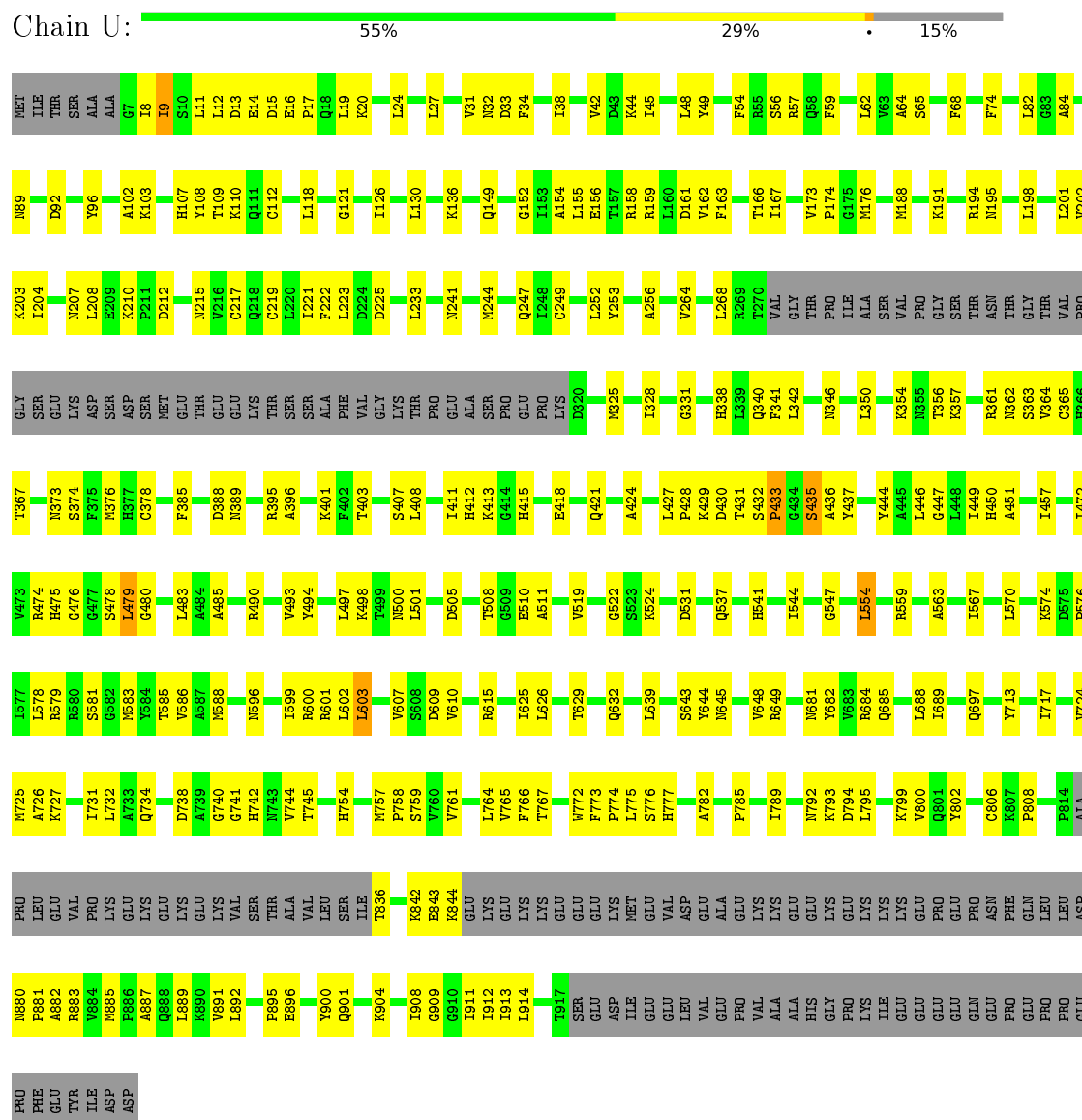


- Molecule 20: Proteasome subunit beta type-4

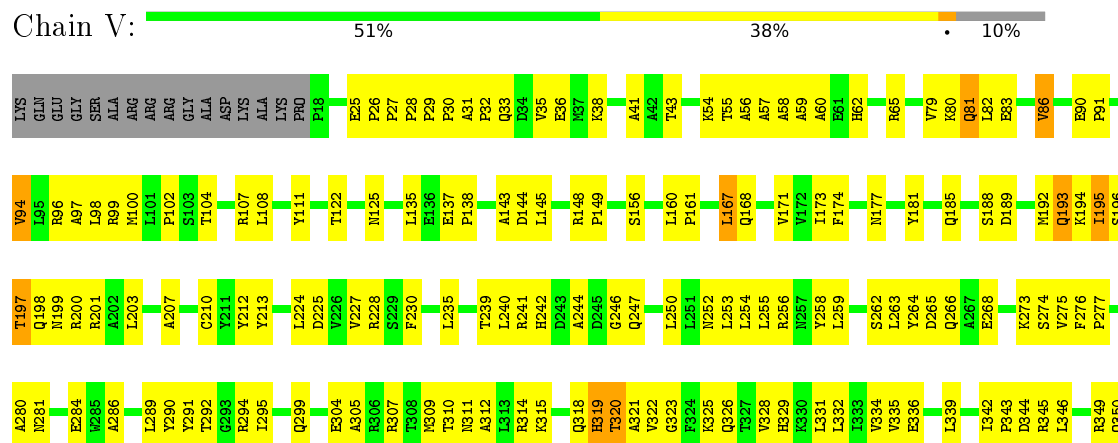
Chain T: 61% 21% 18%

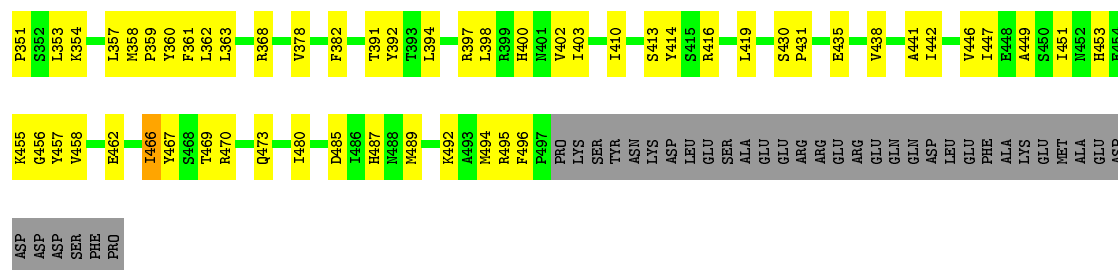


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



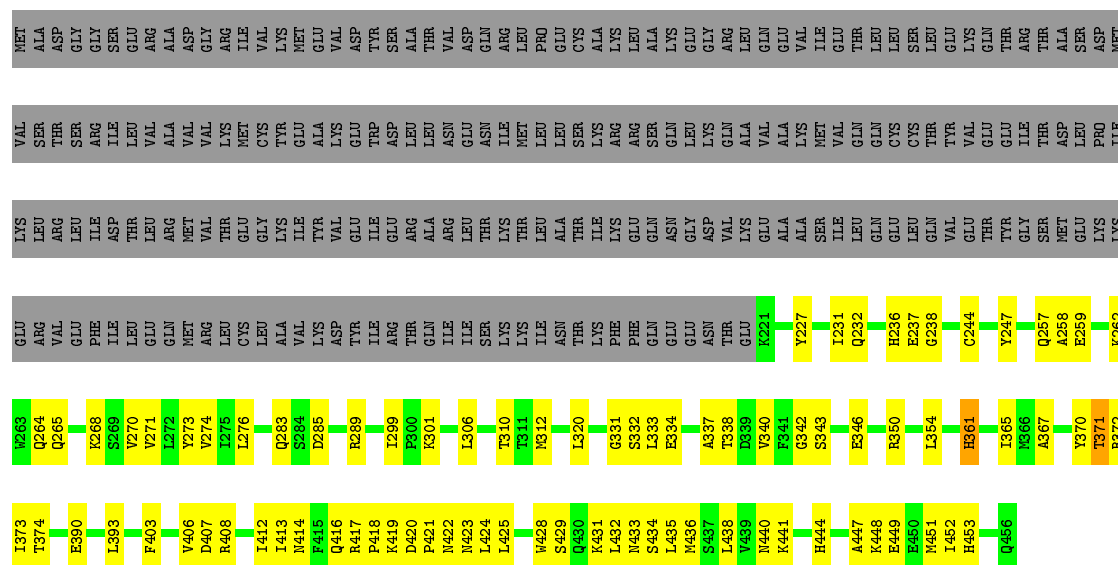
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3





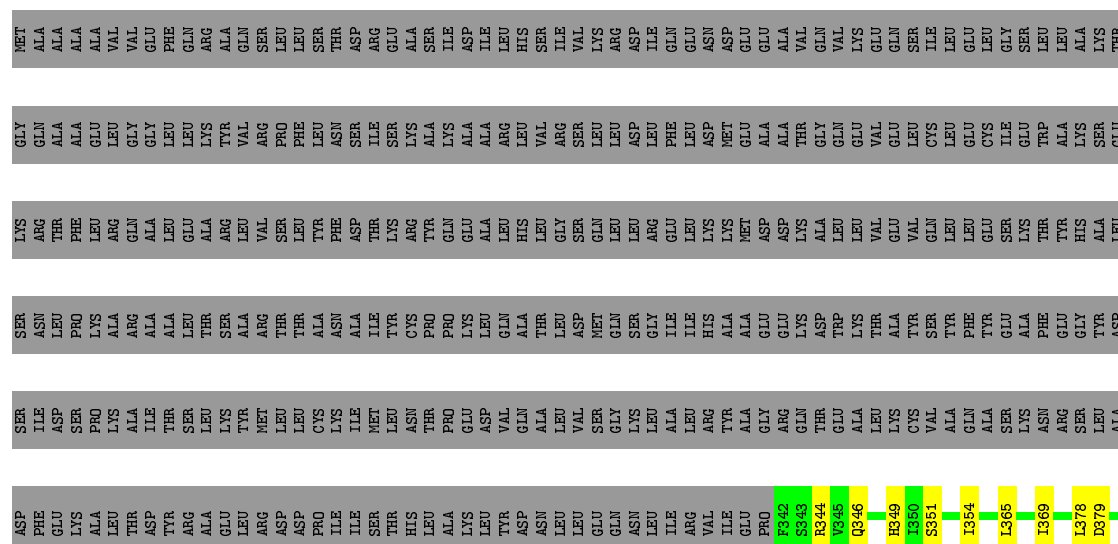
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

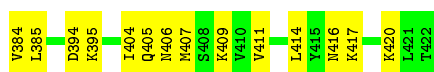
Chain W:



• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

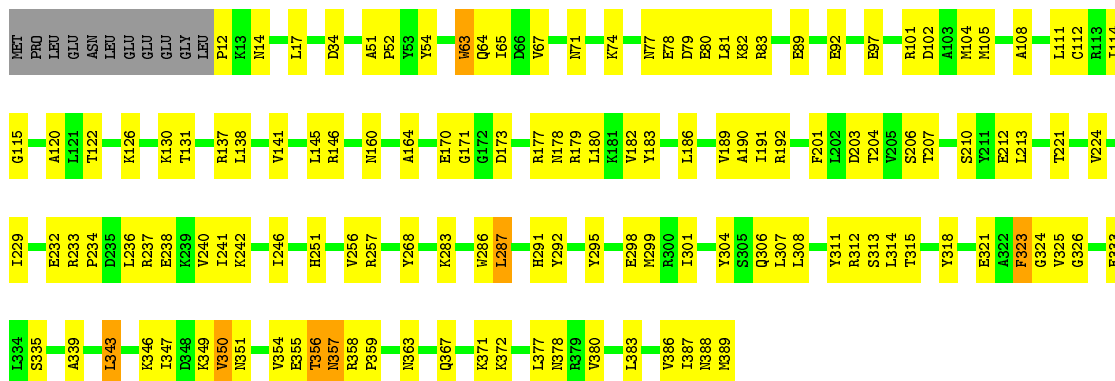
Chain X:





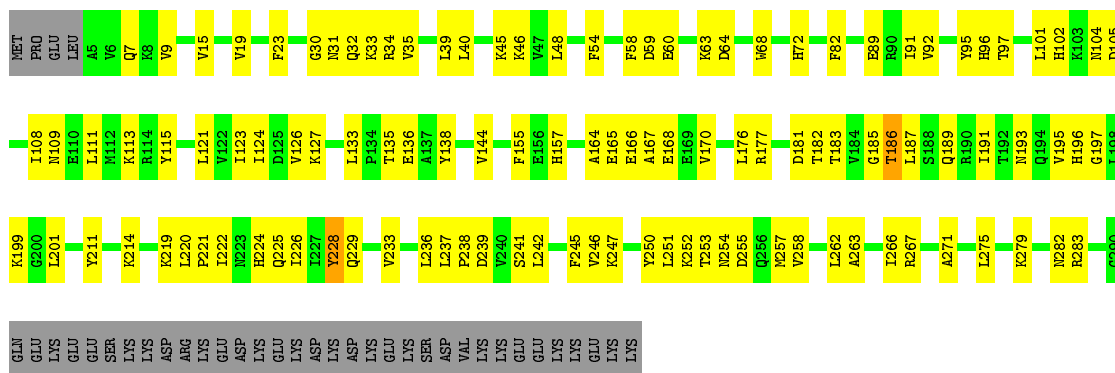
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 63% 33%



- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 54% 34% 12%



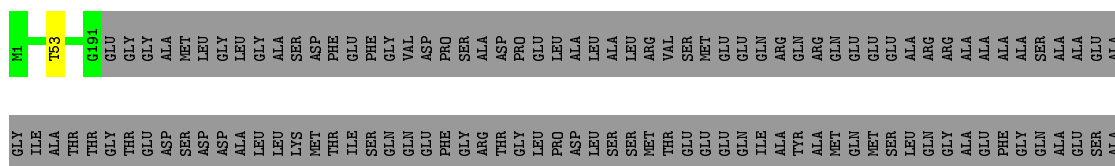
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 98%



- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 50% 49%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 18443 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TECNAI ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | Not provided | 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, ADP

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 | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | A | 0.27 | 0/2886 | 0.54 | 0/3899 |
| 10 | J | 0.23 | 0/1728 | 0.44 | 0/2358 |
| 11 | K | 0.24 | 0/1747 | 0.44 | 0/2364 |
| 12 | L | 0.24 | 0/1885 | 0.44 | 0/2552 |
| 13 | M | 0.23 | 0/1891 | 0.42 | 0/2552 |
| 14 | N | 0.24 | 0/1454 | 0.42 | 0/1967 |
| 15 | O | 0.23 | 0/1670 | 0.43 | 0/2265 |
| 16 | P | 0.24 | 0/1614 | 0.41 | 0/2177 |
| 17 | Q | 0.23 | 0/1603 | 0.41 | 0/2174 |
| 18 | R | 0.23 | 0/1579 | 0.39 | 0/2134 |
| 19 | S | 0.24 | 0/1671 | 0.41 | 0/2253 |
| 2 | B | 0.27 | 0/2700 | 0.55 | 0/3645 |
| 20 | T | 0.25 | 0/1700 | 0.41 | 0/2305 |
| 21 | U | 0.23 | 0/6396 | 0.42 | 0/8646 |
| 22 | V | 0.25 | 0/3929 | 0.52 | 2/5309 (0.0%) |
| 23 | W | 0.24 | 0/1975 | 0.46 | 0/2659 |
| 24 | X | 0.22 | 0/655 | 0.40 | 0/877 |
| 25 | Y | 0.24 | 0/3173 | 0.47 | 2/4273 (0.0%) |
| 26 | Z | 1.86 | 6/2324 (0.3%) | 0.53 | 0/3150 |
| 27 | a | 1.52 | 2/3052 (0.1%) | 0.55 | 4/4130 (0.1%) |
| 28 | b | 0.25 | 0/1478 | 0.43 | 0/2001 |
| 29 | c | 0.25 | 0/2302 | 0.53 | 2/3110 (0.1%) |
| 3 | C | 0.25 | 0/3054 | 0.52 | 1/4107 (0.0%) |
| 30 | d | 0.25 | 0/2162 | 0.51 | 0/2919 |
| 31 | e | 0.24 | 0/198 | 0.53 | 0/258 |
| 32 | f | 0.27 | 1/5413 (0.0%) | 0.53 | 3/7317 (0.0%) |
| 4 | D | 0.26 | 0/3090 | 0.53 | 0/4168 |
| 5 | E | 0.25 | 0/2835 | 0.48 | 0/3821 |
| 6 | F | 0.26 | 0/2903 | 0.54 | 0/3912 |
| 7 | G | 0.23 | 0/1859 | 0.45 | 0/2523 |
| 8 | H | 0.25 | 0/1743 | 0.46 | 0/2372 |
| 9 | I | 0.23 | 0/1942 | 0.45 | 0/2628 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| All | All | 0.51 | 9/74611 (0.0%) | 0.48 | 14/100825 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 2 |
| 21 | U | 0 | 3 |
| 22 | V | 0 | 2 |
| 25 | Y | 0 | 1 |
| 3 | C | 0 | 1 |
| 30 | d | 0 | 1 |
| 32 | f | 0 | 2 |
| 5 | E | 0 | 1 |
| 6 | F | 0 | 2 |
| All | All | 0 | 15 |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27 | a | 215 | GLU | CG-CD | 82.57 | 2.75 | 1.51 |
| 26 | Z | 228 | TYR | CD2-CE2 | 46.09 | 2.08 | 1.39 |
| 26 | Z | 228 | TYR | CD1-CE1 | 45.24 | 2.07 | 1.39 |
| 26 | Z | 228 | TYR | CE1-CZ | 34.72 | 1.83 | 1.38 |
| 26 | Z | 228 | TYR | CE2-CZ | 33.47 | 1.82 | 1.38 |

The worst 5 of 14 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 27 | a | 215 | GLU | OE1-CD-OE2 | -19.13 | 100.35 | 123.30 |
| 27 | a | 215 | GLU | CG-CD-OE1 | 6.35 | 131.00 | 118.30 |
| 29 | c | 243 | SER | C-N-CA | 6.19 | 137.17 | 121.70 |
| 27 | a | 215 | GLU | CB-CG-CD | 6.17 | 130.86 | 114.20 |
| 32 | f | 459 | GLU | N-CA-C | 6.13 | 127.56 | 111.00 |

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | B | 133 | VAL | Peptide |
| 2 | B | 264 | PRO | Peptide |
| 3 | C | 171 | HIS | Peptide |
| 5 | E | 292 | PRO | Peptide |
| 6 | F | 87 | PRO | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2835 | 0 | 2879 | 226 | 0 |
| 2 | B | 2662 | 0 | 2702 | 193 | 0 |
| 3 | C | 3015 | 0 | 3125 | 201 | 0 |
| 4 | D | 3040 | 0 | 3076 | 224 | 0 |
| 5 | E | 2790 | 0 | 2846 | 182 | 0 |
| 6 | F | 2863 | 0 | 2931 | 202 | 0 |
| 7 | G | 1826 | 0 | 1796 | 74 | 0 |
| 8 | H | 1708 | 0 | 1594 | 45 | 0 |
| 9 | I | 1912 | 0 | 1851 | 46 | 0 |
| 10 | J | 1704 | 0 | 1517 | 49 | 0 |
| 11 | K | 1722 | 0 | 1673 | 68 | 0 |
| 12 | L | 1850 | 0 | 1822 | 63 | 0 |
| 13 | M | 1856 | 0 | 1814 | 67 | 0 |
| 14 | N | 1430 | 0 | 1398 | 23 | 0 |
| 15 | O | 1643 | 0 | 1644 | 21 | 0 |
| 16 | P | 1585 | 0 | 1598 | 26 | 0 |
| 17 | Q | 1570 | 0 | 1547 | 50 | 0 |
| 18 | R | 1548 | 0 | 1499 | 31 | 0 |
| 19 | S | 1641 | 0 | 1618 | 25 | 0 |
| 20 | T | 1667 | 0 | 1628 | 42 | 0 |
| 21 | U | 6287 | 0 | 6338 | 191 | 0 |
| 22 | V | 3852 | 0 | 3893 | 181 | 0 |
| 23 | W | 1940 | 0 | 1978 | 73 | 0 |
| 24 | X | 647 | 0 | 676 | 22 | 0 |
| 25 | Y | 3115 | 0 | 3120 | 100 | 0 |
| 26 | Z | 2281 | 0 | 2312 | 95 | 0 |
| 27 | a | 2995 | 0 | 3011 | 0 | 0 |
| 28 | b | 1458 | 0 | 1505 | 0 | 0 |
| 29 | c | 2260 | 0 | 2276 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30 | d | 2116 | 0 | 2146 | 0 | 0 |
| 31 | e | 197 | 0 | 199 | 0 | 0 |
| 32 | f | 5331 | 0 | 5344 | 0 | 0 |
| 33 | A | 27 | 0 | 12 | 5 | 0 |
| 33 | B | 27 | 0 | 12 | 8 | 0 |
| 33 | C | 27 | 0 | 12 | 2 | 0 |
| 33 | D | 27 | 0 | 12 | 4 | 0 |
| 33 | E | 27 | 0 | 12 | 7 | 0 |
| 33 | F | 27 | 0 | 12 | 4 | 0 |
| 34 | c | 1 | 0 | 0 | 0 | 0 |
| All | All | 73509 | 0 | 73428 | 2249 | 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 2249 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) |
|------------------|------------------|--------------------------|-------------------|
| 26:Z:228:TYR:CZ | 26:Z:228:TYR:CE1 | 1.83 | 1.63 |
| 26:Z:228:TYR:CZ | 26:Z:228:TYR:CE2 | 1.82 | 1.60 |
| 26:Z:228:TYR:CD2 | 26:Z:228:TYR:CE2 | 2.08 | 1.42 |
| 26:Z:228:TYR:CD1 | 26:Z:228:TYR:CE1 | 2.07 | 1.40 |
| 1:A:362:MET:HB2 | 2:B:216:ILE:HD11 | 1.47 | 0.97 |

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 | 359/433 (83%) | 304 (85%) | 53 (15%) | 2 (1%) | 30 | 74 |
| 2 | B | 339/440 (77%) | 298 (88%) | 38 (11%) | 3 (1%) | 21 | 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|----------|-------------|-----|
| 3 | C | 382/398 (96%) | 317 (83%) | 62 (16%) | 3 (1%) | 24 | 69 |
| 4 | D | 378/418 (90%) | 328 (87%) | 49 (13%) | 1 (0%) | 46 | 83 |
| 5 | E | 351/403 (87%) | 299 (85%) | 51 (14%) | 1 (0%) | 46 | 83 |
| 6 | F | 362/439 (82%) | 316 (87%) | 45 (12%) | 1 (0%) | 46 | 83 |
| 7 | G | 238/245 (97%) | 221 (93%) | 16 (7%) | 1 (0%) | 39 | 80 |
| 8 | H | 230/233 (99%) | 210 (91%) | 19 (8%) | 1 (0%) | 39 | 80 |
| 9 | I | 248/260 (95%) | 230 (93%) | 18 (7%) | 0 | 100 | 100 |
| 10 | J | 237/247 (96%) | 221 (93%) | 15 (6%) | 1 (0%) | 39 | 80 |
| 11 | K | 224/240 (93%) | 203 (91%) | 20 (9%) | 1 (0%) | 39 | 80 |
| 12 | L | 236/268 (88%) | 222 (94%) | 14 (6%) | 0 | 100 | 100 |
| 13 | M | 238/254 (94%) | 218 (92%) | 20 (8%) | 0 | 100 | 100 |
| 14 | N | 189/238 (79%) | 175 (93%) | 14 (7%) | 0 | 100 | 100 |
| 15 | O | 218/276 (79%) | 209 (96%) | 9 (4%) | 0 | 100 | 100 |
| 16 | P | 202/204 (99%) | 188 (93%) | 14 (7%) | 0 | 100 | 100 |
| 17 | Q | 197/201 (98%) | 183 (93%) | 14 (7%) | 0 | 100 | 100 |
| 18 | R | 199/262 (76%) | 190 (96%) | 9 (4%) | 0 | 100 | 100 |
| 19 | S | 211/240 (88%) | 199 (94%) | 12 (6%) | 0 | 100 | 100 |
| 20 | T | 213/263 (81%) | 204 (96%) | 9 (4%) | 0 | 100 | 100 |
| 21 | U | 798/953 (84%) | 729 (91%) | 67 (8%) | 2 (0%) | 46 | 83 |
| 22 | V | 478/533 (90%) | 416 (87%) | 60 (13%) | 2 (0%) | 39 | 80 |
| 23 | W | 234/456 (51%) | 213 (91%) | 21 (9%) | 0 | 100 | 100 |
| 24 | X | 79/422 (19%) | 75 (95%) | 4 (5%) | 0 | 100 | 100 |
| 25 | Y | 376/389 (97%) | 336 (89%) | 38 (10%) | 2 (0%) | 34 | 77 |
| 26 | Z | 284/324 (88%) | 251 (88%) | 32 (11%) | 1 (0%) | 39 | 80 |
| 27 | a | 369/376 (98%) | 340 (92%) | 27 (7%) | 2 (0%) | 34 | 77 |
| 28 | b | 189/377 (50%) | 178 (94%) | 11 (6%) | 0 | 100 | 100 |
| 29 | c | 285/309 (92%) | 242 (85%) | 39 (14%) | 4 (1%) | 14 | 58 |
| 30 | d | 255/349 (73%) | 219 (86%) | 34 (13%) | 2 (1%) | 24 | 69 |
| 31 | e | 20/70 (29%) | 16 (80%) | 4 (20%) | 0 | 100 | 100 |
| 32 | f | 686/749 (92%) | 574 (84%) | 108 (16%) | 4 (1%) | 30 | 74 |
| All | All | 9304/11269 (83%) | 8324 (90%) | 946 (10%) | 34 (0%) | 43 | 80 |

5 of 34 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 111 | VAL |
| 11 | K | 12 | VAL |
| 21 | U | 364 | VAL |
| 25 | Y | 350 | VAL |
| 29 | c | 244 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | A | 308/372 (83%) | 305 (99%) | 3 (1%) | 82 | 92 |
| 2 | B | 298/385 (77%) | 294 (99%) | 4 (1%) | 76 | 89 |
| 3 | C | 332/346 (96%) | 324 (98%) | 8 (2%) | 57 | 82 |
| 4 | D | 333/366 (91%) | 329 (99%) | 4 (1%) | 78 | 90 |
| 5 | E | 308/353 (87%) | 306 (99%) | 2 (1%) | 90 | 95 |
| 6 | F | 312/379 (82%) | 303 (97%) | 9 (3%) | 50 | 78 |
| 7 | G | 193/209 (92%) | 192 (100%) | 1 (0%) | 92 | 96 |
| 8 | H | 164/190 (86%) | 162 (99%) | 2 (1%) | 78 | 90 |
| 9 | I | 193/220 (88%) | 193 (100%) | 0 | 100 | 100 |
| 10 | J | 152/210 (72%) | 151 (99%) | 1 (1%) | 88 | 94 |
| 11 | K | 186/202 (92%) | 185 (100%) | 1 (0%) | 92 | 96 |
| 12 | L | 198/229 (86%) | 197 (100%) | 1 (0%) | 92 | 96 |
| 13 | M | 192/211 (91%) | 191 (100%) | 1 (0%) | 92 | 96 |
| 14 | N | 148/180 (82%) | 148 (100%) | 0 | 100 | 100 |
| 15 | O | 177/227 (78%) | 177 (100%) | 0 | 100 | 100 |
| 16 | P | 172/173 (99%) | 172 (100%) | 0 | 100 | 100 |
| 17 | Q | 164/171 (96%) | 164 (100%) | 0 | 100 | 100 |
| 18 | R | 153/201 (76%) | 153 (100%) | 0 | 100 | 100 |
| 19 | S | 174/198 (88%) | 174 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 20 | T | 175/214 (82%) | 174 (99%) | 1 (1%) | 90 | 95 |
| 21 | U | 685/816 (84%) | 679 (99%) | 6 (1%) | 84 | 93 |
| 22 | V | 414/459 (90%) | 408 (99%) | 6 (1%) | 74 | 89 |
| 23 | W | 218/416 (52%) | 215 (99%) | 3 (1%) | 74 | 89 |
| 24 | X | 74/362 (20%) | 74 (100%) | 0 | 100 | 100 |
| 25 | Y | 334/344 (97%) | 330 (99%) | 4 (1%) | 78 | 90 |
| 26 | Z | 257/295 (87%) | 254 (99%) | 3 (1%) | 78 | 90 |
| 27 | a | 333/336 (99%) | 333 (100%) | 0 | 100 | 100 |
| 28 | b | 167/312 (54%) | 166 (99%) | 1 (1%) | 90 | 95 |
| 29 | c | 252/267 (94%) | 249 (99%) | 3 (1%) | 78 | 90 |
| 30 | d | 231/293 (79%) | 229 (99%) | 2 (1%) | 84 | 93 |
| 31 | e | 22/63 (35%) | 22 (100%) | 0 | 100 | 100 |
| 32 | f | 582/628 (93%) | 574 (99%) | 8 (1%) | 74 | 89 |
| All | All | 7901/9627 (82%) | 7827 (99%) | 74 (1%) | 85 | 93 |

5 of 74 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 114 | LEU |
| 21 | U | 554 | LEU |
| 32 | f | 371 | CYS |
| 11 | K | 101 | PHE |
| 20 | T | 168 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 392 | ASN |
| 21 | U | 421 | GLN |
| 30 | d | 245 | GLN |
| 7 | G | 123 | GLN |
| 11 | K | 23 | GLN |

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 33 | ADP | A | 501 | - | 24,29,29 | 1.03 | 1 (4%) | 23,45,45 | 1.67 | 1 (4%) |
| 33 | ADP | B | 501 | - | 24,29,29 | 0.99 | 1 (4%) | 23,45,45 | 1.82 | 2 (8%) |
| 33 | ADP | C | 501 | - | 24,29,29 | 1.01 | 1 (4%) | 23,45,45 | 1.65 | 1 (4%) |
| 33 | ADP | D | 501 | - | 24,29,29 | 0.96 | 1 (4%) | 23,45,45 | 1.71 | 1 (4%) |
| 33 | ADP | E | 401 | - | 24,29,29 | 1.02 | 1 (4%) | 23,45,45 | 2.07 | 6 (26%) |
| 33 | ADP | F | 501 | - | 24,29,29 | 1.04 | 1 (4%) | 23,45,45 | 1.74 | 2 (8%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 33 | ADP | A | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 33 | ADP | B | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 33 | ADP | C | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 33 | ADP | D | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 33 | ADP | E | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 33 | ADP | F | 501 | - | - | 0/12/32/32 | 0/3/3/3 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 33 | D | 501 | ADP | C5-C4 | 3.04 | 1.47 | 1.40 |
| 33 | B | 501 | ADP | C5-C4 | 3.06 | 1.47 | 1.40 |
| 33 | E | 401 | ADP | C5-C4 | 3.10 | 1.47 | 1.40 |
| 33 | F | 501 | ADP | C5-C4 | 3.19 | 1.47 | 1.40 |
| 33 | C | 501 | ADP | C5-C4 | 3.20 | 1.47 | 1.40 |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 33 | E | 401 | ADP | N3-C2-N1 | -6.73 | 123.59 | 128.87 |
| 33 | B | 501 | ADP | N3-C2-N1 | -6.70 | 123.61 | 128.87 |
| 33 | D | 501 | ADP | N3-C2-N1 | -6.57 | 123.71 | 128.87 |
| 33 | F | 501 | ADP | N3-C2-N1 | -6.56 | 123.72 | 128.87 |
| 33 | A | 501 | ADP | N3-C2-N1 | -6.31 | 123.92 | 128.87 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 30 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 33 | A | 501 | ADP | 5 | 0 |
| 33 | B | 501 | ADP | 8 | 0 |
| 33 | C | 501 | ADP | 2 | 0 |
| 33 | D | 501 | ADP | 4 | 0 |
| 33 | E | 401 | ADP | 7 | 0 |
| 33 | F | 501 | ADP | 4 | 0 |

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 |
|-----|-------|------------------|
| 32 | f | 3 |
| 27 | a | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | f | 110:ALA | C | 111:LEU | N | 8.67 |
| 1 | f | 79:ASN | C | 80:TYR | N | 7.26 |
| 1 | f | 348:ASP | C | 349:SER | N | 6.44 |
| 1 | a | 341:LEU | C | 342:ASP | N | 5.77 |