# wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 10:28 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 2A69 |
| Title | : | Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic rifapentin |
| Authors | : | Artsimovitch, I.; Vassylyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI) |
| Deposited on | : | 2005-07-02 |
| Resolution | : | 2.50 Å(reported) |

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

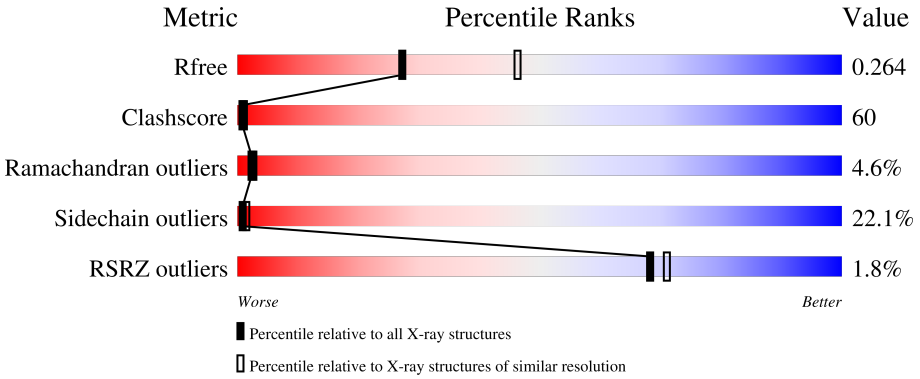
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 4661 (2.50-2.50) |
| Clashscore | 141614 | 5346 (2.50-2.50) |
| Ramachandran outliers | 138981 | 5231 (2.50-2.50) |
| Sidechain outliers | 138945 | 5233 (2.50-2.50) |
| RSRZ outliers | 127900 | 4559 (2.50-2.50) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 315 | 17% 44% 10% • 27% |
| 1 | B | 315 | 4% 18% 43% 11% 27% |
| 1 | K | 315 | % 23% 40% 9% • 27% |
| 1 | L | 315 | 2% 19% 43% 10% 27% |
| 2 | C | 1119 | % 22% 59% 18% • |

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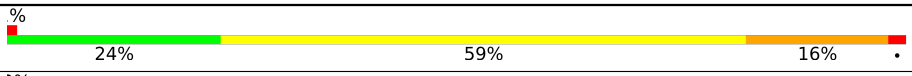
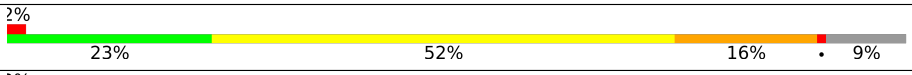
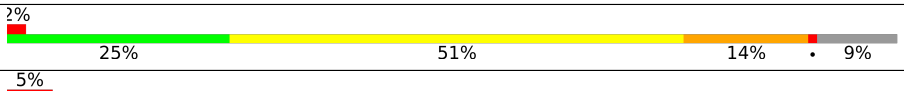
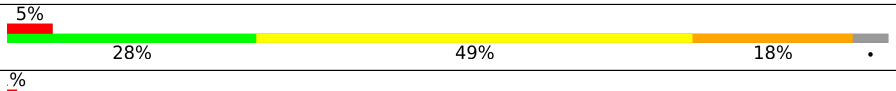
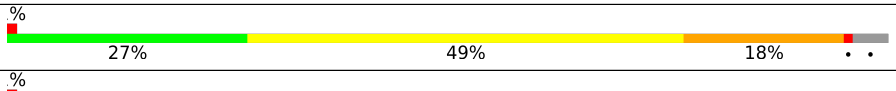
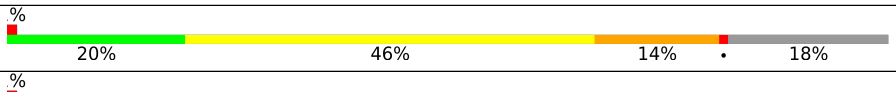
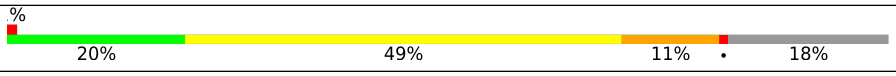
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | M | 1119 |   |
| 3 | D | 1524 |   |
| 3 | N | 1524 |   |
| 4 | E | 99 |   |
| 4 | O | 99 |   |
| 5 | F | 423 |   |
| 5 | P | 423 |   |

# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 60572 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-directed RNA polymerase alpha chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 229 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1806 | 1153 | 313 | 337 | 3 | | | |
| 1 | B | 229 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1806 | 1153 | 313 | 337 | 3 | | | |
| 1 | K | 229 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1806 | 1153 | 313 | 337 | 3 | | | |
| 1 | L | 229 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1806 | 1153 | 313 | 337 | 3 | | | |

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 1119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8829 | 5581 | 1577 | 1647 | 24 | | | |
| 2 | M | 1119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8829 | 5581 | 1577 | 1647 | 24 | | | |

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | D | 1392 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10797 | 6819 | 1925 | 2020 | 33 | | | |
| 3 | N | 1392 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10797 | 6819 | 1925 | 2020 | 33 | | | |

- Molecule 4 is a protein called RNA polymerase omega chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | E | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 488 | 133 | 144 | 4 | | | |
| 4 | O | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 488 | 133 | 144 | 4 | | | |

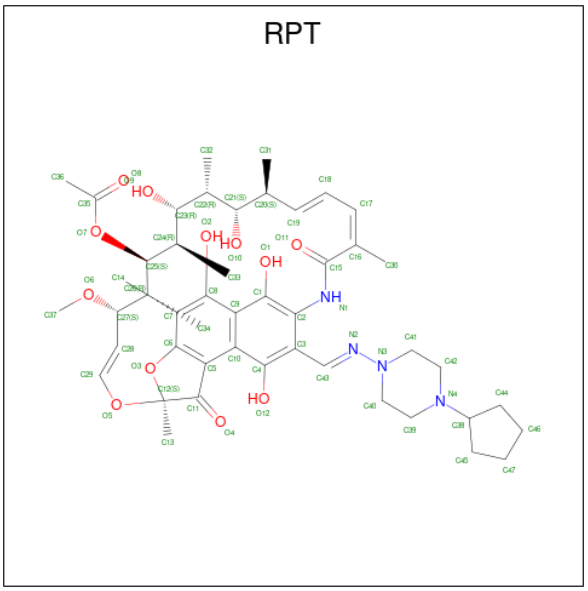
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | F | 345 | Total 2771 | C 1744 | N 504 | O 519 | S 4 | 0 | 0 | 0 |
| 5 | P | 345 | Total 2771 | C 1744 | N 504 | O 519 | S 4 | 0 | 0 | 0 |

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 6 | A | 33 | Total 33 | Mg 33 | 0 | 0 |
| 6 | B | 21 | Total 21 | Mg 21 | 0 | 0 |
| 6 | C | 73 | Total 73 | Mg 73 | 0 | 0 |
| 6 | D | 106 | Total 106 | Mg 106 | 0 | 0 |
| 6 | E | 5 | Total 5 | Mg 5 | 0 | 0 |
| 6 | F | 28 | Total 28 | Mg 28 | 0 | 0 |
| 6 | K | 19 | Total 19 | Mg 19 | 0 | 0 |
| 6 | L | 17 | Total 17 | Mg 17 | 0 | 0 |
| 6 | M | 65 | Total 65 | Mg 65 | 0 | 0 |
| 6 | N | 92 | Total 92 | Mg 92 | 0 | 0 |
| 6 | O | 8 | Total 8 | Mg 8 | 0 | 0 |
| 6 | P | 20 | Total 20 | Mg 20 | 0 | 0 |

- Molecule 7 is RIFAPENTINE (three-letter code: RPT) (formula: $C_{47}H_{64}N_4O_{12}$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 7 | C | 1 | Total C N O<br>63 47 4 12 | 0 | 0 |
| 7 | M | 1 | Total C N O<br>63 47 4 12 | 0 | 0 |

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 8 | D | 2 | Total Zn<br>2 2 | 0 | 0 |
| 8 | N | 2 | Total Zn<br>2 2 | 0 | 0 |

- Molecule 9 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 9 | A | 239 | Total O<br>239 239 | 0 | 0 |
| 9 | B | 258 | Total O<br>258 258 | 0 | 0 |
| 9 | C | 979 | Total O<br>979 979 | 0 | 0 |
| 9 | D | 1252 | Total O<br>1252 1252 | 0 | 0 |
| 9 | E | 117 | Total O<br>117 117 | 0 | 0 |

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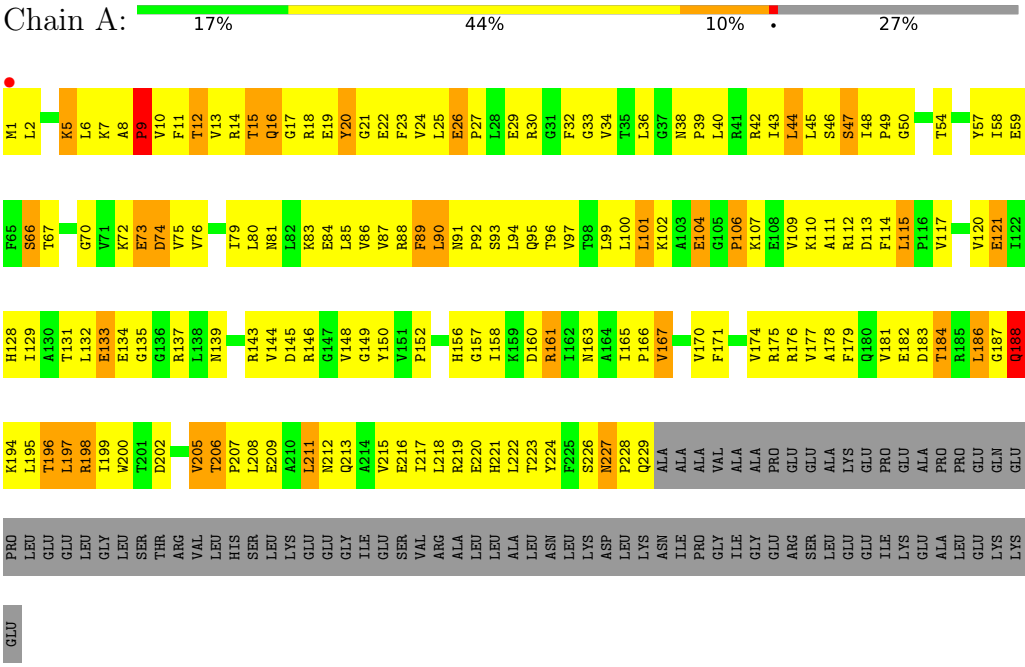
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 9 | F | 420 | Total O<br>420 420 | 0 | 0 |
| 9 | K | 183 | Total O<br>183 183 | 0 | 0 |
| 9 | L | 219 | Total O<br>219 219 | 0 | 0 |
| 9 | M | 998 | Total O<br>998 998 | 0 | 0 |
| 9 | N | 1265 | Total O<br>1265 1265 | 0 | 0 |
| 9 | O | 108 | Total O<br>108 108 | 0 | 0 |
| 9 | P | 361 | Total O<br>361 361 | 0 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

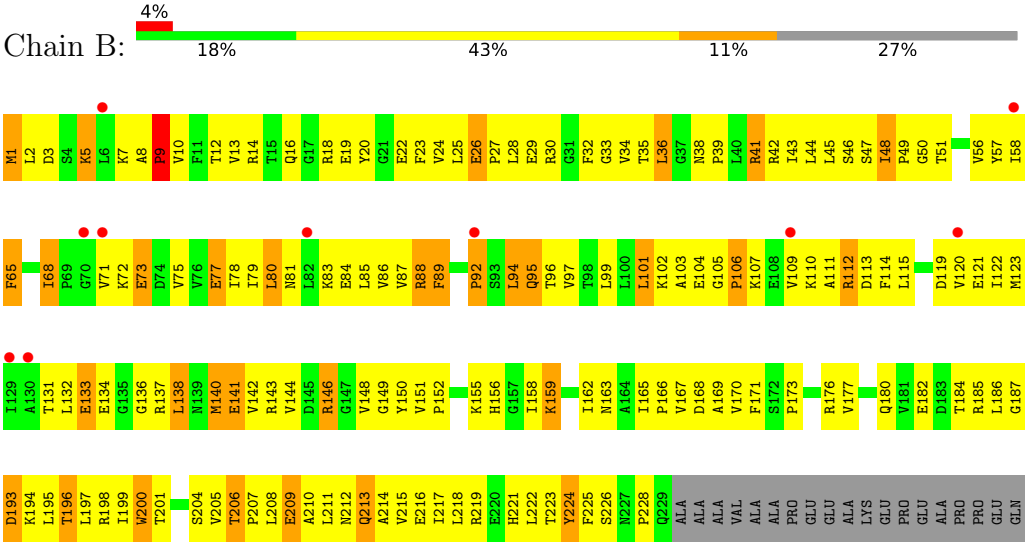
• Molecule 1: DNA-directed RNA polymerase alpha chain

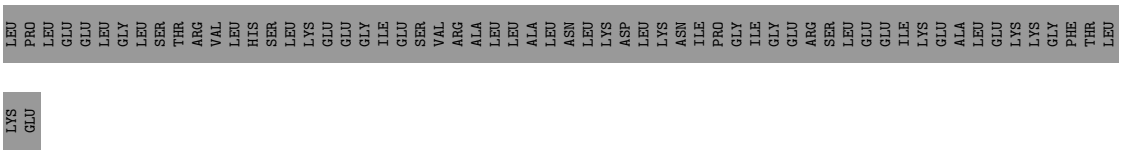
Chain A:




• Molecule 1: DNA-directed RNA polymerase alpha chain

Chain B:

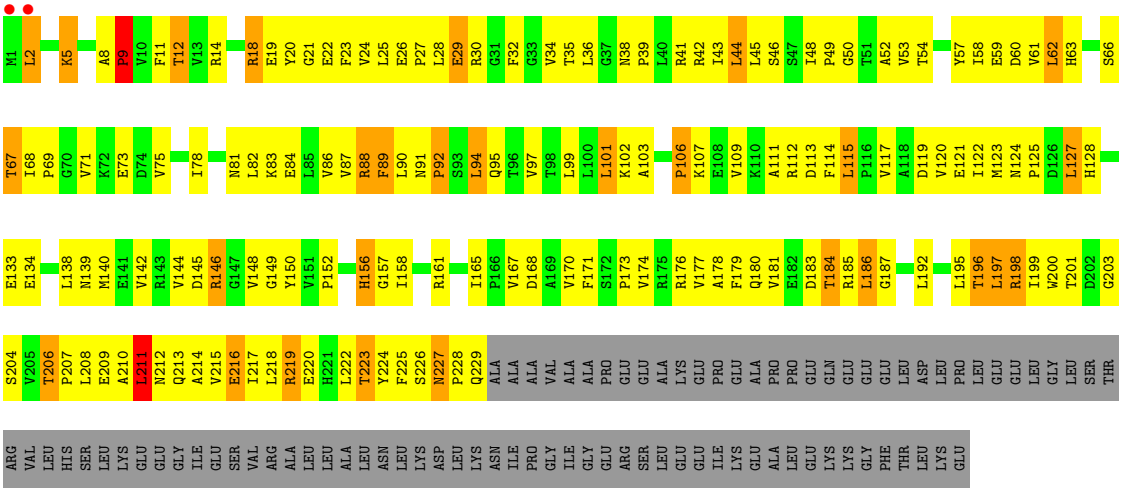






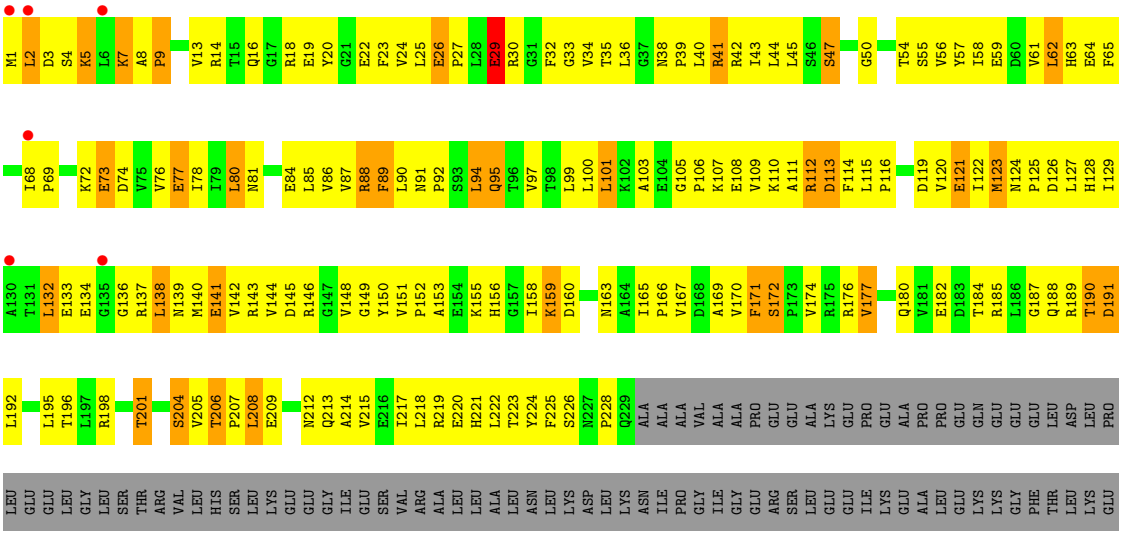
• Molecule 1: DNA-directed RNA polymerase alpha chain

Chain K:

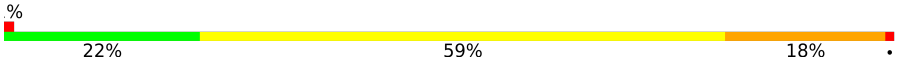
• Molecule 1: DNA-directed RNA polymerase alpha chain

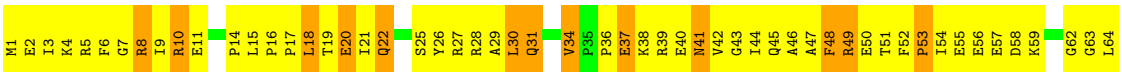
Chain L:

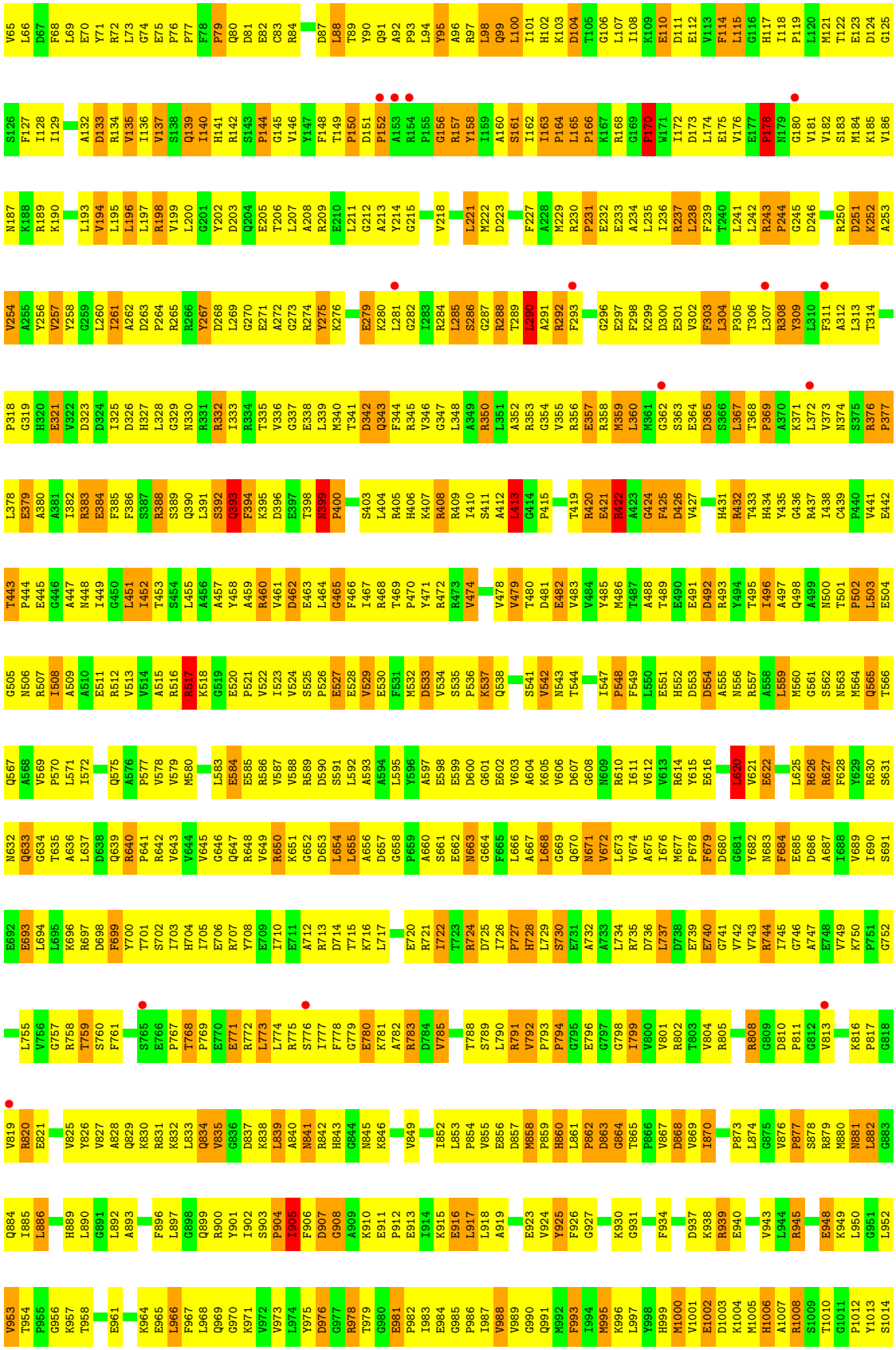



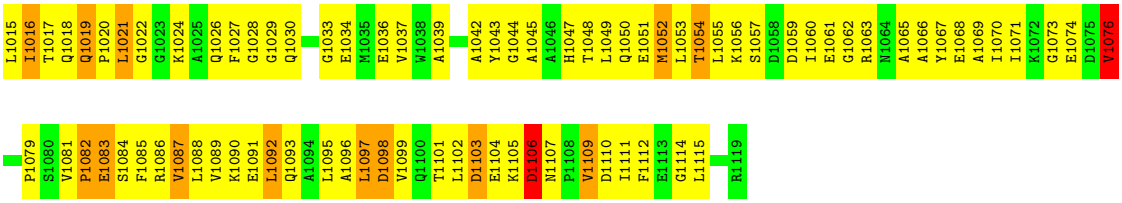
• Molecule 2: DNA-directed RNA polymerase beta chain

Chain C:



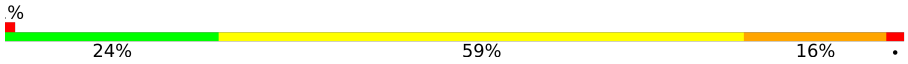


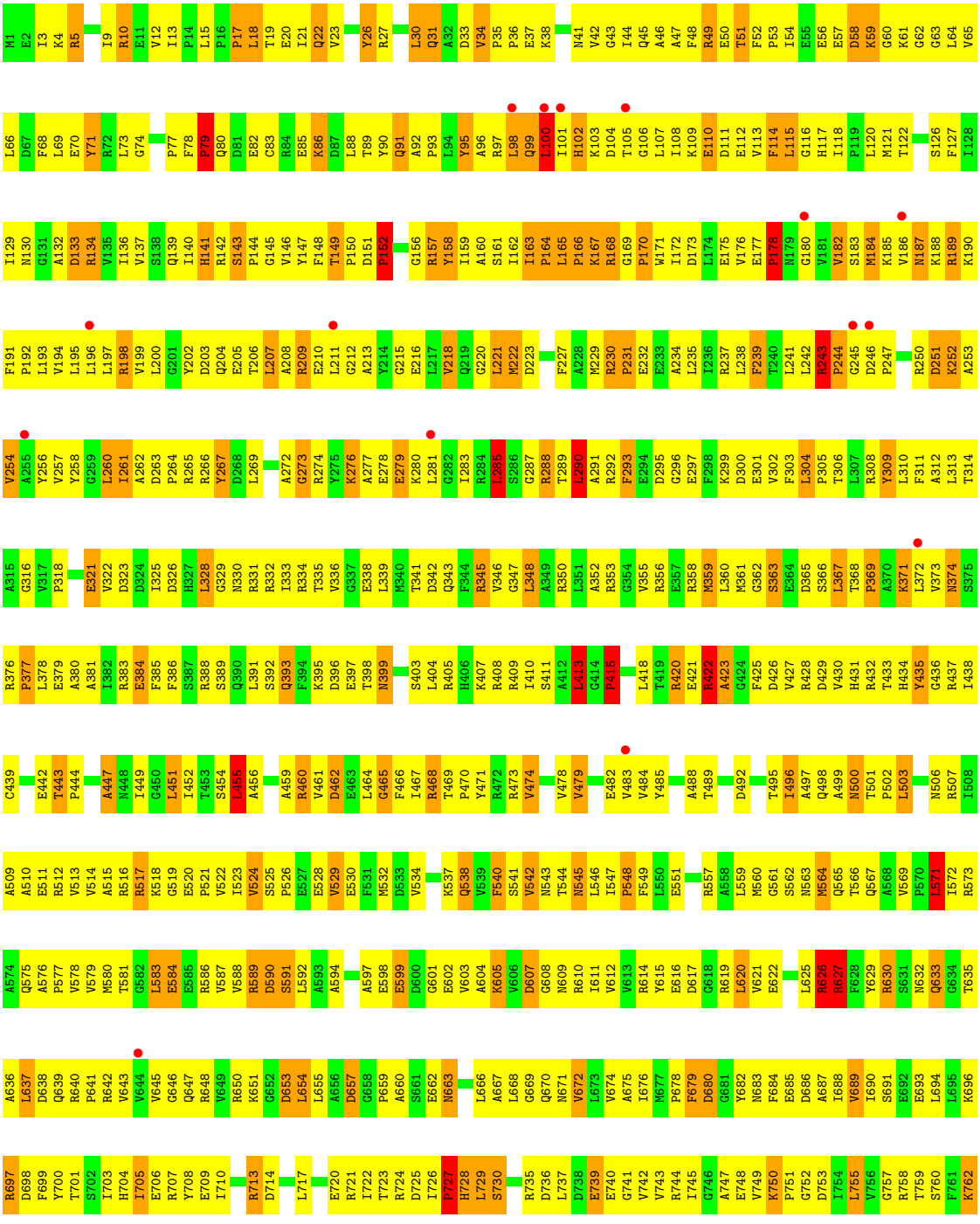


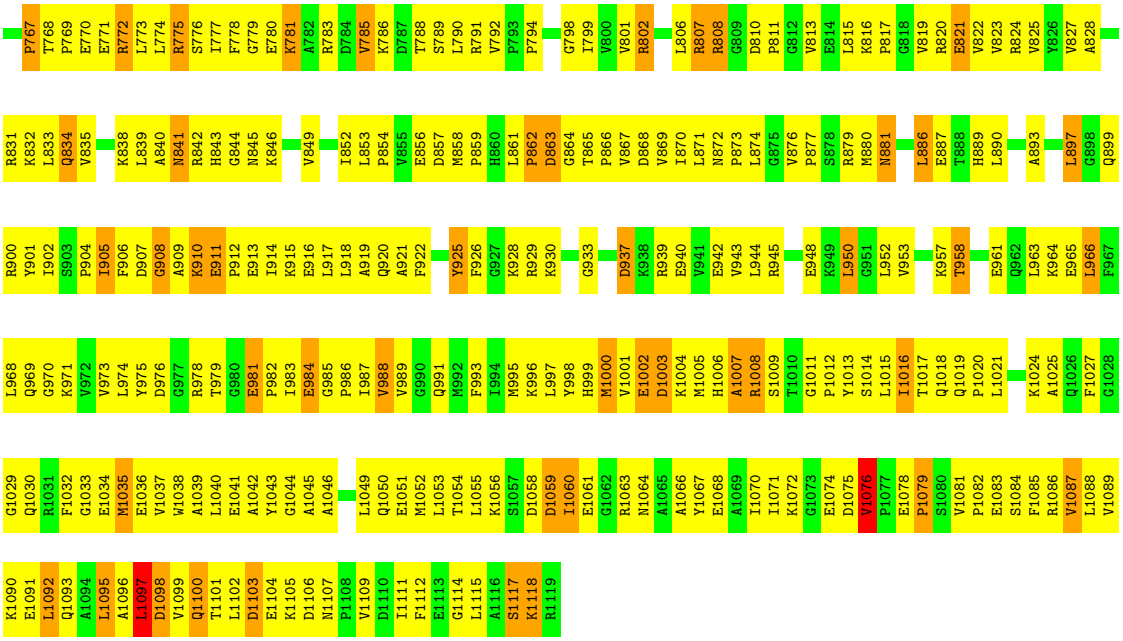


• Molecule 2: DNA-directed RNA polymerase beta chain

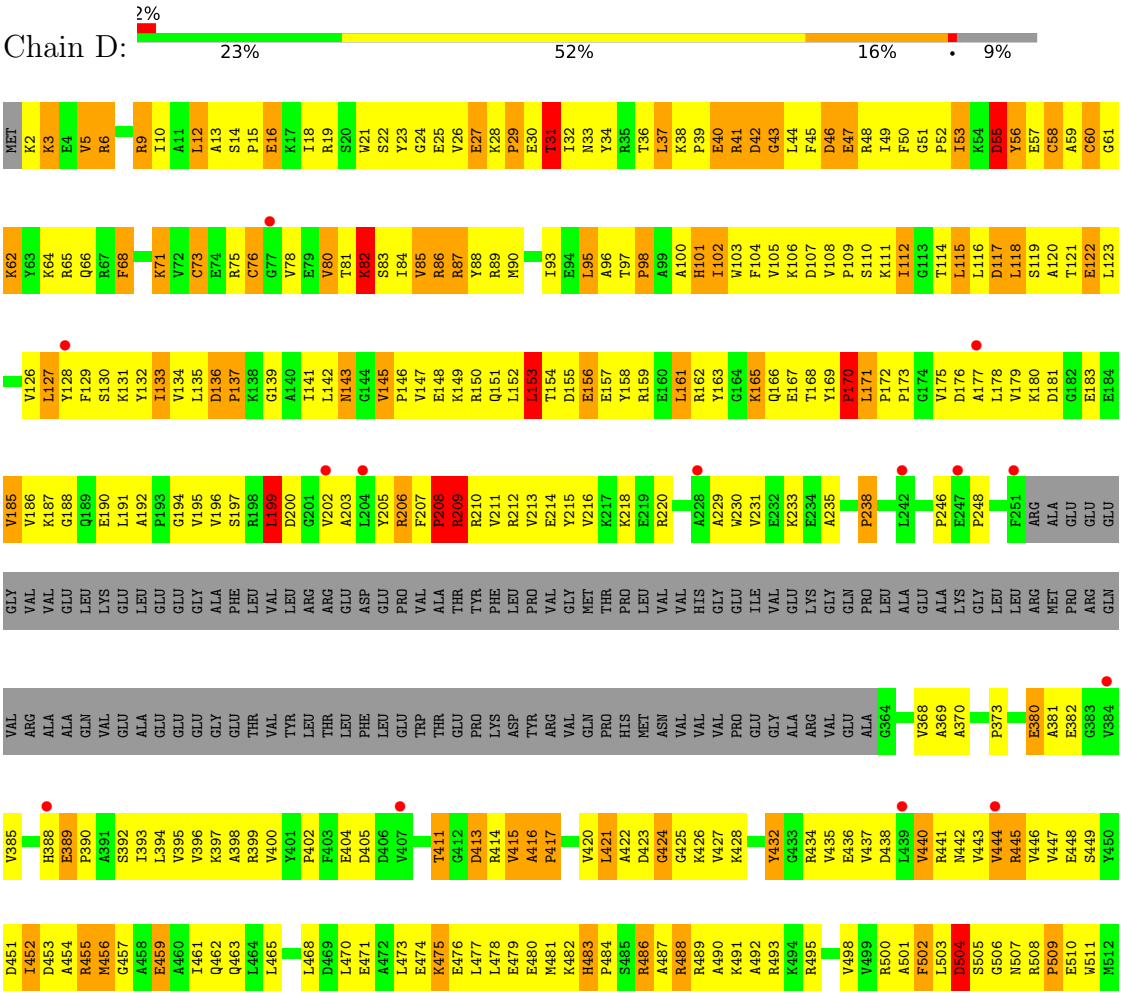
Chain M:

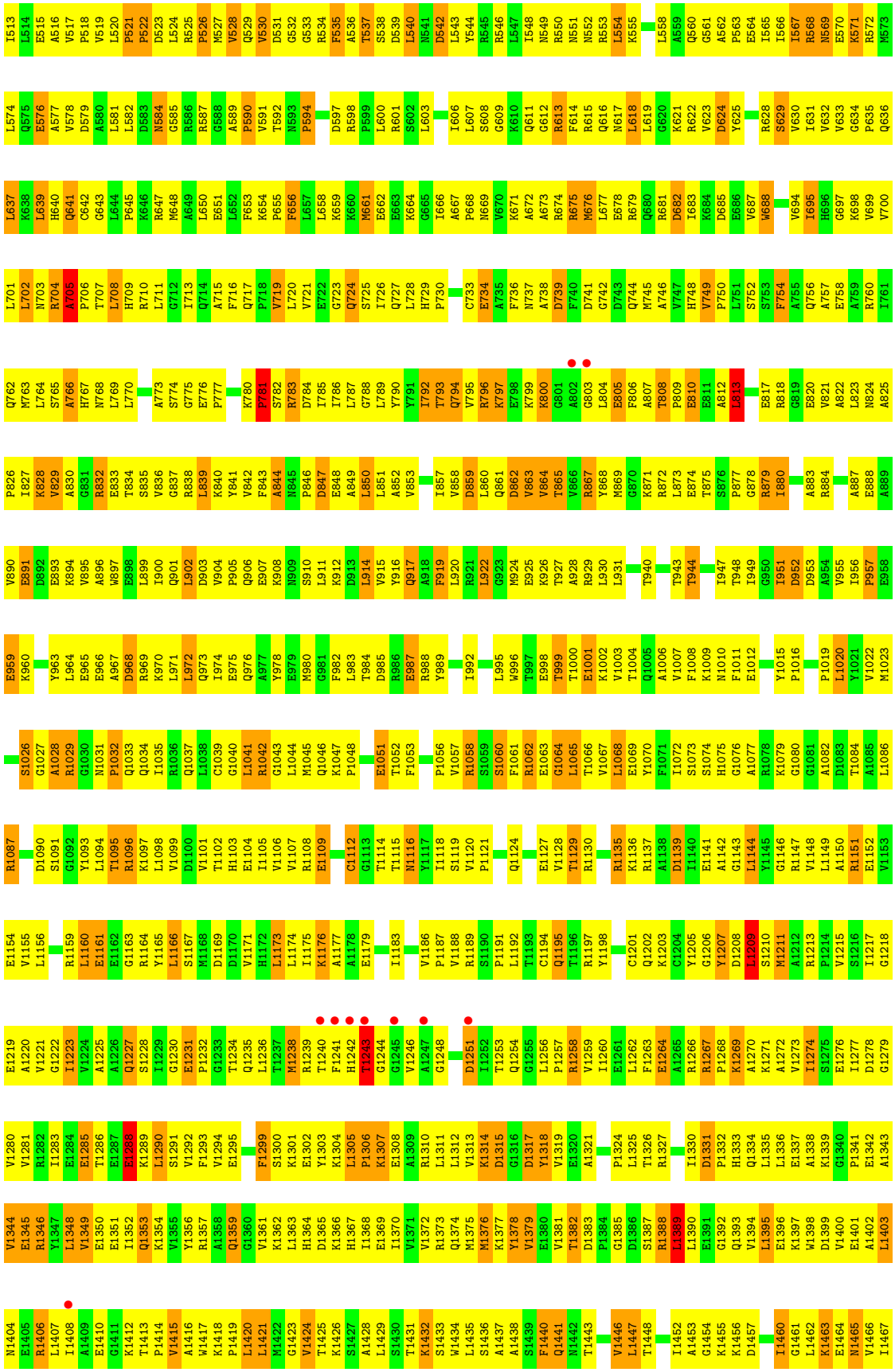


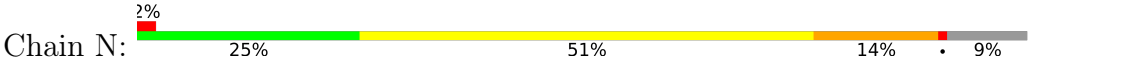


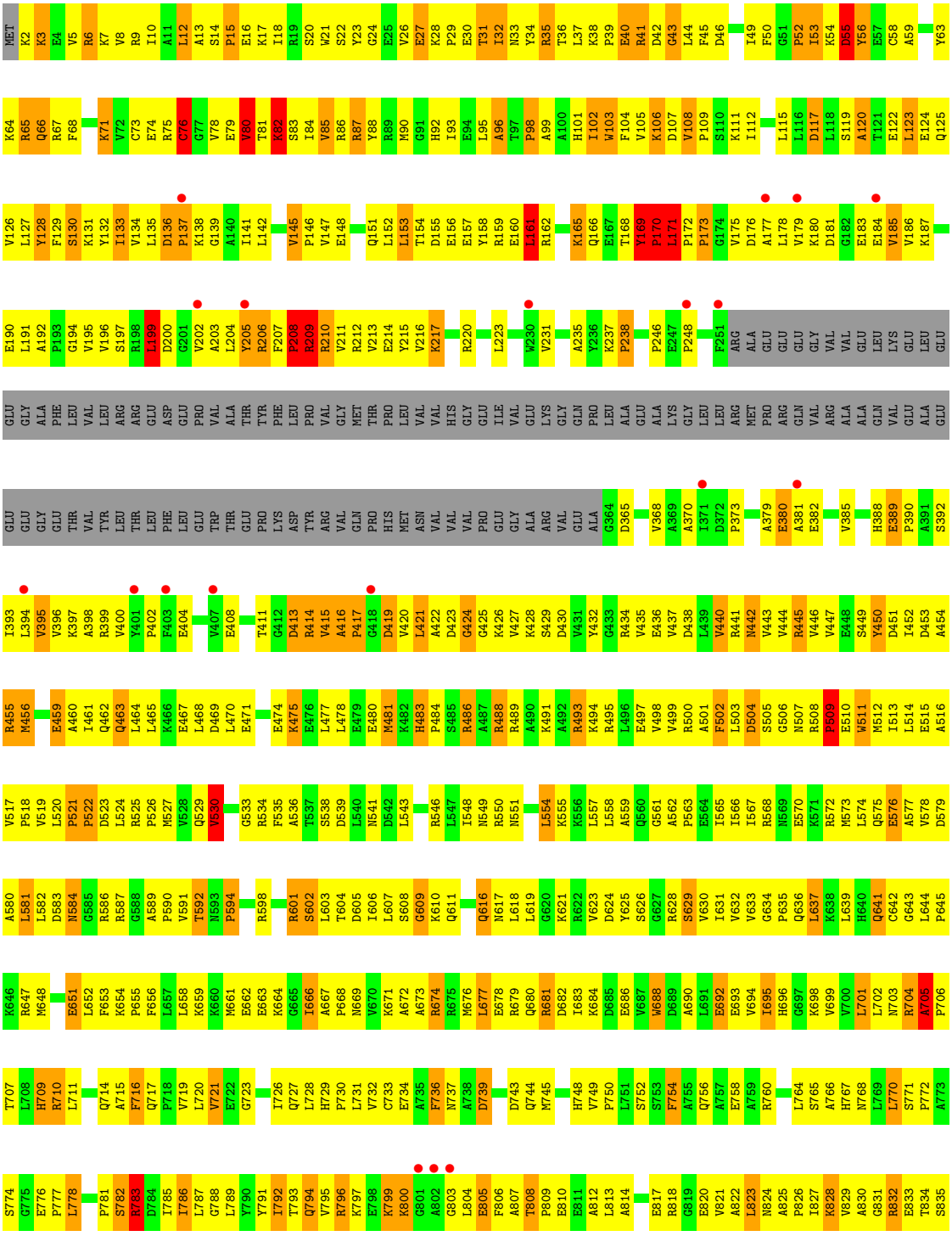
• Molecule 3: DNA-directed RNA polymerase beta' chain

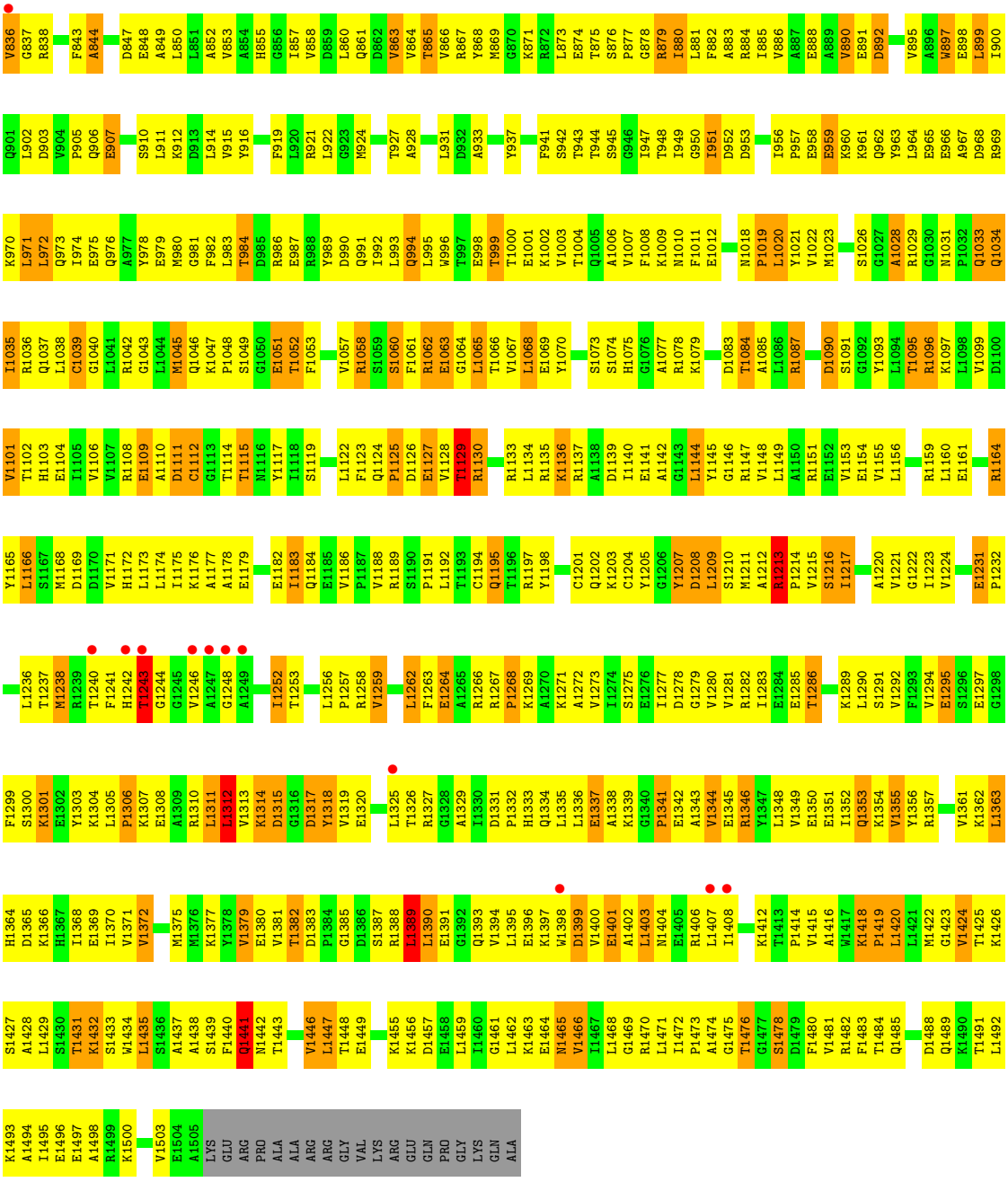




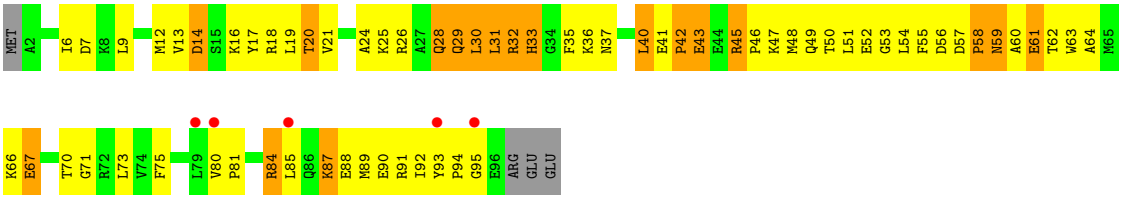
• Molecule 3: DNA-directed RNA polymerase beta' chain



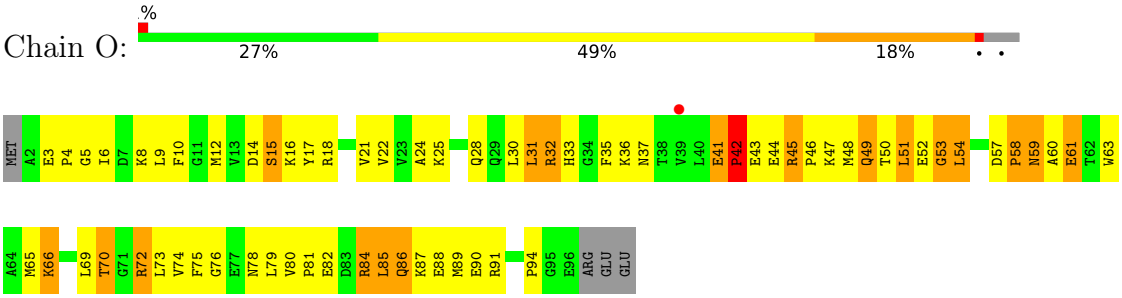


• Molecule 4: RNA polymerase omega chain

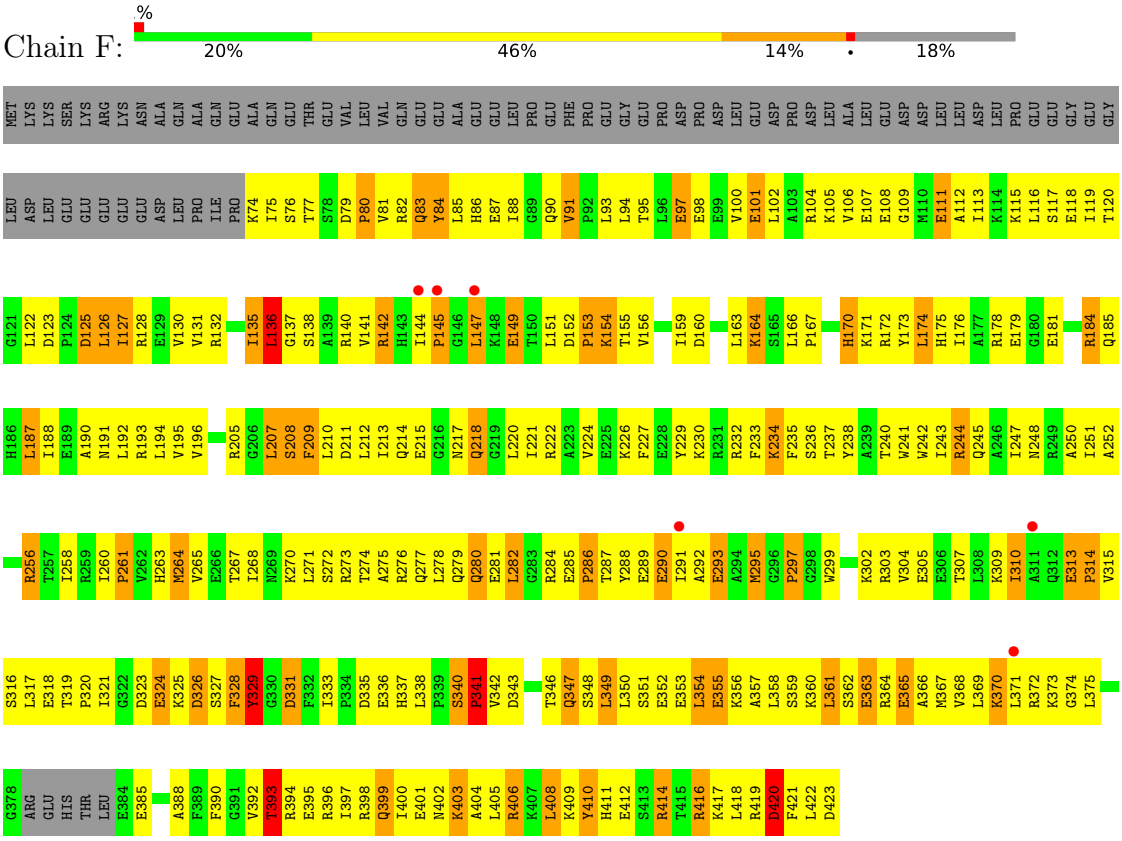
• Molecule 4: RNA polymerase omega chain

Chain O:



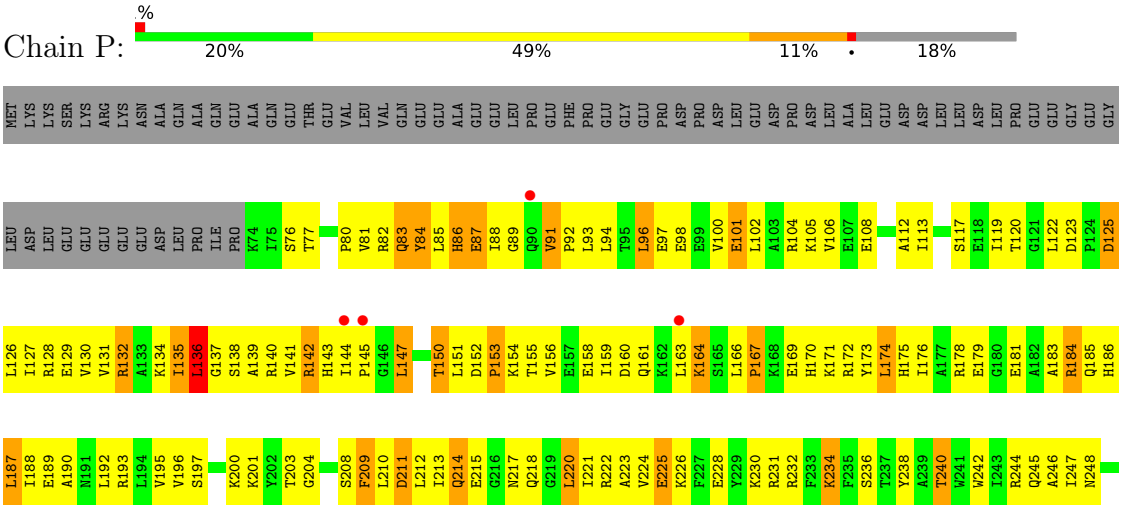

• Molecule 5: RNA polymerase sigma factor rpoD

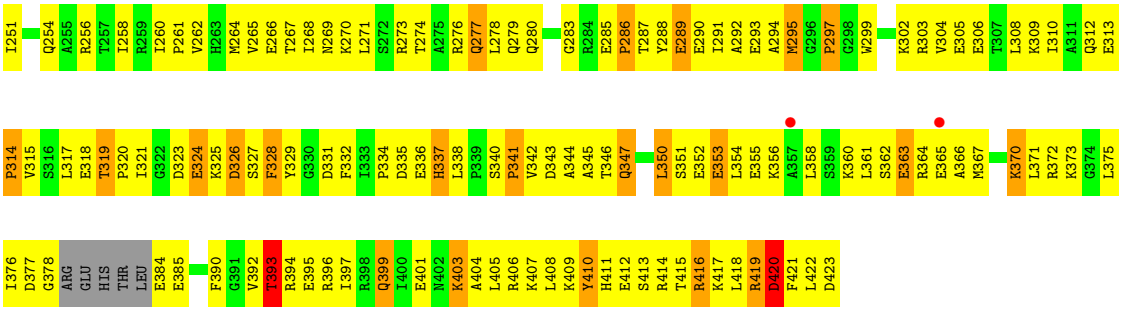
Chain F:




• Molecule 5: RNA polymerase sigma factor rpoD

Chain P:




I251 Q254 A255 R256 T257 I258 R259 I260 P261 V262 H263 M264 V265 E266 T267 I268 N269 K270 L271 S272 R273 T274 A275 R276 Q277 L278 Q279 Q280 G283 R284 E285 P286 T287 Y288 E289 E290 I291 A292 E293 A294 M295 G296 P297 G298 W299 K302 R303 V304 E305 E306 T307 L308 K309 I310 A311 Q312 E313
P314 V315 S316 L317 E318 T319 P320 I321 G322 D323 E324 K325 D326 S327 F328 Y329 G330 D331 F332 I333 P334 D335 E336 H337 L338 P339 S340 P341 V342 D343 A344 A345 T346 Q347 L350 S351 E352 E353 L354 E355 K356 A357 L358 S359 K360 L361 S362 E363 R364 E365 A366 M367 K370 L371 R372 K373 G374 L375
I376 D377 G378 ARG GLU HIS THR LEU E384 E385 F390 G391 V392 T393 R394 E395 R396 I397 R398 Q399 I400 E401 N402 K403 A404 L405 R406 K407 L408 K409 Y410 H411 E412 S413 R414 T415 R416 K417 L418 R419 D420 F421 L422 D423

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 32 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 239.50Å 239.50Å 253.10Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 25.00 – 2.50<br>24.85 – 2.50 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | (Not available) (25.00-2.50)<br>92.5 (24.85-2.50) | Depositor<br>EDS |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.13 (at 2.50Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.230 , 0.267<br>0.228 , 0.264 | Depositor<br>DCC |
| $R_{free}$ test set | 29710 reflections (5.75%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 47.8 | Xtriage |
| Anisotropy | 0.214 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.27 , 76.6 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.40$, $< L^2 > = 0.23$ | Xtriage |
| Estimated twinning fraction | 0.499 for -h,-k,l<br>0.076 for h,-h-k,-l<br>0.076 for -k,-h,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 60572 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 71.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RPT, MG, 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 | 0.81 | 1/1838 (0.1%) | 0.88 | 4/2498 (0.2%) |
| 1 | B | 0.74 | 0/1838 | 0.81 | 2/2498 (0.1%) |
| 1 | K | 0.75 | 0/1838 | 0.86 | 3/2498 (0.1%) |
| 1 | L | 0.73 | 1/1838 (0.1%) | 0.80 | 2/2498 (0.1%) |
| 2 | C | 0.83 | 2/8997 (0.0%) | 0.89 | 7/12164 (0.1%) |
| 2 | M | 0.81 | 0/8997 | 0.88 | 8/12164 (0.1%) |
| 3 | D | 0.84 | 0/10975 | 0.94 | 20/14836 (0.1%) |
| 3 | N | 0.82 | 0/10975 | 0.92 | 17/14836 (0.1%) |
| 4 | E | 0.84 | 0/783 | 0.94 | 0/1054 |
| 4 | O | 0.82 | 0/783 | 0.96 | 2/1054 (0.2%) |
| 5 | F | 0.74 | 0/2812 | 0.82 | 4/3781 (0.1%) |
| 5 | P | 0.71 | 0/2812 | 0.80 | 1/3781 (0.0%) |
| All | All | 0.81 | 4/54486 (0.0%) | 0.89 | 70/73662 (0.1%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 48 | ILE | C-N | 6.06 | 1.45 | 1.34 |
| 1 | L | 172 | SER | N-CA | -5.43 | 1.35 | 1.46 |
| 2 | C | 792 | VAL | CB-CG1 | -5.28 | 1.41 | 1.52 |
| 2 | C | 393 | GLN | CD-OE1 | 5.25 | 1.35 | 1.24 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 1389 | LEU | CA-CB-CG | 8.13 | 133.99 | 115.30 |
| 1 | K | 211 | LEU | CA-CB-CG | 8.11 | 133.95 | 115.30 |
| 1 | B | 138 | LEU | CA-CB-CG | 7.70 | 133.00 | 115.30 |
| 1 | A | 192 | LEU | CA-CB-CG | 7.60 | 132.79 | 115.30 |
| 3 | D | 199 | LEU | CA-CB-CG | -7.59 | 97.84 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | 1806 | 0 | 1861 | 232 | 0 |
| 1 | B | 1806 | 0 | 1861 | 216 | 0 |
| 1 | K | 1806 | 0 | 1861 | 173 | 0 |
| 1 | L | 1806 | 0 | 1861 | 186 | 0 |
| 2 | C | 8829 | 0 | 8933 | 1215 | 0 |
| 2 | M | 8829 | 0 | 8933 | 1174 | 0 |
| 3 | D | 10797 | 0 | 10873 | 1490 | 0 |
| 3 | N | 10797 | 0 | 10873 | 1288 | 0 |
| 4 | E | 769 | 0 | 775 | 89 | 0 |
| 4 | O | 769 | 0 | 775 | 95 | 0 |
| 5 | F | 2771 | 0 | 2844 | 346 | 0 |
| 5 | P | 2771 | 0 | 2844 | 352 | 0 |
| 6 | A | 33 | 0 | 0 | 0 | 0 |
| 6 | B | 21 | 0 | 0 | 0 | 0 |
| 6 | C | 73 | 0 | 0 | 0 | 0 |
| 6 | D | 106 | 0 | 0 | 0 | 0 |
| 6 | E | 5 | 0 | 0 | 0 | 0 |
| 6 | F | 28 | 0 | 0 | 0 | 0 |
| 6 | K | 19 | 0 | 0 | 0 | 0 |
| 6 | L | 17 | 0 | 0 | 0 | 0 |
| 6 | M | 65 | 0 | 0 | 0 | 0 |
| 6 | N | 92 | 0 | 0 | 0 | 0 |
| 6 | O | 8 | 0 | 0 | 0 | 0 |
| 6 | P | 20 | 0 | 0 | 0 | 0 |
| 7 | C | 63 | 0 | 62 | 6 | 0 |
| 7 | M | 63 | 0 | 62 | 7 | 0 |
| 8 | D | 2 | 0 | 0 | 0 | 0 |
| 8 | N | 2 | 0 | 0 | 0 | 0 |
| 9 | A | 239 | 0 | 0 | 50 | 0 |
| 9 | B | 258 | 0 | 0 | 46 | 0 |
| 9 | C | 979 | 0 | 0 | 224 | 0 |
| 9 | D | 1252 | 0 | 0 | 277 | 0 |
| 9 | E | 117 | 0 | 0 | 28 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 9 | F | 420 | 0 | 0 | 94 | 0 |
| 9 | K | 183 | 0 | 0 | 39 | 0 |
| 9 | L | 219 | 0 | 0 | 46 | 0 |
| 9 | M | 998 | 0 | 0 | 249 | 0 |
| 9 | N | 1265 | 0 | 0 | 250 | 0 |
| 9 | O | 108 | 0 | 0 | 26 | 0 |
| 9 | P | 361 | 0 | 0 | 78 | 0 |
| All | All | 60572 | 0 | 54418 | 6470 | 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 60.

The worst 5 of 6470 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:95:GLN:HA | 1:A:146:ARG:HH12 | 1.07 | 1.11 |
| 2:M:952:LEU:HD12 | 2:M:969:GLN:HE22 | 1.13 | 1.11 |
| 3:D:1087:ARG:HG2 | 3:D:1234:THR:HA | 1.27 | 1.07 |
| 1:B:152:PRO:HD2 | 1:B:155:LYS:HD3 | 1.36 | 1.05 |
| 2:M:605:LYS:HB2 | 2:M:610:ARG:HH12 | 1.16 | 1.05 |

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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 227/315 (72%) | 201 (88%) | 21 (9%) | 5 (2%) | 6 10 |
| 1 | B | 227/315 (72%) | 198 (87%) | 23 (10%) | 6 (3%) | 5 8 |
| 1 | K | 227/315 (72%) | 200 (88%) | 23 (10%) | 4 (2%) | 8 14 |
| 1 | L | 227/315 (72%) | 203 (89%) | 20 (9%) | 4 (2%) | 8 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 2 | C | 1117/1119 (100%) | 907 (81%) | 157 (14%) | 53 (5%) | 2 2 |
| 2 | M | 1117/1119 (100%) | 906 (81%) | 158 (14%) | 53 (5%) | 2 2 |
| 3 | D | 1388/1524 (91%) | 1108 (80%) | 207 (15%) | 73 (5%) | 2 2 |
| 3 | N | 1388/1524 (91%) | 1105 (80%) | 208 (15%) | 75 (5%) | 2 2 |
| 4 | E | 93/99 (94%) | 75 (81%) | 15 (16%) | 3 (3%) | 4 5 |
| 4 | O | 93/99 (94%) | 75 (81%) | 15 (16%) | 3 (3%) | 4 5 |
| 5 | F | 341/423 (81%) | 285 (84%) | 38 (11%) | 18 (5%) | 2 2 |
| 5 | P | 341/423 (81%) | 287 (84%) | 38 (11%) | 16 (5%) | 2 2 |
| All | All | 6786/7590 (89%) | 5550 (82%) | 923 (14%) | 313 (5%) | 2 2 |

5 of 313 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 29 | GLU |
| 1 | B | 29 | GLU |
| 1 | B | 48 | ILE |
| 2 | C | 152 | PRO |
| 2 | C | 178 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 | 202/273 (74%) | 159 (79%) | 43 (21%) | 1 2 |
| 1 | B | 202/273 (74%) | 161 (80%) | 41 (20%) | 1 2 |
| 1 | K | 202/273 (74%) | 158 (78%) | 44 (22%) | 1 1 |
| 1 | L | 202/273 (74%) | 160 (79%) | 42 (21%) | 1 2 |
| 2 | C | 941/941 (100%) | 714 (76%) | 227 (24%) | 0 1 |
| 2 | M | 941/941 (100%) | 738 (78%) | 203 (22%) | 1 1 |
| 3 | D | 1123/1279 (88%) | 868 (77%) | 255 (23%) | 1 1 |
| 3 | N | 1123/1279 (88%) | 871 (78%) | 252 (22%) | 1 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 4 | E | 83/87 (95%) | 62 (75%) | 21 (25%) | 0 1 |
| 4 | O | 83/87 (95%) | 65 (78%) | 18 (22%) | 1 1 |
| 5 | F | 295/370 (80%) | 233 (79%) | 62 (21%) | 1 2 |
| 5 | P | 295/370 (80%) | 246 (83%) | 49 (17%) | 2 4 |
| All | All | 5692/6446 (88%) | 4435 (78%) | 1257 (22%) | 1 1 |

5 of 1257 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | M | 1074 | GLU |
| 3 | N | 1306 | PRO |
| 3 | N | 66 | GLN |
| 2 | M | 1060 | ILE |
| 3 | N | 704 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | M | 920 | GLN |
| 3 | N | 1242 | HIS |
| 3 | N | 101 | HIS |
| 3 | N | 748 | HIS |
| 3 | N | 1441 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 493 ligands modelled in this entry, 491 are monoatomic - leaving 2 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 | $\#\|Z\| > 2$ |
| 7 | RPT | M | 8002 | - | 68,68,68 | 2.52 | 22 (32%) | 101,101,101 | 1.22 | 9 (8%) |
| 7 | RPT | C | 8001 | - | 68,68,68 | 2.45 | 22 (32%) | 101,101,101 | 1.23 | 11 (10%) |

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 |
|---|---|---|---|---|---|---|---|
| 7 | RPT | M | 8002 | - | - | 20/64/96/96 | 0/6/6/6 |
| 7 | RPT | C | 8001 | - | - | 12/64/96/96 | 0/6/6/6 |

The worst 5 of 44 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 8002 | RPT | C39-N4 | 6.55 | 1.59 | 1.47 |
| 7 | M | 8002 | RPT | C42-N4 | 6.42 | 1.59 | 1.47 |
| 7 | C | 8001 | RPT | O6-C27 | 6.22 | 1.58 | 1.43 |
| 7 | C | 8001 | RPT | O5-C29 | 6.12 | 1.55 | 1.39 |
| 7 | M | 8002 | RPT | O5-C29 | 5.98 | 1.54 | 1.39 |

The worst 5 of 20 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 8002 | RPT | C24-C23-C22 | 3.73 | 121.68 | 115.43 |
| 7 | C | 8001 | RPT | C24-C23-C22 | 3.28 | 120.92 | 115.43 |
| 7 | M | 8002 | RPT | C20-C21-C22 | 3.25 | 121.58 | 114.96 |
| 7 | C | 8001 | RPT | C25-O7-C35 | 3.23 | 122.72 | 117.72 |
| 7 | C | 8001 | RPT | C2-N1-C15 | 3.10 | 134.26 | 124.11 |

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 7 | C | 8001 | RPT | C26-C27-C28-C29 |
| 7 | C | 8001 | RPT | C26-C27-O6-C37 |
| 7 | C | 8001 | RPT | C28-C27-O6-C37 |
| 7 | M | 8002 | RPT | C28-C27-O6-C37 |
| 7 | M | 8002 | RPT | C44-C38-N4-C39 |

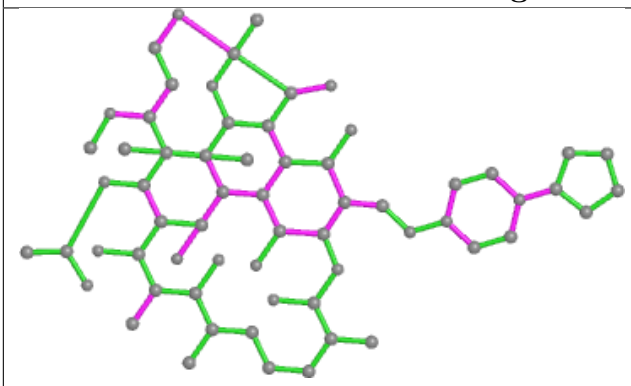
There are no ring outliers.

2 monomers are involved in 13 short contacts:

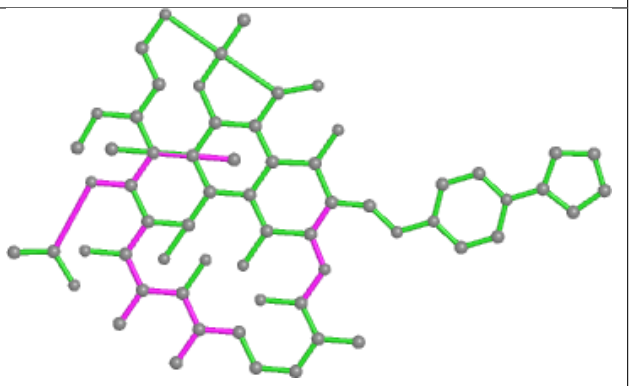
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 7 | M | 8002 | RPT | 7 | 0 |
| 7 | C | 8001 | RPT | 6 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight $> 250$ and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

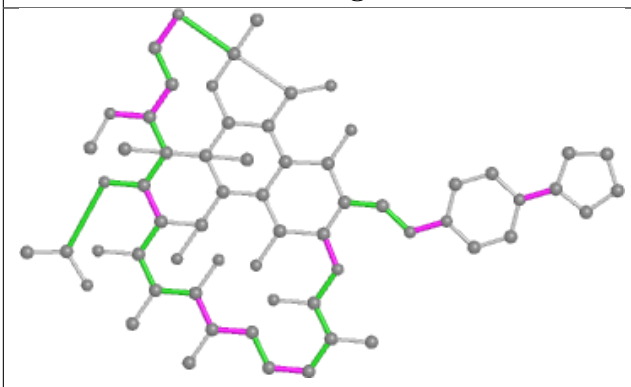
## Ligand RPT M 8002



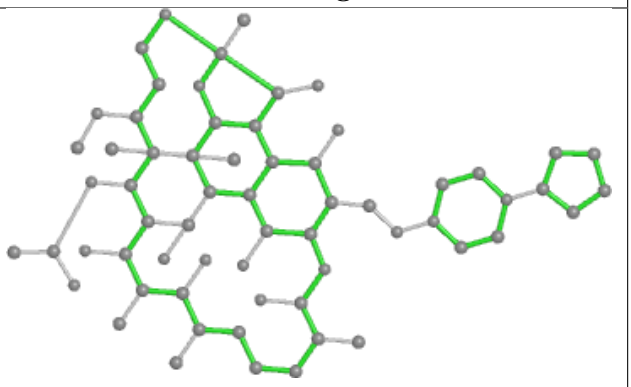
Bond lengths



Bond angles

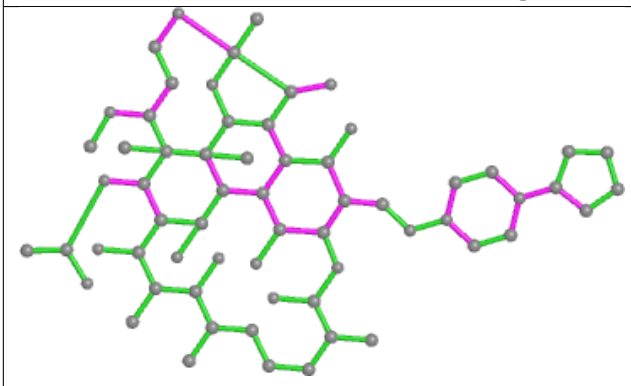


Torsions

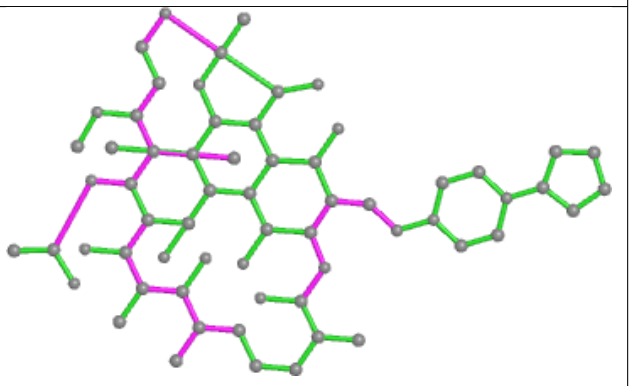


Rings

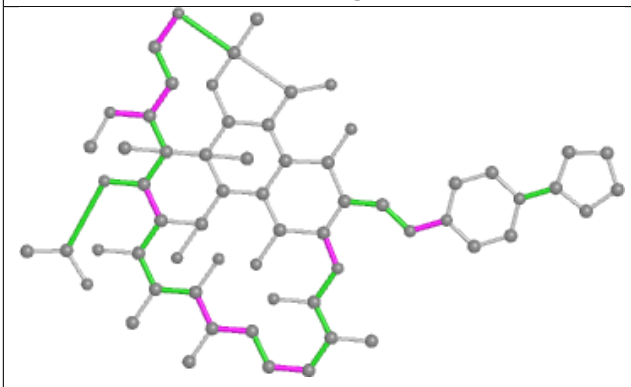
## Ligand RPT C 8001



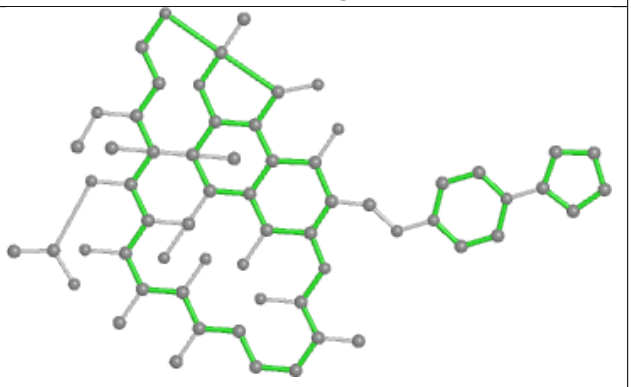
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 229/315 (72%) | -0.31 | 1 (0%) 92 93 | 27, 63, 91, 115 | 0 |
| 1 | B | 229/315 (72%) | -0.11 | 12 (5%) 27 29 | 48, 93, 115, 119 | 0 |
| 1 | K | 229/315 (72%) | -0.30 | 2 (0%) 84 86 | 34, 65, 94, 134 | 0 |
| 1 | L | 229/315 (72%) | -0.21 | 6 (2%) 56 59 | 52, 92, 110, 131 | 0 |
| 2 | C | 1119/1119 (100%) | -0.34 | 14 (1%) 77 79 | 21, 75, 106, 118 | 0 |
| 2 | M | 1119/1119 (100%) | -0.31 | 15 (1%) 77 79 | 25, 79, 109, 122 | 0 |
| 3 | D | 1392/1524 (91%) | -0.27 | 24 (1%) 70 72 | 24, 65, 112, 132 | 0 |
| 3 | N | 1392/1524 (91%) | -0.25 | 31 (2%) 62 65 | 25, 69, 117, 138 | 0 |
| 4 | E | 95/99 (95%) | -0.27 | 5 (5%) 26 28 | 42, 83, 108, 126 | 0 |
| 4 | O | 95/99 (95%) | -0.39 | 1 (1%) 80 82 | 46, 80, 107, 114 | 0 |
| 5 | F | 345/423 (81%) | -0.36 | 6 (1%) 70 72 | 49, 84, 110, 127 | 0 |
| 5 | P | 345/423 (81%) | -0.28 | 6 (1%) 70 72 | 63, 89, 114, 124 | 0 |
| All | All | 6818/7590 (89%) | -0.29 | 123 (1%) 68 71 | 21, 75, 112, 138 | 0 |

The worst 5 of 123 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | N | 802 | ALA | 7.6 |
| 3 | D | 1240 | THR | 5.8 |
| 3 | N | 1249 | ALA | 5.5 |
| 2 | C | 180 | GLY | 5.3 |
| 3 | D | 1245 | GLY | 5.3 |

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 8 | ZN | D | 7058 | 1/1 | 0.87 | 0.07 | 106,106,106,106 | 0 |
| 6 | MG | M | 9256 | 1/1 | 0.89 | 0.17 | 56,56,56,56 | 0 |
| 6 | MG | C | 9362 | 1/1 | 0.90 | 0.15 | 55,55,55,55 | 0 |
| 6 | MG | K | 9470 | 1/1 | 0.91 | 0.13 | 55,55,55,55 | 0 |
| 6 | MG | C | 9168 | 1/1 | 0.91 | 0.10 | 45,45,45,45 | 0 |
| 6 | MG | N | 9192 | 1/1 | 0.91 | 0.12 | 62,62,62,62 | 0 |
| 6 | MG | D | 9161 | 1/1 | 0.91 | 0.09 | 57,57,57,57 | 0 |
| 6 | MG | N | 9221 | 1/1 | 0.92 | 0.13 | 44,44,44,44 | 0 |
| 6 | MG | D | 9330 | 1/1 | 0.92 | 0.14 | 39,39,39,39 | 0 |
| 6 | MG | C | 9350 | 1/1 | 0.93 | 0.07 | 60,60,60,60 | 0 |
| 6 | MG | A | 9078 | 1/1 | 0.93 | 0.13 | 66,66,66,66 | 0 |
| 6 | MG | F | 9390 | 1/1 | 0.93 | 0.07 | 46,46,46,46 | 0 |
| 6 | MG | P | 9226 | 1/1 | 0.93 | 0.08 | 43,43,43,43 | 0 |
| 6 | MG | D | 9001 | 1/1 | 0.93 | 0.10 | 36,36,36,36 | 0 |
| 6 | MG | C | 9149 | 1/1 | 0.94 | 0.16 | 48,48,48,48 | 0 |
| 6 | MG | L | 9182 | 1/1 | 0.94 | 0.05 | 47,47,47,47 | 0 |
| 6 | MG | L | 9414 | 1/1 | 0.94 | 0.13 | 51,51,51,51 | 0 |
| 6 | MG | D | 9102 | 1/1 | 0.94 | 0.13 | 44,44,44,44 | 0 |
| 6 | MG | M | 9263 | 1/1 | 0.94 | 0.10 | 56,56,56,56 | 0 |
| 6 | MG | M | 9411 | 1/1 | 0.94 | 0.09 | 47,47,47,47 | 0 |
| 6 | MG | M | 9447 | 1/1 | 0.94 | 0.07 | 64,64,64,64 | 0 |
| 6 | MG | A | 9357 | 1/1 | 0.94 | 0.11 | 54,54,54,54 | 0 |
| 6 | MG | N | 9194 | 1/1 | 0.94 | 0.12 | 51,51,51,51 | 0 |
| 6 | MG | C | 9049 | 1/1 | 0.94 | 0.10 | 46,46,46,46 | 0 |
| 6 | MG | N | 9313 | 1/1 | 0.94 | 0.10 | 43,43,43,43 | 0 |
| 6 | MG | N | 9427 | 1/1 | 0.94 | 0.14 | 58,58,58,58 | 0 |
| 6 | MG | N | 9449 | 1/1 | 0.94 | 0.09 | 51,51,51,51 | 0 |
| 6 | MG | O | 9420 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 6 | MG | P | 9202 | 1/1 | 0.94 | 0.10 | 49,49,49,49 | 0 |
| 6 | MG | F | 9109 | 1/1 | 0.94 | 0.11 | 60,60,60,60 | 0 |
| 6 | MG | C | 9067 | 1/1 | 0.94 | 0.17 | 57,57,57,57 | 0 |
| 6 | MG | N | 9217 | 1/1 | 0.95 | 0.15 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | C | 9162 | 1/1 | 0.95 | 0.12 | 50,50,50,50 | 0 |
| 6 | MG | N | 9233 | 1/1 | 0.95 | 0.14 | 62,62,62,62 | 0 |
| 6 | MG | N | 9291 | 1/1 | 0.95 | 0.12 | 64,64,64,64 | 0 |
| 6 | MG | M | 9324 | 1/1 | 0.95 | 0.08 | 41,41,41,41 | 0 |
| 6 | MG | N | 9327 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 6 | MG | D | 9014 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 6 | MG | D | 9036 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 6 | MG | M | 9471 | 1/1 | 0.95 | 0.08 | 47,47,47,47 | 0 |
| 6 | MG | D | 9082 | 1/1 | 0.95 | 0.14 | 60,60,60,60 | 0 |
| 6 | MG | F | 9148 | 1/1 | 0.95 | 0.08 | 54,54,54,54 | 0 |
| 6 | MG | P | 9297 | 1/1 | 0.95 | 0.09 | 45,45,45,45 | 0 |
| 6 | MG | N | 9200 | 1/1 | 0.95 | 0.10 | 38,38,38,38 | 0 |
| 6 | MG | M | 9210 | 1/1 | 0.96 | 0.13 | 41,41,41,41 | 0 |
| 6 | MG | M | 9225 | 1/1 | 0.96 | 0.14 | 56,56,56,56 | 0 |
| 6 | MG | M | 9234 | 1/1 | 0.96 | 0.12 | 53,53,53,53 | 0 |
| 6 | MG | B | 9059 | 1/1 | 0.96 | 0.07 | 48,48,48,48 | 0 |
| 6 | MG | M | 9261 | 1/1 | 0.96 | 0.11 | 47,47,47,47 | 0 |
| 6 | MG | B | 9359 | 1/1 | 0.96 | 0.10 | 52,52,52,52 | 0 |
| 6 | MG | M | 9294 | 1/1 | 0.96 | 0.09 | 52,52,52,52 | 0 |
| 6 | MG | D | 9054 | 1/1 | 0.96 | 0.08 | 44,44,44,44 | 0 |
| 6 | MG | M | 9406 | 1/1 | 0.96 | 0.15 | 67,67,67,67 | 0 |
| 6 | MG | D | 9062 | 1/1 | 0.96 | 0.08 | 47,47,47,47 | 0 |
| 6 | MG | C | 9019 | 1/1 | 0.96 | 0.13 | 57,57,57,57 | 0 |
| 6 | MG | D | 9096 | 1/1 | 0.96 | 0.15 | 60,60,60,60 | 0 |
| 6 | MG | C | 9175 | 1/1 | 0.96 | 0.14 | 68,68,68,68 | 0 |
| 6 | MG | C | 9047 | 1/1 | 0.96 | 0.12 | 53,53,53,53 | 0 |
| 6 | MG | C | 9355 | 1/1 | 0.96 | 0.12 | 58,58,58,58 | 0 |
| 6 | MG | D | 9365 | 1/1 | 0.96 | 0.06 | 41,41,41,41 | 0 |
| 6 | MG | D | 9453 | 1/1 | 0.96 | 0.11 | 38,38,38,38 | 0 |
| 6 | MG | E | 9074 | 1/1 | 0.96 | 0.09 | 59,59,59,59 | 0 |
| 6 | MG | A | 9081 | 1/1 | 0.96 | 0.08 | 40,40,40,40 | 0 |
| 6 | MG | N | 9292 | 1/1 | 0.96 | 0.12 | 56,56,56,56 | 0 |
| 6 | MG | C | 9372 | 1/1 | 0.96 | 0.09 | 61,61,61,61 | 0 |
| 6 | MG | N | 9326 | 1/1 | 0.96 | 0.14 | 62,62,62,62 | 0 |
| 6 | MG | F | 9172 | 1/1 | 0.96 | 0.11 | 51,51,51,51 | 0 |
| 6 | MG | N | 9426 | 1/1 | 0.96 | 0.09 | 41,41,41,41 | 0 |
| 6 | MG | F | 9370 | 1/1 | 0.96 | 0.09 | 46,46,46,46 | 0 |
| 6 | MG | C | 9381 | 1/1 | 0.96 | 0.08 | 53,53,53,53 | 0 |
| 6 | MG | O | 9198 | 1/1 | 0.96 | 0.12 | 36,36,36,36 | 0 |
| 6 | MG | C | 9391 | 1/1 | 0.96 | 0.06 | 60,60,60,60 | 0 |
| 6 | MG | A | 9013 | 1/1 | 0.96 | 0.12 | 44,44,44,44 | 0 |
| 6 | MG | P | 9209 | 1/1 | 0.96 | 0.15 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | L | 9218 | 1/1 | 0.96 | 0.09 | 33,33,33,33 | 0 |
| 6 | MG | L | 9278 | 1/1 | 0.96 | 0.11 | 44,44,44,44 | 0 |
| 7 | RPT | C | 8001 | 63/63 | 0.96 | 0.23 | 26,40,66,82 | 0 |
| 7 | RPT | M | 8002 | 63/63 | 0.96 | 0.22 | 33,45,55,57 | 0 |
| 6 | MG | D | 9009 | 1/1 | 0.96 | 0.09 | 43,43,43,43 | 0 |
| 6 | MG | K | 9188 | 1/1 | 0.97 | 0.12 | 40,40,40,40 | 0 |
| 6 | MG | K | 9251 | 1/1 | 0.97 | 0.11 | 43,43,43,43 | 0 |
| 6 | MG | K | 9257 | 1/1 | 0.97 | 0.10 | 58,58,58,58 | 0 |
| 6 | MG | K | 9410 | 1/1 | 0.97 | 0.15 | 36,36,36,36 | 0 |
| 6 | MG | K | 9433 | 1/1 | 0.97 | 0.07 | 50,50,50,50 | 0 |
| 6 | MG | C | 9122 | 1/1 | 0.97 | 0.10 | 56,56,56,56 | 0 |
| 6 | MG | D | 9017 | 1/1 | 0.97 | 0.10 | 42,42,42,42 | 0 |
| 6 | MG | D | 9030 | 1/1 | 0.97 | 0.09 | 48,48,48,48 | 0 |
| 6 | MG | L | 9245 | 1/1 | 0.97 | 0.09 | 62,62,62,62 | 0 |
| 6 | MG | L | 9252 | 1/1 | 0.97 | 0.09 | 45,45,45,45 | 0 |
| 6 | MG | A | 9125 | 1/1 | 0.97 | 0.12 | 36,36,36,36 | 0 |
| 6 | MG | L | 9289 | 1/1 | 0.97 | 0.14 | 62,62,62,62 | 0 |
| 6 | MG | D | 9041 | 1/1 | 0.97 | 0.13 | 47,47,47,47 | 0 |
| 6 | MG | M | 9196 | 1/1 | 0.97 | 0.09 | 42,42,42,42 | 0 |
| 6 | MG | M | 9201 | 1/1 | 0.97 | 0.10 | 45,45,45,45 | 0 |
| 6 | MG | C | 9160 | 1/1 | 0.97 | 0.09 | 44,44,44,44 | 0 |
| 6 | MG | M | 9219 | 1/1 | 0.97 | 0.09 | 47,47,47,47 | 0 |
| 6 | MG | B | 9103 | 1/1 | 0.97 | 0.12 | 43,43,43,43 | 0 |
| 6 | MG | D | 9073 | 1/1 | 0.97 | 0.12 | 34,34,34,34 | 0 |
| 6 | MG | M | 9237 | 1/1 | 0.97 | 0.15 | 52,52,52,52 | 0 |
| 6 | MG | B | 9104 | 1/1 | 0.97 | 0.10 | 45,45,45,45 | 0 |
| 6 | MG | D | 9087 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 6 | MG | D | 9095 | 1/1 | 0.97 | 0.15 | 30,30,30,30 | 0 |
| 6 | MG | M | 9273 | 1/1 | 0.97 | 0.12 | 44,44,44,44 | 0 |
| 6 | MG | M | 9275 | 1/1 | 0.97 | 0.12 | 55,55,55,55 | 0 |
| 6 | MG | A | 9153 | 1/1 | 0.97 | 0.15 | 66,66,66,66 | 0 |
| 6 | MG | C | 9178 | 1/1 | 0.97 | 0.09 | 39,39,39,39 | 0 |
| 6 | MG | D | 9127 | 1/1 | 0.97 | 0.14 | 48,48,48,48 | 0 |
| 6 | MG | D | 9158 | 1/1 | 0.97 | 0.12 | 60,60,60,60 | 0 |
| 6 | MG | M | 9412 | 1/1 | 0.97 | 0.14 | 43,43,43,43 | 0 |
| 6 | MG | B | 9458 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 6 | MG | D | 9165 | 1/1 | 0.97 | 0.07 | 32,32,32,32 | 0 |
| 6 | MG | M | 9475 | 1/1 | 0.97 | 0.05 | 62,62,62,62 | 0 |
| 6 | MG | D | 9166 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 6 | MG | D | 9167 | 1/1 | 0.97 | 0.12 | 49,49,49,49 | 0 |
| 6 | MG | D | 9174 | 1/1 | 0.97 | 0.12 | 47,47,47,47 | 0 |
| 6 | MG | N | 9211 | 1/1 | 0.97 | 0.10 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | D | 9177 | 1/1 | 0.97 | 0.13 | 64,64,64,64 | 0 |
| 6 | MG | A | 9156 | 1/1 | 0.97 | 0.08 | 43,43,43,43 | 0 |
| 6 | MG | N | 9232 | 1/1 | 0.97 | 0.08 | 47,47,47,47 | 0 |
| 6 | MG | D | 9346 | 1/1 | 0.97 | 0.07 | 47,47,47,47 | 0 |
| 6 | MG | N | 9276 | 1/1 | 0.97 | 0.08 | 61,61,61,61 | 0 |
| 6 | MG | D | 9348 | 1/1 | 0.97 | 0.14 | 57,57,57,57 | 0 |
| 6 | MG | C | 9360 | 1/1 | 0.97 | 0.13 | 53,53,53,53 | 0 |
| 6 | MG | D | 9367 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 6 | MG | D | 9373 | 1/1 | 0.97 | 0.12 | 51,51,51,51 | 0 |
| 6 | MG | D | 9388 | 1/1 | 0.97 | 0.09 | 37,37,37,37 | 0 |
| 6 | MG | N | 9422 | 1/1 | 0.97 | 0.14 | 56,56,56,56 | 0 |
| 6 | MG | N | 9425 | 1/1 | 0.97 | 0.12 | 46,46,46,46 | 0 |
| 6 | MG | C | 9022 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 6 | MG | A | 9171 | 1/1 | 0.97 | 0.11 | 58,58,58,58 | 0 |
| 6 | MG | F | 9060 | 1/1 | 0.97 | 0.10 | 41,41,41,41 | 0 |
| 6 | MG | N | 9450 | 1/1 | 0.97 | 0.10 | 48,48,48,48 | 0 |
| 6 | MG | N | 9473 | 1/1 | 0.97 | 0.12 | 51,51,51,51 | 0 |
| 6 | MG | F | 9099 | 1/1 | 0.97 | 0.13 | 56,56,56,56 | 0 |
| 6 | MG | A | 9352 | 1/1 | 0.97 | 0.10 | 46,46,46,46 | 0 |
| 6 | MG | P | 9189 | 1/1 | 0.97 | 0.11 | 49,49,49,49 | 0 |
| 6 | MG | F | 9123 | 1/1 | 0.97 | 0.09 | 37,37,37,37 | 0 |
| 6 | MG | A | 9066 | 1/1 | 0.97 | 0.14 | 47,47,47,47 | 0 |
| 6 | MG | P | 9216 | 1/1 | 0.97 | 0.13 | 48,48,48,48 | 0 |
| 6 | MG | C | 9107 | 1/1 | 0.97 | 0.09 | 42,42,42,42 | 0 |
| 6 | MG | D | 9006 | 1/1 | 0.97 | 0.12 | 40,40,40,40 | 0 |
| 6 | MG | P | 9325 | 1/1 | 0.97 | 0.12 | 49,49,49,49 | 0 |
| 6 | MG | F | 9376 | 1/1 | 0.97 | 0.19 | 62,62,62,62 | 0 |
| 6 | MG | F | 9389 | 1/1 | 0.97 | 0.11 | 53,53,53,53 | 0 |
| 6 | MG | C | 9119 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 6 | MG | F | 9387 | 1/1 | 0.98 | 0.10 | 53,53,53,53 | 0 |
| 6 | MG | C | 9112 | 1/1 | 0.98 | 0.11 | 39,39,39,39 | 0 |
| 6 | MG | D | 9052 | 1/1 | 0.98 | 0.07 | 65,65,65,65 | 0 |
| 6 | MG | B | 9080 | 1/1 | 0.98 | 0.10 | 56,56,56,56 | 0 |
| 6 | MG | K | 9191 | 1/1 | 0.98 | 0.15 | 32,32,32,32 | 0 |
| 6 | MG | K | 9213 | 1/1 | 0.98 | 0.11 | 43,43,43,43 | 0 |
| 6 | MG | B | 9093 | 1/1 | 0.98 | 0.15 | 40,40,40,40 | 0 |
| 6 | MG | D | 9063 | 1/1 | 0.98 | 0.08 | 33,33,33,33 | 0 |
| 6 | MG | K | 9264 | 1/1 | 0.98 | 0.08 | 42,42,42,42 | 0 |
| 6 | MG | K | 9290 | 1/1 | 0.98 | 0.12 | 51,51,51,51 | 0 |
| 6 | MG | K | 9301 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 6 | MG | K | 9405 | 1/1 | 0.98 | 0.11 | 56,56,56,56 | 0 |
| 6 | MG | D | 9064 | 1/1 | 0.98 | 0.14 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | D | 9069 | 1/1 | 0.98 | 0.12 | 48,48,48,48 | 0 |
| 6 | MG | K | 9438 | 1/1 | 0.98 | 0.10 | 52,52,52,52 | 0 |
| 6 | MG | C | 9128 | 1/1 | 0.98 | 0.12 | 52,52,52,52 | 0 |
| 6 | MG | C | 9138 | 1/1 | 0.98 | 0.08 | 43,43,43,43 | 0 |
| 6 | MG | C | 9142 | 1/1 | 0.98 | 0.15 | 48,48,48,48 | 0 |
| 6 | MG | A | 9012 | 1/1 | 0.98 | 0.10 | 47,47,47,47 | 0 |
| 6 | MG | L | 9246 | 1/1 | 0.98 | 0.12 | 52,52,52,52 | 0 |
| 6 | MG | C | 9154 | 1/1 | 0.98 | 0.07 | 43,43,43,43 | 0 |
| 6 | MG | A | 9068 | 1/1 | 0.98 | 0.12 | 39,39,39,39 | 0 |
| 6 | MG | L | 9283 | 1/1 | 0.98 | 0.12 | 59,59,59,59 | 0 |
| 6 | MG | D | 9108 | 1/1 | 0.98 | 0.15 | 51,51,51,51 | 0 |
| 6 | MG | L | 9309 | 1/1 | 0.98 | 0.13 | 49,49,49,49 | 0 |
| 6 | MG | L | 9314 | 1/1 | 0.98 | 0.07 | 56,56,56,56 | 0 |
| 6 | MG | D | 9113 | 1/1 | 0.98 | 0.11 | 34,34,34,34 | 0 |
| 6 | MG | L | 9421 | 1/1 | 0.98 | 0.12 | 53,53,53,53 | 0 |
| 6 | MG | D | 9118 | 1/1 | 0.98 | 0.11 | 44,44,44,44 | 0 |
| 6 | MG | D | 9121 | 1/1 | 0.98 | 0.09 | 35,35,35,35 | 0 |
| 6 | MG | M | 9205 | 1/1 | 0.98 | 0.11 | 38,38,38,38 | 0 |
| 6 | MG | A | 9010 | 1/1 | 0.98 | 0.12 | 30,30,30,30 | 0 |
| 6 | MG | M | 9212 | 1/1 | 0.98 | 0.08 | 32,32,32,32 | 0 |
| 6 | MG | D | 9132 | 1/1 | 0.98 | 0.10 | 43,43,43,43 | 0 |
| 6 | MG | D | 9135 | 1/1 | 0.98 | 0.14 | 50,50,50,50 | 0 |
| 6 | MG | D | 9137 | 1/1 | 0.98 | 0.08 | 47,47,47,47 | 0 |
| 6 | MG | D | 9152 | 1/1 | 0.98 | 0.12 | 67,67,67,67 | 0 |
| 6 | MG | M | 9239 | 1/1 | 0.98 | 0.07 | 34,34,34,34 | 0 |
| 6 | MG | M | 9241 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 6 | MG | M | 9247 | 1/1 | 0.98 | 0.07 | 51,51,51,51 | 0 |
| 6 | MG | M | 9250 | 1/1 | 0.98 | 0.07 | 38,38,38,38 | 0 |
| 6 | MG | B | 9457 | 1/1 | 0.98 | 0.07 | 43,43,43,43 | 0 |
| 6 | MG | A | 9016 | 1/1 | 0.98 | 0.14 | 36,36,36,36 | 0 |
| 6 | MG | D | 9163 | 1/1 | 0.98 | 0.14 | 52,52,52,52 | 0 |
| 6 | MG | B | 9478 | 1/1 | 0.98 | 0.12 | 61,61,61,61 | 0 |
| 6 | MG | C | 9340 | 1/1 | 0.98 | 0.09 | 60,60,60,60 | 0 |
| 6 | MG | M | 9284 | 1/1 | 0.98 | 0.14 | 54,54,54,54 | 0 |
| 6 | MG | C | 9004 | 1/1 | 0.98 | 0.10 | 39,39,39,39 | 0 |
| 6 | MG | M | 9305 | 1/1 | 0.98 | 0.09 | 46,46,46,46 | 0 |
| 6 | MG | M | 9310 | 1/1 | 0.98 | 0.07 | 46,46,46,46 | 0 |
| 6 | MG | D | 9173 | 1/1 | 0.98 | 0.07 | 48,48,48,48 | 0 |
| 6 | MG | C | 9015 | 1/1 | 0.98 | 0.09 | 38,38,38,38 | 0 |
| 6 | MG | M | 9407 | 1/1 | 0.98 | 0.14 | 35,35,35,35 | 0 |
| 6 | MG | A | 9111 | 1/1 | 0.98 | 0.09 | 35,35,35,35 | 0 |
| 6 | MG | C | 9021 | 1/1 | 0.98 | 0.09 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | M | 9424 | 1/1 | 0.98 | 0.13 | 34,34,34,34 | 0 |
| 6 | MG | M | 9434 | 1/1 | 0.98 | 0.11 | 34,34,34,34 | 0 |
| 6 | MG | M | 9440 | 1/1 | 0.98 | 0.10 | 50,50,50,50 | 0 |
| 6 | MG | M | 9441 | 1/1 | 0.98 | 0.07 | 45,45,45,45 | 0 |
| 6 | MG | D | 9338 | 1/1 | 0.98 | 0.10 | 42,42,42,42 | 0 |
| 6 | MG | M | 9452 | 1/1 | 0.98 | 0.13 | 42,42,42,42 | 0 |
| 6 | MG | D | 9344 | 1/1 | 0.98 | 0.11 | 55,55,55,55 | 0 |
| 6 | MG | A | 9384 | 1/1 | 0.98 | 0.14 | 39,39,39,39 | 0 |
| 6 | MG | N | 9181 | 1/1 | 0.98 | 0.16 | 47,47,47,47 | 0 |
| 6 | MG | N | 9184 | 1/1 | 0.98 | 0.10 | 29,29,29,29 | 0 |
| 6 | MG | N | 9185 | 1/1 | 0.98 | 0.14 | 56,56,56,56 | 0 |
| 6 | MG | C | 9025 | 1/1 | 0.98 | 0.14 | 39,39,39,39 | 0 |
| 6 | MG | D | 9349 | 1/1 | 0.98 | 0.13 | 33,33,33,33 | 0 |
| 6 | MG | C | 9037 | 1/1 | 0.98 | 0.16 | 51,51,51,51 | 0 |
| 6 | MG | N | 9204 | 1/1 | 0.98 | 0.19 | 44,44,44,44 | 0 |
| 6 | MG | C | 9394 | 1/1 | 0.98 | 0.09 | 33,33,33,33 | 0 |
| 6 | MG | N | 9214 | 1/1 | 0.98 | 0.10 | 33,33,33,33 | 0 |
| 6 | MG | N | 9215 | 1/1 | 0.98 | 0.12 | 32,32,32,32 | 0 |
| 6 | MG | D | 9369 | 1/1 | 0.98 | 0.10 | 49,49,49,49 | 0 |
| 6 | MG | C | 9461 | 1/1 | 0.98 | 0.07 | 50,50,50,50 | 0 |
| 6 | MG | N | 9231 | 1/1 | 0.98 | 0.11 | 52,52,52,52 | 0 |
| 6 | MG | D | 9374 | 1/1 | 0.98 | 0.10 | 41,41,41,41 | 0 |
| 6 | MG | D | 9379 | 1/1 | 0.98 | 0.11 | 47,47,47,47 | 0 |
| 6 | MG | N | 9236 | 1/1 | 0.98 | 0.10 | 39,39,39,39 | 0 |
| 6 | MG | N | 9243 | 1/1 | 0.98 | 0.09 | 35,35,35,35 | 0 |
| 6 | MG | N | 9253 | 1/1 | 0.98 | 0.12 | 42,42,42,42 | 0 |
| 6 | MG | N | 9259 | 1/1 | 0.98 | 0.15 | 34,34,34,34 | 0 |
| 6 | MG | N | 9265 | 1/1 | 0.98 | 0.14 | 61,61,61,61 | 0 |
| 6 | MG | N | 9267 | 1/1 | 0.98 | 0.12 | 42,42,42,42 | 0 |
| 6 | MG | N | 9270 | 1/1 | 0.98 | 0.05 | 39,39,39,39 | 0 |
| 6 | MG | C | 9464 | 1/1 | 0.98 | 0.06 | 48,48,48,48 | 0 |
| 6 | MG | N | 9286 | 1/1 | 0.98 | 0.14 | 31,31,31,31 | 0 |
| 6 | MG | N | 9287 | 1/1 | 0.98 | 0.09 | 53,53,53,53 | 0 |
| 6 | MG | D | 9392 | 1/1 | 0.98 | 0.12 | 52,52,52,52 | 0 |
| 6 | MG | D | 9397 | 1/1 | 0.98 | 0.12 | 51,51,51,51 | 0 |
| 6 | MG | N | 9293 | 1/1 | 0.98 | 0.15 | 42,42,42,42 | 0 |
| 6 | MG | N | 9298 | 1/1 | 0.98 | 0.05 | 55,55,55,55 | 0 |
| 6 | MG | A | 9460 | 1/1 | 0.98 | 0.07 | 55,55,55,55 | 0 |
| 6 | MG | N | 9322 | 1/1 | 0.98 | 0.10 | 54,54,54,54 | 0 |
| 6 | MG | D | 9459 | 1/1 | 0.98 | 0.05 | 54,54,54,54 | 0 |
| 6 | MG | E | 9007 | 1/1 | 0.98 | 0.11 | 40,40,40,40 | 0 |
| 6 | MG | N | 9404 | 1/1 | 0.98 | 0.12 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | N | 9415 | 1/1 | 0.98 | 0.07 | 42,42,42,42 | 0 |
| 6 | MG | N | 9419 | 1/1 | 0.98 | 0.11 | 51,51,51,51 | 0 |
| 6 | MG | E | 9045 | 1/1 | 0.98 | 0.12 | 61,61,61,61 | 0 |
| 6 | MG | N | 9423 | 1/1 | 0.98 | 0.17 | 58,58,58,58 | 0 |
| 6 | MG | A | 9477 | 1/1 | 0.98 | 0.18 | 52,52,52,52 | 0 |
| 6 | MG | E | 9479 | 1/1 | 0.98 | 0.10 | 62,62,62,62 | 0 |
| 6 | MG | F | 9008 | 1/1 | 0.98 | 0.09 | 40,40,40,40 | 0 |
| 6 | MG | N | 9428 | 1/1 | 0.98 | 0.10 | 42,42,42,42 | 0 |
| 6 | MG | N | 9429 | 1/1 | 0.98 | 0.10 | 45,45,45,45 | 0 |
| 6 | MG | N | 9435 | 1/1 | 0.98 | 0.23 | 53,53,53,53 | 0 |
| 6 | MG | N | 9445 | 1/1 | 0.98 | 0.10 | 51,51,51,51 | 0 |
| 6 | MG | C | 9065 | 1/1 | 0.98 | 0.10 | 37,37,37,37 | 0 |
| 6 | MG | F | 9098 | 1/1 | 0.98 | 0.11 | 54,54,54,54 | 0 |
| 6 | MG | N | 9465 | 1/1 | 0.98 | 0.08 | 49,49,49,49 | 0 |
| 6 | MG | B | 9056 | 1/1 | 0.98 | 0.13 | 43,43,43,43 | 0 |
| 6 | MG | O | 9197 | 1/1 | 0.98 | 0.04 | 57,57,57,57 | 0 |
| 6 | MG | F | 9105 | 1/1 | 0.98 | 0.14 | 36,36,36,36 | 0 |
| 6 | MG | O | 9296 | 1/1 | 0.98 | 0.11 | 42,42,42,42 | 0 |
| 6 | MG | C | 9090 | 1/1 | 0.98 | 0.10 | 47,47,47,47 | 0 |
| 6 | MG | O | 9439 | 1/1 | 0.98 | 0.16 | 56,56,56,56 | 0 |
| 6 | MG | D | 9018 | 1/1 | 0.98 | 0.11 | 39,39,39,39 | 0 |
| 6 | MG | D | 9024 | 1/1 | 0.98 | 0.14 | 36,36,36,36 | 0 |
| 6 | MG | F | 9159 | 1/1 | 0.98 | 0.15 | 57,57,57,57 | 0 |
| 6 | MG | D | 9028 | 1/1 | 0.98 | 0.13 | 34,34,34,34 | 0 |
| 6 | MG | F | 9356 | 1/1 | 0.98 | 0.14 | 37,37,37,37 | 0 |
| 6 | MG | P | 9228 | 1/1 | 0.98 | 0.09 | 43,43,43,43 | 0 |
| 6 | MG | P | 9235 | 1/1 | 0.98 | 0.16 | 40,40,40,40 | 0 |
| 6 | MG | P | 9280 | 1/1 | 0.98 | 0.10 | 51,51,51,51 | 0 |
| 6 | MG | P | 9282 | 1/1 | 0.98 | 0.09 | 56,56,56,56 | 0 |
| 6 | MG | P | 9285 | 1/1 | 0.98 | 0.09 | 56,56,56,56 | 0 |
| 6 | MG | F | 9363 | 1/1 | 0.98 | 0.12 | 53,53,53,53 | 0 |
| 6 | MG | C | 9092 | 1/1 | 0.98 | 0.06 | 44,44,44,44 | 0 |
| 6 | MG | F | 9375 | 1/1 | 0.98 | 0.13 | 36,36,36,36 | 0 |
| 6 | MG | A | 9027 | 1/1 | 0.98 | 0.08 | 37,37,37,37 | 0 |
| 6 | MG | F | 9383 | 1/1 | 0.98 | 0.11 | 48,48,48,48 | 0 |
| 6 | MG | B | 9131 | 1/1 | 0.99 | 0.08 | 33,33,33,33 | 0 |
| 6 | MG | L | 9183 | 1/1 | 0.99 | 0.13 | 37,37,37,37 | 0 |
| 6 | MG | B | 9136 | 1/1 | 0.99 | 0.10 | 47,47,47,47 | 0 |
| 6 | MG | B | 9358 | 1/1 | 0.99 | 0.07 | 39,39,39,39 | 0 |
| 6 | MG | C | 9143 | 1/1 | 0.99 | 0.10 | 35,35,35,35 | 0 |
| 6 | MG | D | 9120 | 1/1 | 0.99 | 0.08 | 31,31,31,31 | 0 |
| 6 | MG | C | 9145 | 1/1 | 0.99 | 0.13 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | A | 9354 | 1/1 | 0.99 | 0.09 | 37,37,37,37 | 0 |
| 6 | MG | D | 9129 | 1/1 | 0.99 | 0.14 | 42,42,42,42 | 0 |
| 6 | MG | L | 9306 | 1/1 | 0.99 | 0.11 | 57,57,57,57 | 0 |
| 6 | MG | L | 9307 | 1/1 | 0.99 | 0.10 | 35,35,35,35 | 0 |
| 6 | MG | D | 9130 | 1/1 | 0.99 | 0.09 | 51,51,51,51 | 0 |
| 6 | MG | B | 9378 | 1/1 | 0.99 | 0.13 | 47,47,47,47 | 0 |
| 6 | MG | D | 9133 | 1/1 | 0.99 | 0.13 | 42,42,42,42 | 0 |
| 6 | MG | D | 9134 | 1/1 | 0.99 | 0.13 | 47,47,47,47 | 0 |
| 6 | MG | L | 9437 | 1/1 | 0.99 | 0.06 | 40,40,40,40 | 0 |
| 6 | MG | L | 9466 | 1/1 | 0.99 | 0.10 | 49,49,49,49 | 0 |
| 6 | MG | M | 9190 | 1/1 | 0.99 | 0.16 | 29,29,29,29 | 0 |
| 6 | MG | M | 9195 | 1/1 | 0.99 | 0.08 | 34,34,34,34 | 0 |
| 6 | MG | A | 9075 | 1/1 | 0.99 | 0.10 | 36,36,36,36 | 0 |
| 6 | MG | A | 9368 | 1/1 | 0.99 | 0.13 | 43,43,43,43 | 0 |
| 6 | MG | M | 9203 | 1/1 | 0.99 | 0.11 | 32,32,32,32 | 0 |
| 6 | MG | D | 9140 | 1/1 | 0.99 | 0.13 | 40,40,40,40 | 0 |
| 6 | MG | M | 9208 | 1/1 | 0.99 | 0.10 | 39,39,39,39 | 0 |
| 6 | MG | D | 9141 | 1/1 | 0.99 | 0.06 | 50,50,50,50 | 0 |
| 6 | MG | D | 9144 | 1/1 | 0.99 | 0.12 | 39,39,39,39 | 0 |
| 6 | MG | D | 9146 | 1/1 | 0.99 | 0.10 | 31,31,31,31 | 0 |
| 6 | MG | M | 9220 | 1/1 | 0.99 | 0.11 | 51,51,51,51 | 0 |
| 6 | MG | M | 9222 | 1/1 | 0.99 | 0.10 | 35,35,35,35 | 0 |
| 6 | MG | M | 9224 | 1/1 | 0.99 | 0.13 | 40,40,40,40 | 0 |
| 6 | MG | D | 9147 | 1/1 | 0.99 | 0.10 | 41,41,41,41 | 0 |
| 6 | MG | M | 9227 | 1/1 | 0.99 | 0.12 | 35,35,35,35 | 0 |
| 6 | MG | D | 9150 | 1/1 | 0.99 | 0.14 | 31,31,31,31 | 0 |
| 6 | MG | D | 9151 | 1/1 | 0.99 | 0.15 | 57,57,57,57 | 0 |
| 6 | MG | C | 9164 | 1/1 | 0.99 | 0.10 | 49,49,49,49 | 0 |
| 6 | MG | A | 9380 | 1/1 | 0.99 | 0.11 | 44,44,44,44 | 0 |
| 6 | MG | M | 9242 | 1/1 | 0.99 | 0.11 | 35,35,35,35 | 0 |
| 6 | MG | C | 9169 | 1/1 | 0.99 | 0.13 | 42,42,42,42 | 0 |
| 6 | MG | C | 9170 | 1/1 | 0.99 | 0.06 | 41,41,41,41 | 0 |
| 6 | MG | C | 9003 | 1/1 | 0.99 | 0.13 | 38,38,38,38 | 0 |
| 6 | MG | M | 9260 | 1/1 | 0.99 | 0.12 | 36,36,36,36 | 0 |
| 6 | MG | C | 9176 | 1/1 | 0.99 | 0.09 | 28,28,28,28 | 0 |
| 6 | MG | A | 9124 | 1/1 | 0.99 | 0.12 | 39,39,39,39 | 0 |
| 6 | MG | M | 9268 | 1/1 | 0.99 | 0.09 | 32,32,32,32 | 0 |
| 6 | MG | M | 9272 | 1/1 | 0.99 | 0.17 | 45,45,45,45 | 0 |
| 6 | MG | A | 9395 | 1/1 | 0.99 | 0.14 | 50,50,50,50 | 0 |
| 6 | MG | A | 9002 | 1/1 | 0.99 | 0.17 | 31,31,31,31 | 0 |
| 6 | MG | M | 9281 | 1/1 | 0.99 | 0.11 | 49,49,49,49 | 0 |
| 6 | MG | C | 9353 | 1/1 | 0.99 | 0.10 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | D | 9328 | 1/1 | 0.99 | 0.12 | 30,30,30,30 | 0 |
| 6 | MG | M | 9295 | 1/1 | 0.99 | 0.08 | 42,42,42,42 | 0 |
| 6 | MG | M | 9299 | 1/1 | 0.99 | 0.09 | 43,43,43,43 | 0 |
| 6 | MG | M | 9300 | 1/1 | 0.99 | 0.09 | 39,39,39,39 | 0 |
| 6 | MG | D | 9329 | 1/1 | 0.99 | 0.12 | 33,33,33,33 | 0 |
| 6 | MG | C | 9020 | 1/1 | 0.99 | 0.10 | 34,34,34,34 | 0 |
| 6 | MG | M | 9312 | 1/1 | 0.99 | 0.12 | 37,37,37,37 | 0 |
| 6 | MG | D | 9331 | 1/1 | 0.99 | 0.18 | 43,43,43,43 | 0 |
| 6 | MG | M | 9400 | 1/1 | 0.99 | 0.12 | 40,40,40,40 | 0 |
| 6 | MG | D | 9333 | 1/1 | 0.99 | 0.07 | 33,33,33,33 | 0 |
| 6 | MG | D | 9334 | 1/1 | 0.99 | 0.10 | 54,54,54,54 | 0 |
| 6 | MG | M | 9409 | 1/1 | 0.99 | 0.10 | 36,36,36,36 | 0 |
| 6 | MG | D | 9335 | 1/1 | 0.99 | 0.06 | 52,52,52,52 | 0 |
| 6 | MG | D | 9336 | 1/1 | 0.99 | 0.10 | 53,53,53,53 | 0 |
| 6 | MG | M | 9416 | 1/1 | 0.99 | 0.11 | 45,45,45,45 | 0 |
| 6 | MG | D | 9337 | 1/1 | 0.99 | 0.15 | 53,53,53,53 | 0 |
| 6 | MG | A | 9043 | 1/1 | 0.99 | 0.17 | 37,37,37,37 | 0 |
| 6 | MG | D | 9339 | 1/1 | 0.99 | 0.14 | 37,37,37,37 | 0 |
| 6 | MG | D | 9341 | 1/1 | 0.99 | 0.10 | 41,41,41,41 | 0 |
| 6 | MG | M | 9442 | 1/1 | 0.99 | 0.07 | 59,59,59,59 | 0 |
| 6 | MG | D | 9343 | 1/1 | 0.99 | 0.10 | 59,59,59,59 | 0 |
| 6 | MG | B | 9032 | 1/1 | 0.99 | 0.06 | 34,34,34,34 | 0 |
| 6 | MG | C | 9366 | 1/1 | 0.99 | 0.14 | 41,41,41,41 | 0 |
| 6 | MG | M | 9474 | 1/1 | 0.99 | 0.14 | 49,49,49,49 | 0 |
| 6 | MG | D | 9347 | 1/1 | 0.99 | 0.09 | 49,49,49,49 | 0 |
| 6 | MG | M | 9486 | 1/1 | 0.99 | 0.07 | 48,48,48,48 | 0 |
| 6 | MG | N | 9179 | 1/1 | 0.99 | 0.12 | 33,33,33,33 | 0 |
| 6 | MG | C | 9371 | 1/1 | 0.99 | 0.15 | 54,54,54,54 | 0 |
| 6 | MG | B | 9033 | 1/1 | 0.99 | 0.14 | 33,33,33,33 | 0 |
| 6 | MG | D | 9351 | 1/1 | 0.99 | 0.06 | 43,43,43,43 | 0 |
| 6 | MG | N | 9186 | 1/1 | 0.99 | 0.12 | 49,49,49,49 | 0 |
| 6 | MG | N | 9187 | 1/1 | 0.99 | 0.18 | 33,33,33,33 | 0 |
| 6 | MG | D | 9364 | 1/1 | 0.99 | 0.12 | 47,47,47,47 | 0 |
| 6 | MG | C | 9377 | 1/1 | 0.99 | 0.09 | 44,44,44,44 | 0 |
| 6 | MG | N | 9199 | 1/1 | 0.99 | 0.11 | 35,35,35,35 | 0 |
| 6 | MG | C | 9026 | 1/1 | 0.99 | 0.13 | 42,42,42,42 | 0 |
| 6 | MG | C | 9031 | 1/1 | 0.99 | 0.10 | 40,40,40,40 | 0 |
| 6 | MG | N | 9206 | 1/1 | 0.99 | 0.16 | 31,31,31,31 | 0 |
| 6 | MG | N | 9207 | 1/1 | 0.99 | 0.13 | 41,41,41,41 | 0 |
| 6 | MG | B | 9040 | 1/1 | 0.99 | 0.16 | 36,36,36,36 | 0 |
| 6 | MG | C | 9454 | 1/1 | 0.99 | 0.09 | 55,55,55,55 | 0 |
| 6 | MG | C | 9455 | 1/1 | 0.99 | 0.11 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | D | 9385 | 1/1 | 0.99 | 0.13 | 35,35,35,35 | 0 |
| 6 | MG | D | 9386 | 1/1 | 0.99 | 0.11 | 40,40,40,40 | 0 |
| 6 | MG | N | 9229 | 1/1 | 0.99 | 0.07 | 41,41,41,41 | 0 |
| 6 | MG | C | 9042 | 1/1 | 0.99 | 0.07 | 47,47,47,47 | 0 |
| 6 | MG | C | 9462 | 1/1 | 0.99 | 0.08 | 43,43,43,43 | 0 |
| 6 | MG | D | 9396 | 1/1 | 0.99 | 0.10 | 62,62,62,62 | 0 |
| 6 | MG | C | 9463 | 1/1 | 0.99 | 0.09 | 55,55,55,55 | 0 |
| 6 | MG | N | 9238 | 1/1 | 0.99 | 0.11 | 43,43,43,43 | 0 |
| 6 | MG | N | 9240 | 1/1 | 0.99 | 0.14 | 46,46,46,46 | 0 |
| 6 | MG | C | 9044 | 1/1 | 0.99 | 0.14 | 34,34,34,34 | 0 |
| 6 | MG | D | 9456 | 1/1 | 0.99 | 0.10 | 55,55,55,55 | 0 |
| 6 | MG | C | 9046 | 1/1 | 0.99 | 0.11 | 38,38,38,38 | 0 |
| 6 | MG | N | 9262 | 1/1 | 0.99 | 0.09 | 51,51,51,51 | 0 |
| 6 | MG | D | 9480 | 1/1 | 0.99 | 0.10 | 55,55,55,55 | 0 |
| 6 | MG | D | 9005 | 1/1 | 0.99 | 0.11 | 40,40,40,40 | 0 |
| 6 | MG | N | 9269 | 1/1 | 0.99 | 0.07 | 42,42,42,42 | 0 |
| 6 | MG | A | 9088 | 1/1 | 0.99 | 0.07 | 36,36,36,36 | 0 |
| 6 | MG | N | 9274 | 1/1 | 0.99 | 0.18 | 40,40,40,40 | 0 |
| 6 | MG | A | 9097 | 1/1 | 0.99 | 0.16 | 34,34,34,34 | 0 |
| 6 | MG | N | 9279 | 1/1 | 0.99 | 0.11 | 54,54,54,54 | 0 |
| 6 | MG | E | 9155 | 1/1 | 0.99 | 0.14 | 44,44,44,44 | 0 |
| 6 | MG | D | 9011 | 1/1 | 0.99 | 0.12 | 33,33,33,33 | 0 |
| 6 | MG | N | 9288 | 1/1 | 0.99 | 0.09 | 49,49,49,49 | 0 |
| 6 | MG | C | 9050 | 1/1 | 0.99 | 0.15 | 37,37,37,37 | 0 |
| 6 | MG | F | 9035 | 1/1 | 0.99 | 0.10 | 40,40,40,40 | 0 |
| 6 | MG | F | 9048 | 1/1 | 0.99 | 0.10 | 41,41,41,41 | 0 |
| 6 | MG | C | 9051 | 1/1 | 0.99 | 0.12 | 37,37,37,37 | 0 |
| 6 | MG | N | 9302 | 1/1 | 0.99 | 0.10 | 31,31,31,31 | 0 |
| 6 | MG | N | 9303 | 1/1 | 0.99 | 0.08 | 54,54,54,54 | 0 |
| 6 | MG | N | 9304 | 1/1 | 0.99 | 0.11 | 47,47,47,47 | 0 |
| 6 | MG | N | 9308 | 1/1 | 0.99 | 0.15 | 55,55,55,55 | 0 |
| 6 | MG | C | 9053 | 1/1 | 0.99 | 0.12 | 30,30,30,30 | 0 |
| 6 | MG | N | 9316 | 1/1 | 0.99 | 0.08 | 37,37,37,37 | 0 |
| 6 | MG | N | 9317 | 1/1 | 0.99 | 0.09 | 43,43,43,43 | 0 |
| 6 | MG | N | 9318 | 1/1 | 0.99 | 0.11 | 34,34,34,34 | 0 |
| 6 | MG | D | 9023 | 1/1 | 0.99 | 0.14 | 34,34,34,34 | 0 |
| 6 | MG | N | 9323 | 1/1 | 0.99 | 0.09 | 38,38,38,38 | 0 |
| 6 | MG | C | 9055 | 1/1 | 0.99 | 0.11 | 38,38,38,38 | 0 |
| 6 | MG | C | 9061 | 1/1 | 0.99 | 0.07 | 34,34,34,34 | 0 |
| 6 | MG | N | 9398 | 1/1 | 0.99 | 0.15 | 48,48,48,48 | 0 |
| 6 | MG | N | 9402 | 1/1 | 0.99 | 0.07 | 45,45,45,45 | 0 |
| 6 | MG | N | 9403 | 1/1 | 0.99 | 0.12 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | D | 9029 | 1/1 | 0.99 | 0.12 | 33,33,33,33 | 0 |
| 6 | MG | F | 9139 | 1/1 | 0.99 | 0.10 | 38,38,38,38 | 0 |
| 6 | MG | N | 9417 | 1/1 | 0.99 | 0.09 | 39,39,39,39 | 0 |
| 6 | MG | N | 9418 | 1/1 | 0.99 | 0.10 | 49,49,49,49 | 0 |
| 6 | MG | A | 9332 | 1/1 | 0.99 | 0.06 | 35,35,35,35 | 0 |
| 6 | MG | F | 9157 | 1/1 | 0.99 | 0.11 | 42,42,42,42 | 0 |
| 6 | MG | D | 9034 | 1/1 | 0.99 | 0.08 | 41,41,41,41 | 0 |
| 6 | MG | B | 9083 | 1/1 | 0.99 | 0.13 | 40,40,40,40 | 0 |
| 6 | MG | D | 9038 | 1/1 | 0.99 | 0.14 | 39,39,39,39 | 0 |
| 6 | MG | D | 9039 | 1/1 | 0.99 | 0.12 | 44,44,44,44 | 0 |
| 6 | MG | C | 9071 | 1/1 | 0.99 | 0.11 | 42,42,42,42 | 0 |
| 6 | MG | C | 9079 | 1/1 | 0.99 | 0.11 | 38,38,38,38 | 0 |
| 6 | MG | N | 9430 | 1/1 | 0.99 | 0.08 | 57,57,57,57 | 0 |
| 6 | MG | N | 9431 | 1/1 | 0.99 | 0.12 | 39,39,39,39 | 0 |
| 6 | MG | C | 9086 | 1/1 | 0.99 | 0.14 | 39,39,39,39 | 0 |
| 6 | MG | N | 9443 | 1/1 | 0.99 | 0.13 | 54,54,54,54 | 0 |
| 6 | MG | N | 9444 | 1/1 | 0.99 | 0.15 | 49,49,49,49 | 0 |
| 6 | MG | F | 9382 | 1/1 | 0.99 | 0.09 | 40,40,40,40 | 0 |
| 6 | MG | N | 9448 | 1/1 | 0.99 | 0.09 | 51,51,51,51 | 0 |
| 6 | MG | D | 9058 | 1/1 | 0.99 | 0.08 | 38,38,38,38 | 0 |
| 6 | MG | A | 9342 | 1/1 | 0.99 | 0.12 | 39,39,39,39 | 0 |
| 6 | MG | N | 9451 | 1/1 | 0.99 | 0.06 | 41,41,41,41 | 0 |
| 6 | MG | B | 9094 | 1/1 | 0.99 | 0.15 | 38,38,38,38 | 0 |
| 6 | MG | N | 9467 | 1/1 | 0.99 | 0.12 | 35,35,35,35 | 0 |
| 6 | MG | N | 9468 | 1/1 | 0.99 | 0.10 | 55,55,55,55 | 0 |
| 6 | MG | N | 9472 | 1/1 | 0.99 | 0.15 | 56,56,56,56 | 0 |
| 6 | MG | A | 9345 | 1/1 | 0.99 | 0.12 | 41,41,41,41 | 0 |
| 6 | MG | N | 9476 | 1/1 | 0.99 | 0.09 | 54,54,54,54 | 0 |
| 6 | MG | N | 9484 | 1/1 | 0.99 | 0.07 | 37,37,37,37 | 0 |
| 6 | MG | F | 9393 | 1/1 | 0.99 | 0.12 | 38,38,38,38 | 0 |
| 6 | MG | F | 9481 | 1/1 | 0.99 | 0.08 | 57,57,57,57 | 0 |
| 6 | MG | O | 9254 | 1/1 | 0.99 | 0.08 | 39,39,39,39 | 0 |
| 6 | MG | A | 9106 | 1/1 | 0.99 | 0.12 | 38,38,38,38 | 0 |
| 6 | MG | D | 9070 | 1/1 | 0.99 | 0.07 | 33,33,33,33 | 0 |
| 6 | MG | D | 9072 | 1/1 | 0.99 | 0.14 | 32,32,32,32 | 0 |
| 6 | MG | O | 9483 | 1/1 | 0.99 | 0.09 | 63,63,63,63 | 0 |
| 6 | MG | K | 9223 | 1/1 | 0.99 | 0.09 | 32,32,32,32 | 0 |
| 6 | MG | K | 9244 | 1/1 | 0.99 | 0.07 | 44,44,44,44 | 0 |
| 6 | MG | C | 9114 | 1/1 | 0.99 | 0.09 | 30,30,30,30 | 0 |
| 6 | MG | D | 9077 | 1/1 | 0.99 | 0.11 | 35,35,35,35 | 0 |
| 6 | MG | C | 9115 | 1/1 | 0.99 | 0.11 | 36,36,36,36 | 0 |
| 6 | MG | D | 9084 | 1/1 | 0.99 | 0.11 | 37,37,37,37 | 0 |

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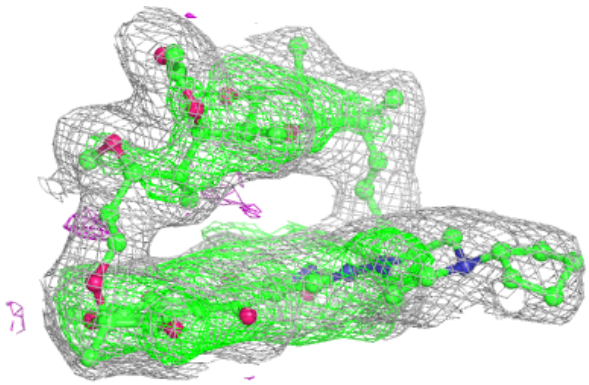
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | MG | D | 9085 | 1/1 | 0.99 | 0.18 | 49,49,49,49 | 0 |
| 6 | MG | P | 9255 | 1/1 | 0.99 | 0.12 | 34,34,34,34 | 0 |
| 6 | MG | P | 9277 | 1/1 | 0.99 | 0.09 | 41,41,41,41 | 0 |
| 6 | MG | B | 9110 | 1/1 | 0.99 | 0.12 | 49,49,49,49 | 0 |
| 6 | MG | D | 9089 | 1/1 | 0.99 | 0.09 | 36,36,36,36 | 0 |
| 6 | MG | K | 9413 | 1/1 | 0.99 | 0.10 | 54,54,54,54 | 0 |
| 6 | MG | K | 9432 | 1/1 | 0.99 | 0.13 | 49,49,49,49 | 0 |
| 6 | MG | P | 9315 | 1/1 | 0.99 | 0.08 | 35,35,35,35 | 0 |
| 6 | MG | B | 9116 | 1/1 | 0.99 | 0.09 | 38,38,38,38 | 0 |
| 6 | MG | P | 9399 | 1/1 | 0.99 | 0.11 | 34,34,34,34 | 0 |
| 6 | MG | P | 9436 | 1/1 | 0.99 | 0.11 | 49,49,49,49 | 0 |
| 6 | MG | P | 9446 | 1/1 | 0.99 | 0.13 | 34,34,34,34 | 0 |
| 6 | MG | C | 9126 | 1/1 | 0.99 | 0.10 | 46,46,46,46 | 0 |
| 6 | MG | K | 9469 | 1/1 | 0.99 | 0.12 | 50,50,50,50 | 0 |
| 6 | MG | D | 9100 | 1/1 | 0.99 | 0.08 | 43,43,43,43 | 0 |
| 8 | ZN | D | 7112 | 1/1 | 0.99 | 0.10 | 80,80,80,80 | 0 |
| 8 | ZN | N | 7059 | 1/1 | 0.99 | 0.12 | 93,93,93,93 | 0 |
| 8 | ZN | N | 7113 | 1/1 | 0.99 | 0.13 | 84,84,84,84 | 0 |
| 6 | MG | K | 9180 | 1/1 | 1.00 | 0.11 | 42,42,42,42 | 0 |
| 6 | MG | N | 9408 | 1/1 | 1.00 | 0.14 | 45,45,45,45 | 0 |
| 6 | MG | M | 9248 | 1/1 | 1.00 | 0.08 | 48,48,48,48 | 0 |
| 6 | MG | N | 9249 | 1/1 | 1.00 | 0.10 | 45,45,45,45 | 0 |
| 6 | MG | M | 9401 | 1/1 | 1.00 | 0.10 | 37,37,37,37 | 0 |
| 6 | MG | P | 9258 | 1/1 | 1.00 | 0.14 | 51,51,51,51 | 0 |
| 6 | MG | F | 9101 | 1/1 | 1.00 | 0.12 | 44,44,44,44 | 0 |
| 6 | MG | C | 9076 | 1/1 | 1.00 | 0.12 | 33,33,33,33 | 0 |
| 6 | MG | M | 9485 | 1/1 | 1.00 | 0.07 | 54,54,54,54 | 0 |
| 6 | MG | N | 9311 | 1/1 | 1.00 | 0.10 | 39,39,39,39 | 0 |
| 6 | MG | M | 9230 | 1/1 | 1.00 | 0.11 | 50,50,50,50 | 0 |
| 6 | MG | D | 9091 | 1/1 | 1.00 | 0.13 | 27,27,27,27 | 0 |
| 6 | MG | F | 9057 | 1/1 | 1.00 | 0.09 | 30,30,30,30 | 0 |
| 6 | MG | N | 9271 | 1/1 | 1.00 | 0.07 | 43,43,43,43 | 0 |
| 6 | MG | O | 9266 | 1/1 | 1.00 | 0.08 | 47,47,47,47 | 0 |
| 6 | MG | C | 9361 | 1/1 | 1.00 | 0.10 | 41,41,41,41 | 0 |
| 6 | MG | P | 9482 | 1/1 | 1.00 | 0.11 | 48,48,48,48 | 0 |
| 6 | MG | C | 9487 | 1/1 | 1.00 | 0.11 | 32,32,32,32 | 0 |
| 6 | MG | D | 9117 | 1/1 | 1.00 | 0.13 | 48,48,48,48 | 0 |
| 6 | MG | M | 9319 | 1/1 | 1.00 | 0.12 | 41,41,41,41 | 0 |
| 6 | MG | M | 9320 | 1/1 | 1.00 | 0.11 | 34,34,34,34 | 0 |
| 6 | MG | N | 9193 | 1/1 | 1.00 | 0.15 | 34,34,34,34 | 0 |
| 6 | MG | M | 9321 | 1/1 | 1.00 | 0.12 | 41,41,41,41 | 0 |

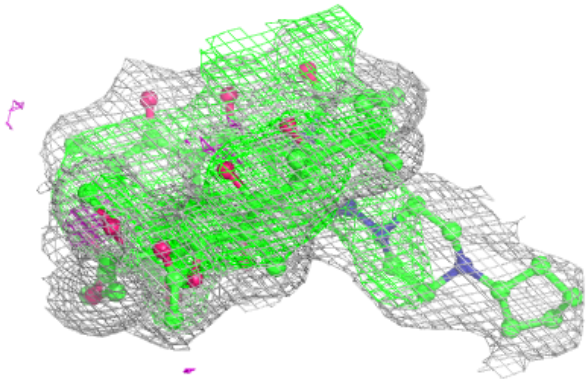
The following is a graphical depiction of the model fit to experimental electron density of all

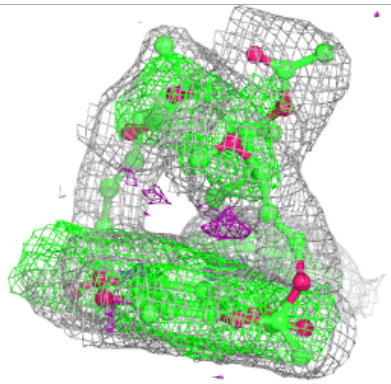
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around RPT C 8001:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

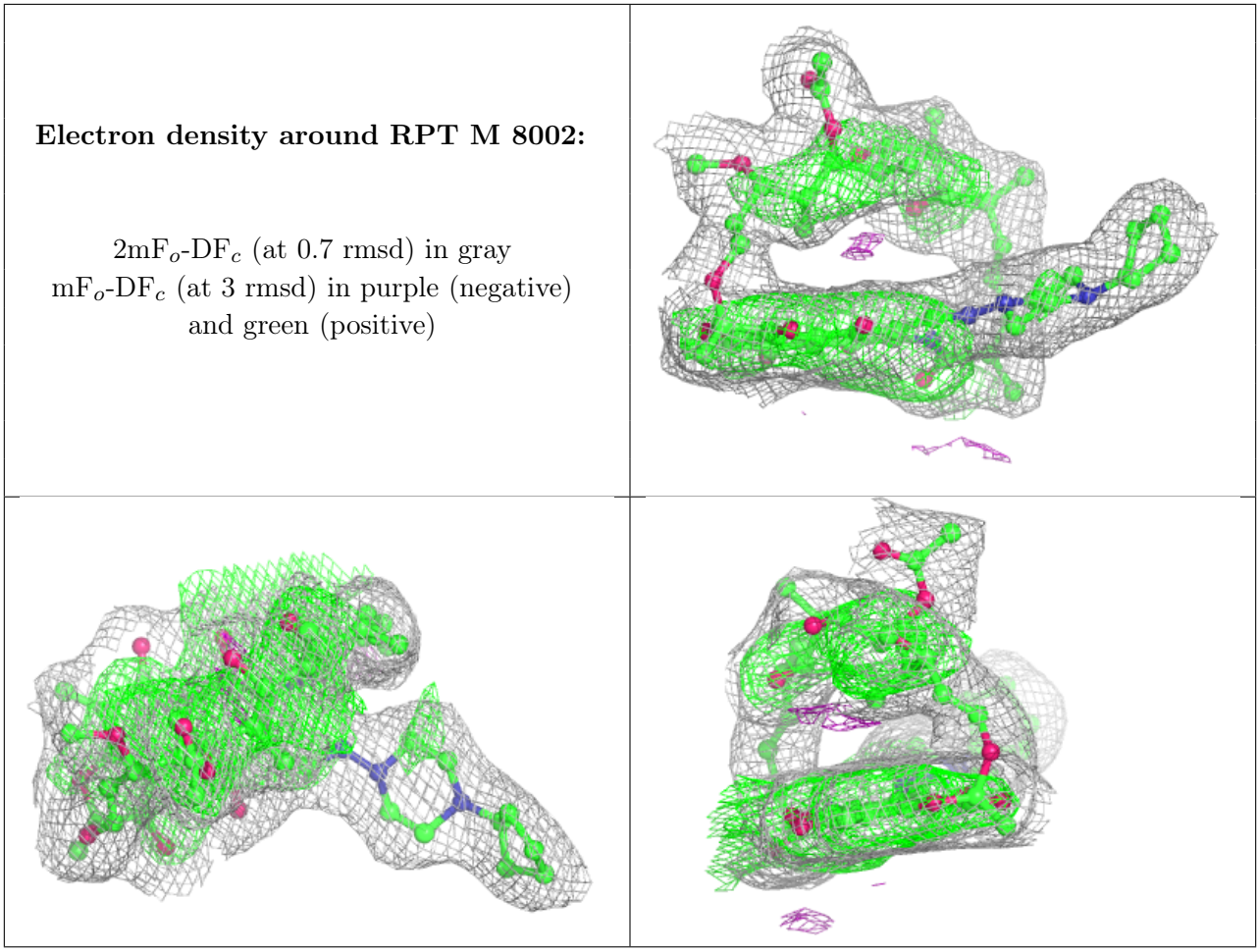






**Electron density around RPT M 8002:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.