



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 12:53 AM UTC

PDB ID : 4TNW / pdb\_00004tnw  
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab and POPC in a lipid-modulated conformation  
Authors : Althoff, T.; Hibbs, R.E.; Banerjee, S.; Gouaux, E.  
Deposited on : 2014-06-05  
Resolution : 3.20 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

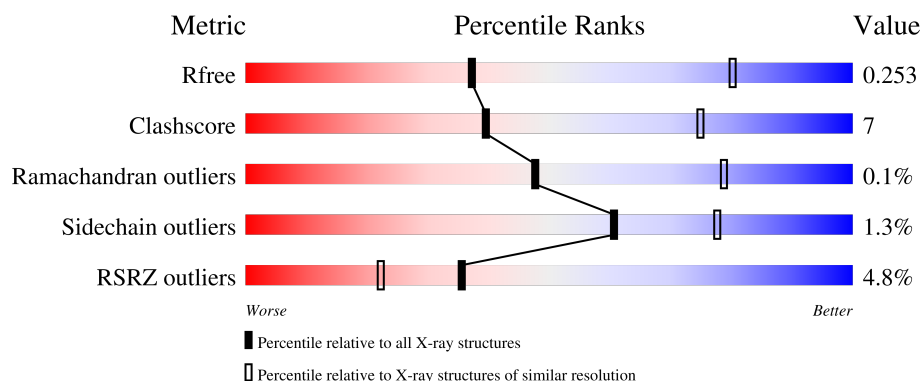
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 347    | <div> <div>9%</div> <div>78%</div> <div>20%</div> <div>..</div> </div> |
| 1   | B     | 347    | <div> <div>4%</div> <div>77%</div> <div>21%</div> <div>..</div> </div> |
| 1   | C     | 347    | <div> <div>6%</div> <div>76%</div> <div>21%</div> <div>..</div> </div> |
| 1   | D     | 347    | <div> <div>5%</div> <div>79%</div> <div>18%</div> <div>..</div> </div> |
| 1   | E     | 347    | <div> <div>5%</div> <div>78%</div> <div>18%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | P     | 347    | <div> <div>5%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>  |
| 1   | Q     | 347    | <div> <div>4%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>  |
| 1   | R     | 347    | <div> <div>3%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>   |
| 1   | S     | 347    | <div> <div>4%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>  |
| 1   | T     | 347    | <div> <div>6%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>   |
| 2   | F     | 224    | <div> <div>5%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>  |
| 2   | G     | 224    | <div> <div>6%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>   |
| 2   | H     | 224    | <div> <div>5%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>   |
| 2   | I     | 224    | <div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>   |
| 2   | J     | 224    | <div> <div>12%</div> <div>84%</div> <div>14%</div> <div>..</div> </div> |
| 2   | U     | 224    | <div> <div>4%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>  |
| 2   | V     | 224    | <div> <div>3%</div> <div>86%</div> <div>14%</div> <div></div> </div>    |
| 2   | W     | 224    | <div> <div>4%</div> <div>89%</div> <div>11%</div> <div></div> </div>    |
| 2   | X     | 224    | <div> <div>5%</div> <div>88%</div> <div>12%</div> <div></div> </div>    |
| 2   | Y     | 224    | <div> <div>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>  |
| 3   | K     | 215    | <div> <div>7%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>   |
| 3   | L     | 215    | <div> <div>6%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>  |
| 3   | M     | 215    | <div> <div>4%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>   |
| 3   | N     | 215    | <div> <div>3%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>   |
| 3   | O     | 215    | <div> <div>3%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>   |
| 3   | Z     | 215    | <div> <div>4%</div> <div>89%</div> <div>11%</div> <div></div> </div>    |
| 3   | f     | 215    | <div> <div>6%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>   |
| 3   | g     | 215    | <div> <div>5%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>  |
| 3   | h     | 215    | <div> <div>2%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>   |
| 3   | i     | 215    | <div> <div>%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>    |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 60818 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 Avermectin-sensitive glutamate-gated chloride channel GluCl alpha.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 342      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2744  | 1786 | 449 | 494 | 15 |         |         |       |
| 1   | B     | 341      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2734  | 1780 | 446 | 493 | 15 |         |         |       |
| 1   | C     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2724  | 1774 | 443 | 492 | 15 |         |         |       |
| 1   | D     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2724  | 1774 | 443 | 492 | 15 |         |         |       |
| 1   | E     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2724  | 1774 | 443 | 492 | 15 |         |         |       |
| 1   | P     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2724  | 1774 | 443 | 492 | 15 |         |         |       |
| 1   | Q     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2724  | 1774 | 443 | 492 | 15 |         |         |       |
| 1   | R     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2724  | 1774 | 443 | 492 | 15 |         |         |       |
| 1   | S     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2724  | 1774 | 443 | 492 | 15 |         |         |       |
| 1   | T     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2724  | 1774 | 443 | 492 | 15 |         |         |       |

There are 110 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| A     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| A     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| A     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| A     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| A     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| A     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| A     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| A     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| A     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| B     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| B     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| B     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| B     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| B     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| B     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| B     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| B     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| B     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| B     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| B     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| C     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| C     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| C     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| C     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| C     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| C     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| C     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| C     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| C     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| C     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| C     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| D     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| D     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| D     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| D     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| D     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| D     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| D     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| D     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| D     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| D     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| D     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| E     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| E     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| E     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| E     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| E     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| E     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| E     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| E     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| E     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| E     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| P     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| P     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| P     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| P     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| P     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| P     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| P     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| P     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| P     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| P     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| P     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| Q     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| Q     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| Q     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| Q     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| Q     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| Q     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| Q     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| Q     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| Q     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| Q     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| Q     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| R     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| R     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| R     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| R     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| R     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| R     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| R     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| R     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| R     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| R     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| R     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| S     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| S     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| S     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| S     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| S     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| S     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| S     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| S     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| S     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| S     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| S     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |
| T     | 303     | ALA      | -      | linker         | UNP G5EBR3 |
| T     | 304     | GLY      | -      | linker         | UNP G5EBR3 |
| T     | 305     | THR      | -      | linker         | UNP G5EBR3 |
| T     | 340     | HIS      | -      | expression tag | UNP G5EBR3 |
| T     | 341     | HIS      | -      | expression tag | UNP G5EBR3 |
| T     | 342     | HIS      | -      | expression tag | UNP G5EBR3 |
| T     | 343     | HIS      | -      | expression tag | UNP G5EBR3 |
| T     | 344     | HIS      | -      | expression tag | UNP G5EBR3 |
| T     | 345     | HIS      | -      | expression tag | UNP G5EBR3 |
| T     | 346     | HIS      | -      | expression tag | UNP G5EBR3 |
| T     | 347     | HIS      | -      | expression tag | UNP G5EBR3 |

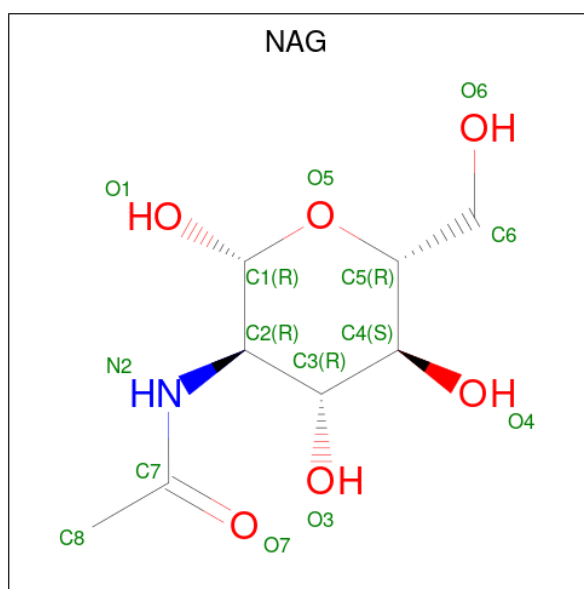
- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | F     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1682  | 1067 | 273 | 334 | 8 |         |         |       |
| 2   | G     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1693  | 1073 | 277 | 335 | 8 |         |         |       |
| 2   | H     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1701  | 1077 | 278 | 338 | 8 |         |         |       |
| 2   | I     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1693  | 1073 | 277 | 335 | 8 |         |         |       |
| 2   | U     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1682  | 1067 | 273 | 334 | 8 |         |         |       |
| 2   | V     | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1707  | 1080 | 279 | 339 | 9 |         |         |       |
| 2   | W     | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1707  | 1080 | 279 | 339 | 9 |         |         |       |
| 2   | X     | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1707  | 1080 | 279 | 339 | 9 |         |         |       |
| 2   | Y     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1682  | 1067 | 273 | 334 | 8 |         |         |       |
| 2   | J     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1693  | 1073 | 277 | 335 | 8 |         |         |       |

- Molecule 3 is a protein called Mouse monoclonal Fab fragment, light chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | K     | 210      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1590  | 999  | 266 | 319 | 6 |         |         |       |
| 3   | L     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1601  | 1005 | 270 | 320 | 6 |         |         |       |
| 3   | N     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1601  | 1005 | 270 | 320 | 6 |         |         |       |
| 3   | O     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1601  | 1005 | 270 | 320 | 6 |         |         |       |
| 3   | Z     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1626  | 1018 | 274 | 327 | 7 |         |         |       |
| 3   | f     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1626  | 1018 | 274 | 327 | 7 |         |         |       |
| 3   | g     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1601  | 1005 | 270 | 320 | 6 |         |         |       |
| 3   | h     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1601  | 1005 | 270 | 320 | 6 |         |         |       |
| 3   | i     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1620  | 1015 | 273 | 325 | 7 |         |         |       |
| 3   | M     | 210      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1590  | 999  | 266 | 319 | 6 |         |         |       |

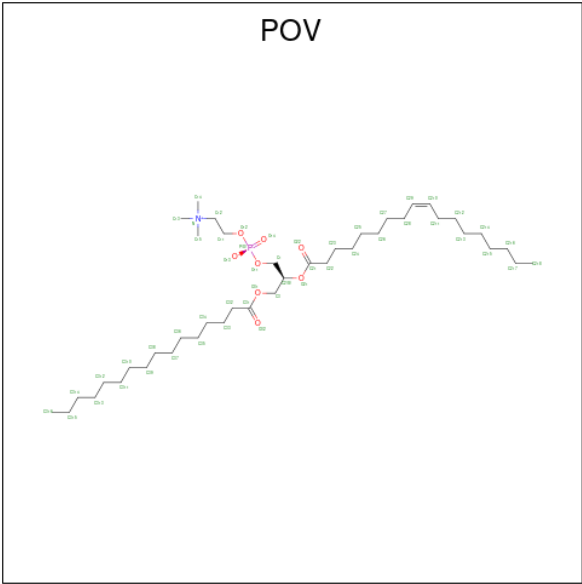
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).





| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | P     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | Q     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | S     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | T     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 5   | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 14 | 1 | 7 | 1 |         |         |
| 5   | D     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 26    | 16 | 1 | 8 | 1 |         |         |

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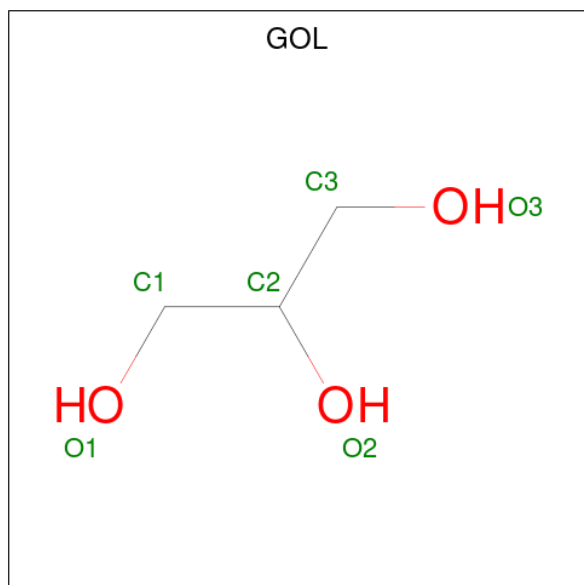
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| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 5   | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |         |
| 5   | Q     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |         |
| 5   | R     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 34    | 24 | 1 | 8 | 1 |         |         |
| 5   | R     | 1        | Total | C  | O | P |   | 0       | 0       |
|     |       |          | 35    | 26 | 8 | 1 |   |         |         |
| 5   | T     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |         |

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

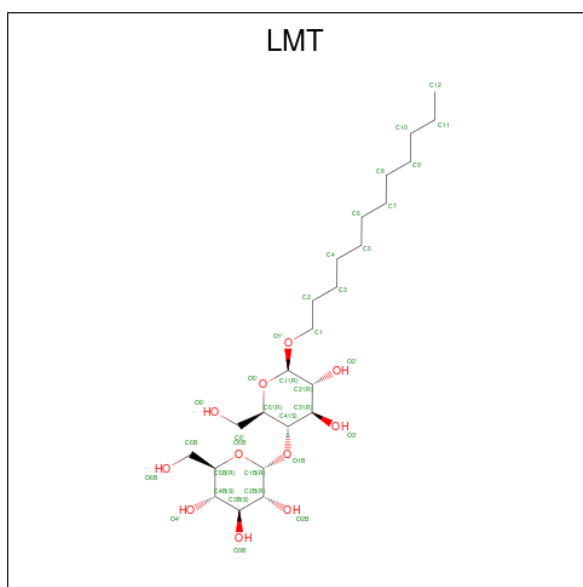
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | P     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



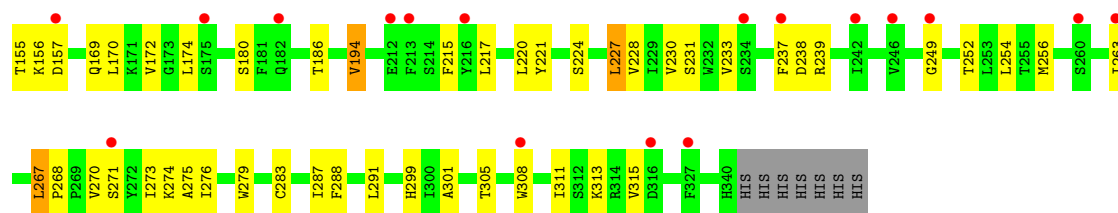
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 8 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).

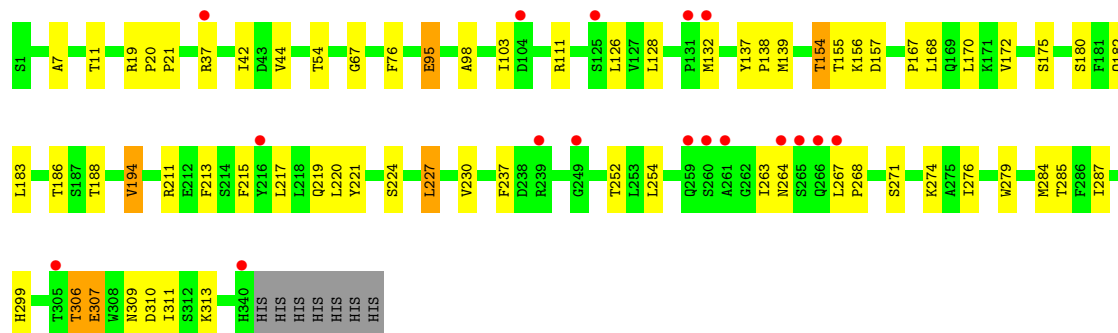
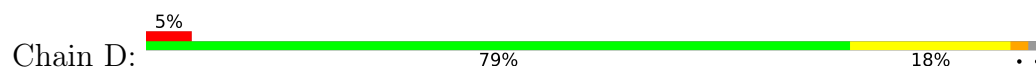


| Mol | Chain | Residues | Atoms       |         |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|---------|
| 8   | B     | 1        | Total<br>23 | C<br>12 | O<br>11 | 0       | 0       |
| 8   | C     | 1        | Total<br>23 | C<br>12 | O<br>11 | 0       | 0       |
| 8   | D     | 1        | Total<br>23 | C<br>12 | O<br>11 | 0       | 0       |
| 8   | E     | 1        | Total<br>23 | C<br>12 | O<br>11 | 0       | 0       |
| 8   | P     | 1        | Total<br>23 | C<br>12 | O<br>11 | 0       | 0       |
| 8   | S     | 1        | Total<br>23 | C<br>12 | O<br>11 | 0       | 0       |
| 8   | T     | 1        | Total<br>23 | C<br>12 | O<br>11 | 0       | 0       |

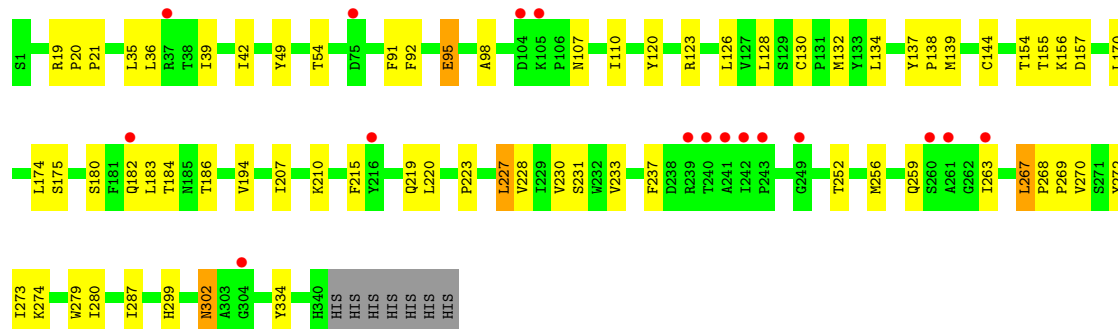
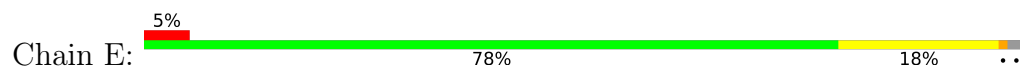




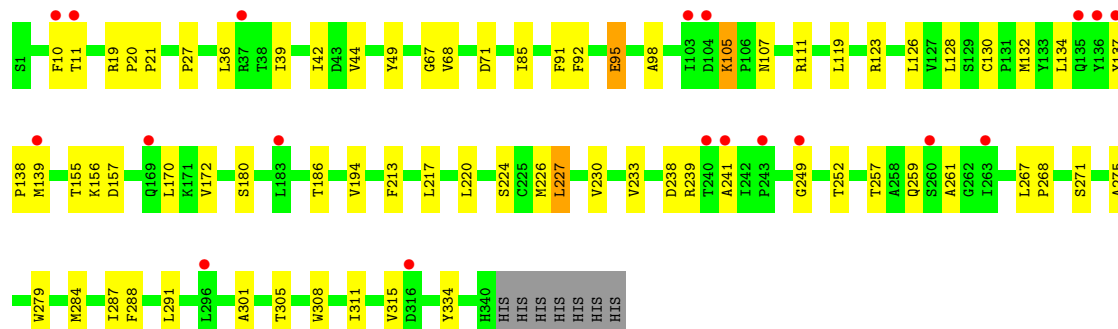
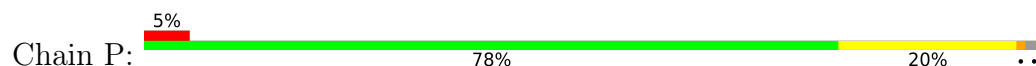
● Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



● Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



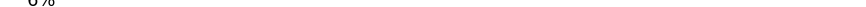
● Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

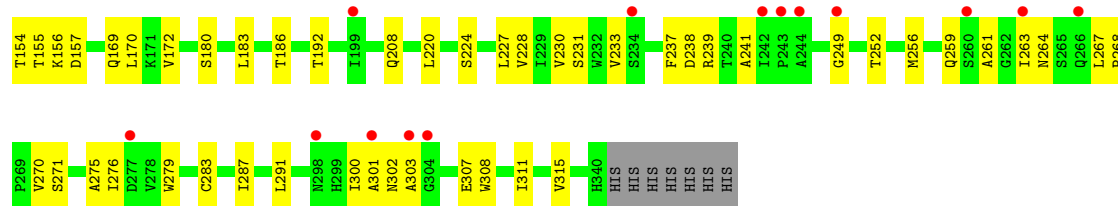


- Chain Q:
- 
- 4% 78% 19% ..
- 
- S1 L9 F10 T11 R19 N33 L36 L39 T42 D43 V44 B56 Y66 G67 F76 I85 F92 E95 K96 G97 A98 I103 M107 R111 I112 L119 R123 L126 V127 L128 S129 C130 P131 M132 Y133 L134 P138 M139 D140 V141 Q142
- 
- W279 C283 I287 L291 N298 N302 A303 G304 F308 I311 V315 H340 HIS HIS HIS HIS HIS HIS HIS HIS HIS

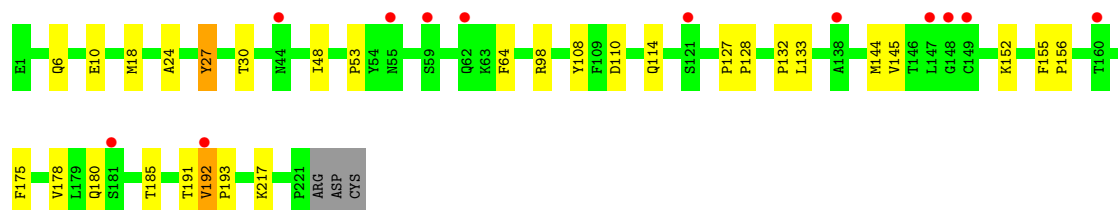
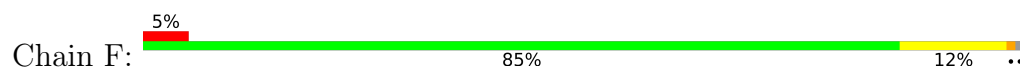
- Chain R:
- 
- | Category | Percentage |
|----------|------------|
| Green    | 77%        |
| Yellow   | 21%        |
| Grey     | 3%         |

- Chain S:
- 
- 4% 78% 20%
- S1 I5 A7 H8 L9 F10 R19 P20 R33 R37 T38 I42 Y49 Q52 R56 D75 T85 W86 W87 E95 A98 Y99 K100 D104 R111 I112 H113 N114 L119 L126 V127 L128 M132 Y133 L134 Y137 P138 M139 C144

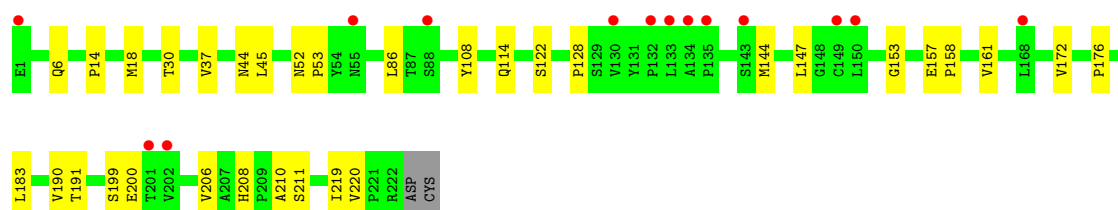
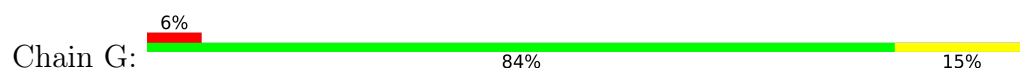
- Chain T: 



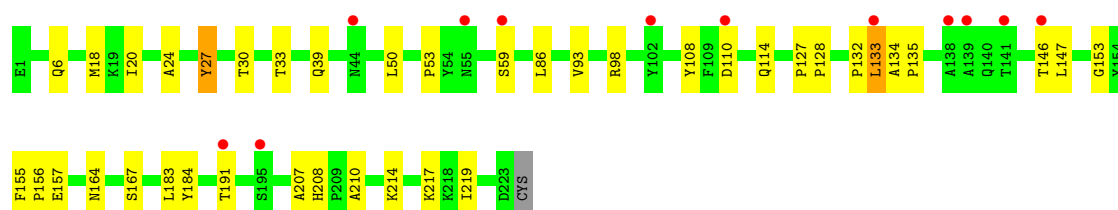
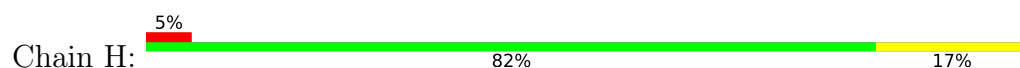
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



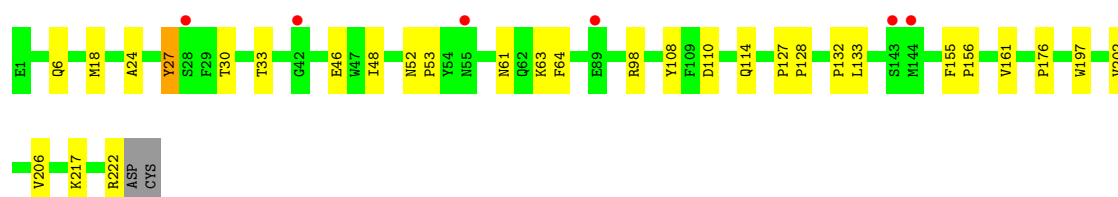
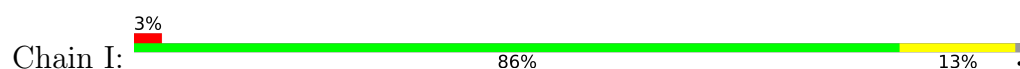
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



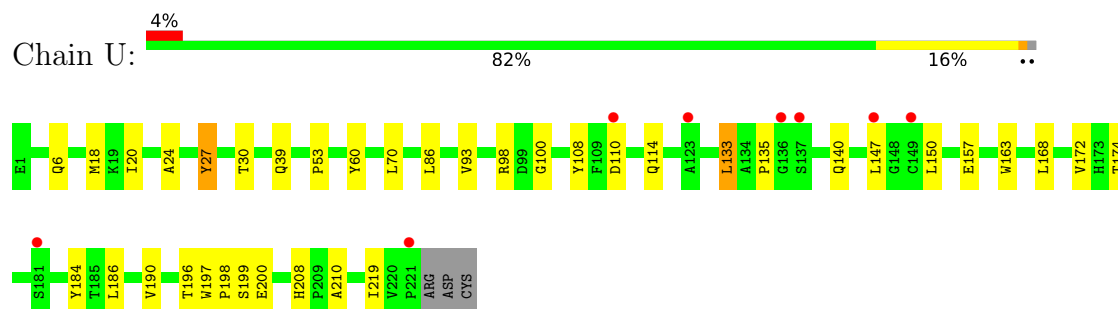
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



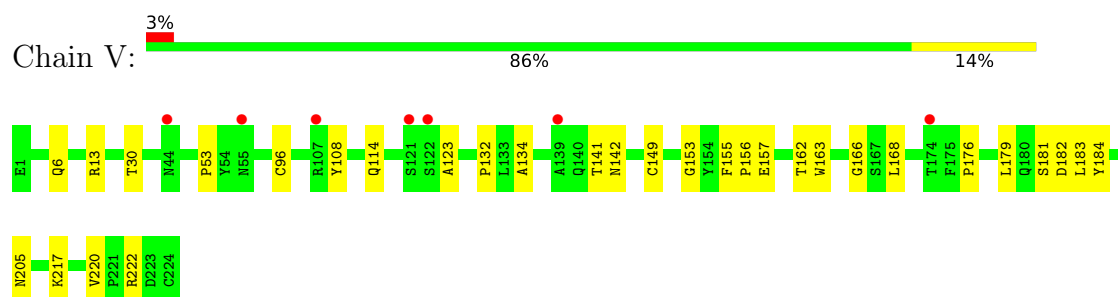
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



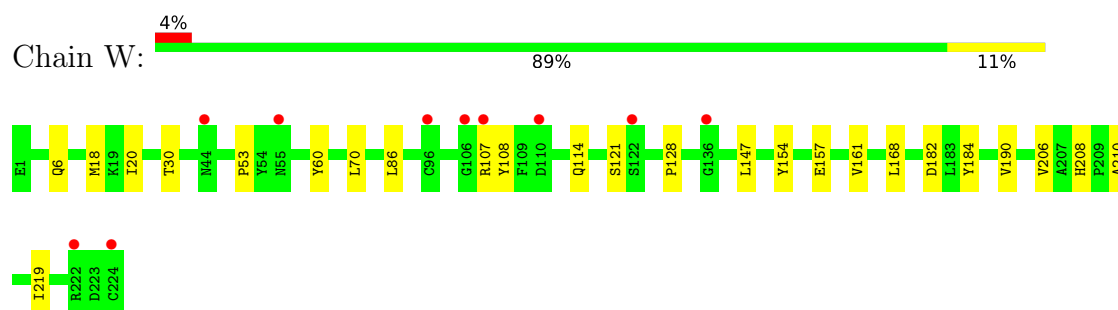
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



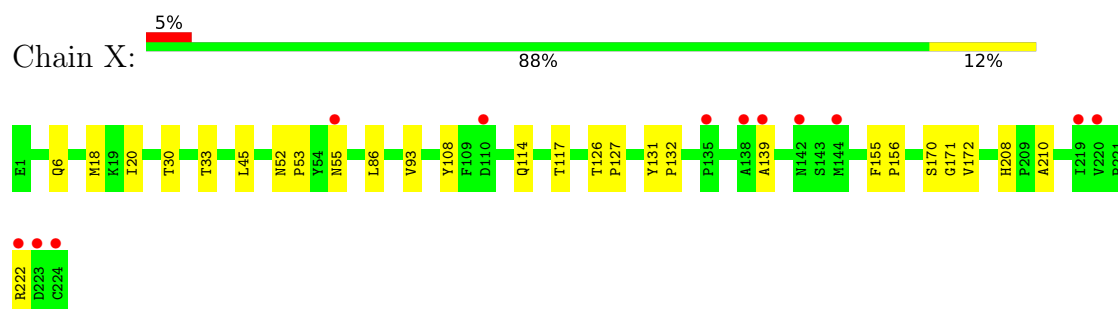
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



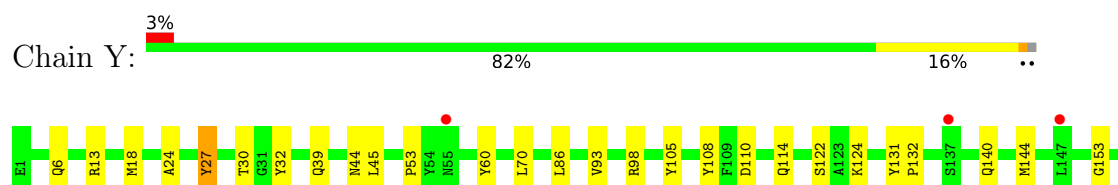
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



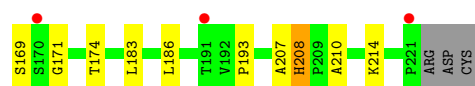
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



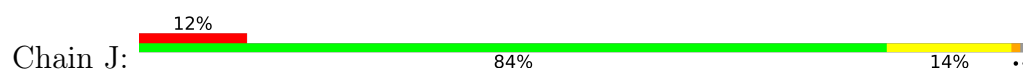
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



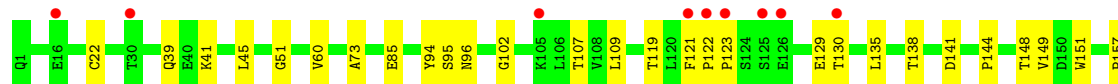
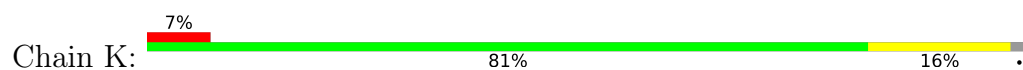




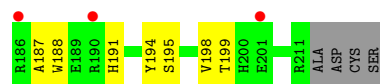
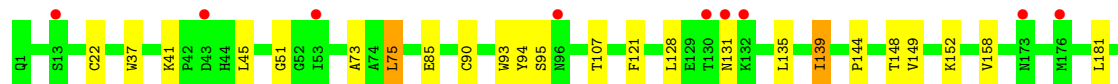
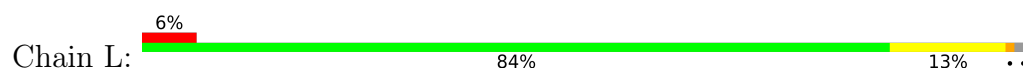
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



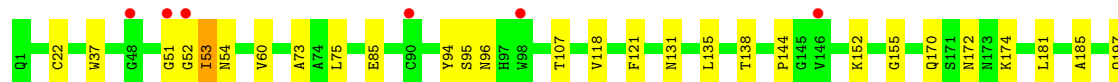
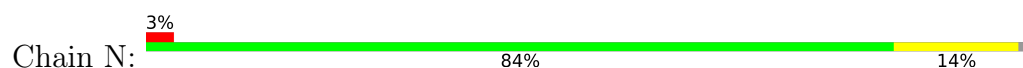
- Molecule 3: Mouse monoclonal Fab fragment, light chain



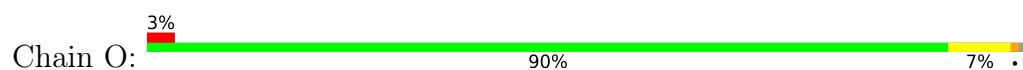
- Molecule 3: Mouse monoclonal Fab fragment, light chain

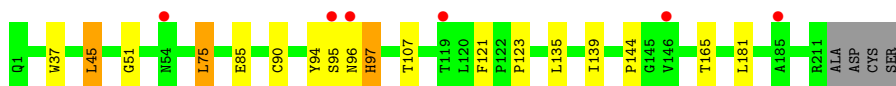


- Molecule 3: Mouse monoclonal Fab fragment, light chain

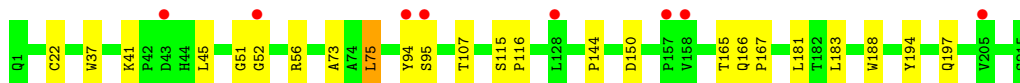
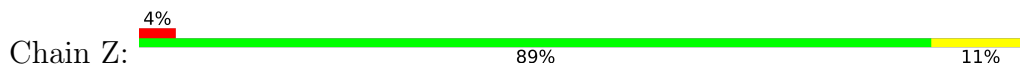


- Molecule 3: Mouse monoclonal Fab fragment, light chain

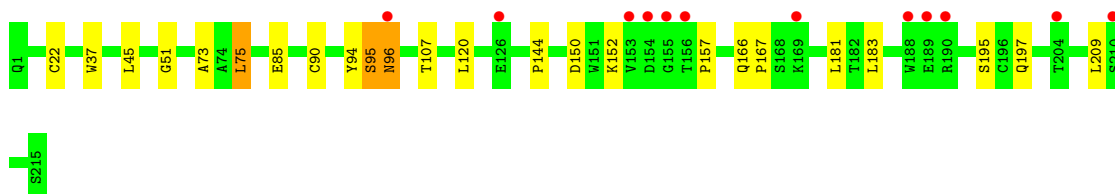
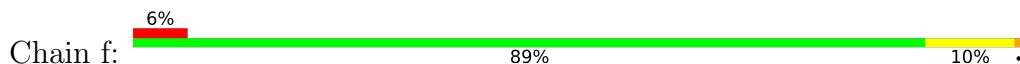




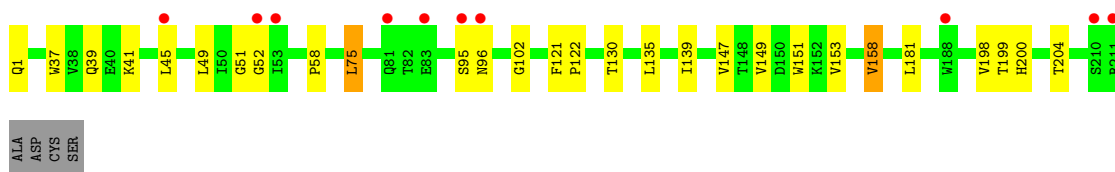
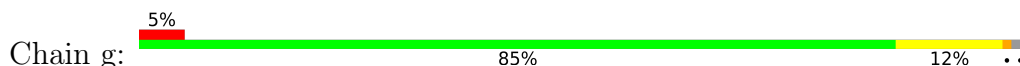
- Molecule 3: Mouse monoclonal Fab fragment, light chain



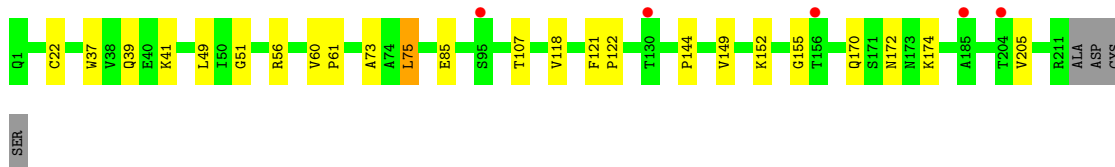
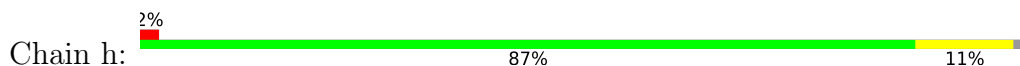
- Molecule 3: Mouse monoclonal Fab fragment, light chain



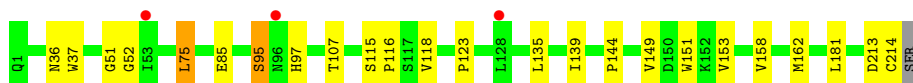
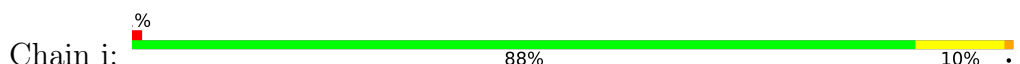
- Molecule 3: Mouse monoclonal Fab fragment, light chain



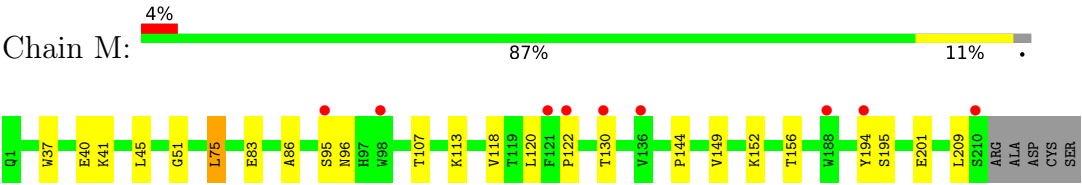
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 453.75Å 192.87Å 196.14Å<br>90.00° 92.27° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 58.70 – 3.20<br>58.70 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 77.6 (58.70-3.20)<br>92.3 (58.70-3.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.25 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.8.4_1496)                          | Depositor        |
| R, $R_{free}$                                                           | 0.227 , 0.251<br>0.232 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 14870 reflections (5.00%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 84.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.036                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 69.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction                                             | 0.021 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 60818                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 115.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: LMT, POV, GOL, NAG, CL

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     | 0.32         | 0/2819      | 0.78        | 3/3847 (0.1%)   |
| 1   | B     | 0.31         | 0/2808      | 0.77        | 3/3832 (0.1%)   |
| 1   | C     | 0.31         | 0/2797      | 0.78        | 2/3817 (0.1%)   |
| 1   | D     | 0.33         | 0/2797      | 0.82        | 5/3817 (0.1%)   |
| 1   | E     | 0.32         | 0/2797      | 0.79        | 5/3817 (0.1%)   |
| 1   | P     | 0.32         | 0/2797      | 0.79        | 4/3817 (0.1%)   |
| 1   | Q     | 0.32         | 0/2797      | 0.77        | 4/3817 (0.1%)   |
| 1   | R     | 0.32         | 0/2797      | 0.77        | 3/3817 (0.1%)   |
| 1   | S     | 0.32         | 0/2797      | 0.76        | 0/3817          |
| 1   | T     | 0.32         | 0/2797      | 0.78        | 1/3817 (0.0%)   |
| 2   | F     | 0.26         | 0/1728      | 0.71        | 2/2360 (0.1%)   |
| 2   | G     | 0.29         | 0/1739      | 0.72        | 0/2374          |
| 2   | H     | 0.26         | 0/1747      | 0.72        | 0/2385          |
| 2   | I     | 0.25         | 0/1739      | 0.70        | 0/2374          |
| 2   | J     | 0.30         | 0/1739      | 0.75        | 2/2374 (0.1%)   |
| 2   | U     | 0.26         | 0/1728      | 0.69        | 0/2360          |
| 2   | V     | 0.27         | 0/1753      | 0.72        | 1/2393 (0.0%)   |
| 2   | W     | 0.26         | 0/1753      | 0.72        | 0/2393          |
| 2   | X     | 0.26         | 0/1753      | 0.74        | 1/2393 (0.0%)   |
| 2   | Y     | 0.26         | 0/1728      | 0.72        | 3/2360 (0.1%)   |
| 3   | K     | 0.27         | 0/1628      | 0.71        | 2/2226 (0.1%)   |
| 3   | L     | 0.28         | 0/1639      | 0.74        | 1/2240 (0.0%)   |
| 3   | M     | 0.29         | 0/1628      | 0.77        | 4/2226 (0.2%)   |
| 3   | N     | 0.29         | 0/1639      | 0.73        | 2/2240 (0.1%)   |
| 3   | O     | 0.27         | 0/1639      | 0.70        | 0/2240          |
| 3   | Z     | 0.28         | 0/1664      | 0.73        | 1/2274 (0.0%)   |
| 3   | f     | 0.28         | 0/1664      | 0.71        | 0/2274          |
| 3   | g     | 0.28         | 0/1639      | 0.72        | 0/2240          |
| 3   | h     | 0.27         | 0/1639      | 0.70        | 0/2240          |
| 3   | i     | 0.27         | 0/1658      | 0.71        | 0/2266          |
| All | All   | 0.30         | 0/61847     | 0.75        | 49/84447 (0.1%) |

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | P     | 11  | THR  | N-CA-C | -9.03 | 100.59      | 111.69   |
| 1   | D     | 67  | GLY  | N-CA-C | 7.89  | 123.66      | 110.56   |
| 1   | T     | 11  | THR  | N-CA-C | -7.79 | 102.42      | 112.23   |
| 1   | C     | 267 | LEU  | CA-C-N | 6.80  | 124.56      | 119.66   |
| 1   | C     | 267 | LEU  | C-N-CA | 6.80  | 124.56      | 119.66   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 2744  | 0        | 2744     | 48      | 0            |
| 1   | B     | 2734  | 0        | 2737     | 52      | 0            |
| 1   | C     | 2724  | 0        | 2729     | 54      | 0            |
| 1   | D     | 2724  | 0        | 2729     | 47      | 0            |
| 1   | E     | 2724  | 0        | 2730     | 49      | 0            |
| 1   | P     | 2724  | 0        | 2730     | 48      | 0            |
| 1   | Q     | 2724  | 0        | 2730     | 44      | 0            |
| 1   | R     | 2724  | 0        | 2731     | 48      | 0            |
| 1   | S     | 2724  | 0        | 2730     | 54      | 0            |
| 1   | T     | 2724  | 0        | 2730     | 56      | 0            |
| 2   | F     | 1682  | 0        | 1632     | 26      | 0            |
| 2   | G     | 1693  | 0        | 1645     | 23      | 0            |
| 2   | H     | 1701  | 0        | 1649     | 27      | 0            |
| 2   | I     | 1693  | 0        | 1645     | 24      | 0            |
| 2   | J     | 1693  | 0        | 1645     | 23      | 0            |
| 2   | U     | 1682  | 0        | 1632     | 23      | 0            |
| 2   | V     | 1707  | 0        | 1653     | 20      | 0            |
| 2   | W     | 1707  | 0        | 1653     | 16      | 0            |
| 2   | X     | 1707  | 0        | 1653     | 17      | 0            |
| 2   | Y     | 1682  | 0        | 1632     | 25      | 0            |
| 3   | K     | 1590  | 0        | 1542     | 25      | 0            |
| 3   | L     | 1601  | 0        | 1555     | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | M     | 1590  | 0        | 1542     | 12      | 0            |
| 3   | N     | 1601  | 0        | 1555     | 21      | 0            |
| 3   | O     | 1601  | 0        | 1555     | 17      | 0            |
| 3   | Z     | 1626  | 0        | 1573     | 13      | 0            |
| 3   | f     | 1626  | 0        | 1573     | 19      | 0            |
| 3   | g     | 1601  | 0        | 1555     | 18      | 0            |
| 3   | h     | 1601  | 0        | 1555     | 13      | 0            |
| 3   | i     | 1620  | 0        | 1568     | 14      | 0            |
| 4   | A     | 14    | 0        | 13       | 0       | 0            |
| 4   | B     | 14    | 0        | 13       | 0       | 0            |
| 4   | C     | 14    | 0        | 13       | 0       | 0            |
| 4   | D     | 14    | 0        | 13       | 0       | 0            |
| 4   | E     | 14    | 0        | 13       | 0       | 0            |
| 4   | P     | 14    | 0        | 13       | 0       | 0            |
| 4   | Q     | 14    | 0        | 13       | 0       | 0            |
| 4   | S     | 14    | 0        | 13       | 1       | 0            |
| 4   | T     | 14    | 0        | 13       | 0       | 0            |
| 5   | A     | 23    | 0        | 26       | 1       | 0            |
| 5   | D     | 26    | 0        | 26       | 5       | 0            |
| 5   | P     | 42    | 0        | 61       | 4       | 0            |
| 5   | Q     | 46    | 0        | 67       | 6       | 0            |
| 5   | R     | 69    | 0        | 83       | 6       | 0            |
| 5   | T     | 43    | 0        | 63       | 3       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | P     | 1     | 0        | 0        | 0       | 0            |
| 7   | B     | 6     | 0        | 8        | 0       | 0            |
| 8   | B     | 23    | 0        | 21       | 0       | 0            |
| 8   | C     | 23    | 0        | 21       | 0       | 0            |
| 8   | D     | 23    | 0        | 21       | 1       | 0            |
| 8   | E     | 23    | 0        | 21       | 0       | 0            |
| 8   | P     | 23    | 0        | 21       | 0       | 0            |
| 8   | S     | 23    | 0        | 21       | 1       | 0            |
| 8   | T     | 23    | 0        | 21       | 1       | 0            |
| All | All   | 60818 | 0        | 59930    | 812     | 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 7.

The worst 5 of 812 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:D:306:THR:HA   | 1:D:309:ASN:HB2 | 1.53                     | 0.90              |
| 1:Q:302:ASN:HD22 | 1:R:241:ALA:HB2 | 1.36                     | 0.89              |
| 1:T:37:ARG:NH2   | 1:T:54:THR:OG1  | 2.10                     | 0.84              |
| 1:C:305:THR:HG22 | 1:C:308:TRP:HD1 | 1.43                     | 0.83              |
| 1:R:156:LYS:HA   | 3:Z:95:SER:HB2  | 1.61                     | 0.83              |

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     | 340/347 (98%) | 327 (96%) | 13 (4%) | 0        | 100         | 100 |
| 1   | B     | 339/347 (98%) | 325 (96%) | 14 (4%) | 0        | 100         | 100 |
| 1   | C     | 338/347 (97%) | 324 (96%) | 14 (4%) | 0        | 100         | 100 |
| 1   | D     | 338/347 (97%) | 328 (97%) | 10 (3%) | 0        | 100         | 100 |
| 1   | E     | 338/347 (97%) | 325 (96%) | 13 (4%) | 0        | 100         | 100 |
| 1   | P     | 338/347 (97%) | 326 (96%) | 12 (4%) | 0        | 100         | 100 |
| 1   | Q     | 338/347 (97%) | 326 (96%) | 12 (4%) | 0        | 100         | 100 |
| 1   | R     | 338/347 (97%) | 326 (96%) | 12 (4%) | 0        | 100         | 100 |
| 1   | S     | 338/347 (97%) | 325 (96%) | 12 (4%) | 1 (0%)   | 36          | 68  |
| 1   | T     | 338/347 (97%) | 326 (96%) | 12 (4%) | 0        | 100         | 100 |
| 2   | F     | 219/224 (98%) | 206 (94%) | 13 (6%) | 0        | 100         | 100 |
| 2   | G     | 220/224 (98%) | 203 (92%) | 17 (8%) | 0        | 100         | 100 |
| 2   | H     | 221/224 (99%) | 206 (93%) | 15 (7%) | 0        | 100         | 100 |
| 2   | I     | 220/224 (98%) | 206 (94%) | 14 (6%) | 0        | 100         | 100 |
| 2   | J     | 220/224 (98%) | 203 (92%) | 16 (7%) | 1 (0%)   | 24          | 59  |
| 2   | U     | 219/224 (98%) | 205 (94%) | 14 (6%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | V     | 222/224 (99%)   | 203 (91%)  | 19 (9%)  | 0        | 100         | 100 |
| 2   | W     | 222/224 (99%)   | 209 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 2   | X     | 222/224 (99%)   | 206 (93%)  | 16 (7%)  | 0        | 100         | 100 |
| 2   | Y     | 219/224 (98%)   | 202 (92%)  | 17 (8%)  | 0        | 100         | 100 |
| 3   | K     | 208/215 (97%)   | 193 (93%)  | 14 (7%)  | 1 (0%)   | 24          | 59  |
| 3   | L     | 209/215 (97%)   | 198 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 3   | M     | 208/215 (97%)   | 193 (93%)  | 15 (7%)  | 0        | 100         | 100 |
| 3   | N     | 209/215 (97%)   | 194 (93%)  | 14 (7%)  | 1 (0%)   | 24          | 59  |
| 3   | O     | 209/215 (97%)   | 194 (93%)  | 15 (7%)  | 0        | 100         | 100 |
| 3   | Z     | 213/215 (99%)   | 193 (91%)  | 19 (9%)  | 1 (0%)   | 24          | 59  |
| 3   | f     | 213/215 (99%)   | 195 (92%)  | 16 (8%)  | 2 (1%)   | 14          | 47  |
| 3   | g     | 209/215 (97%)   | 196 (94%)  | 11 (5%)  | 2 (1%)   | 12          | 45  |
| 3   | h     | 209/215 (97%)   | 194 (93%)  | 15 (7%)  | 0        | 100         | 100 |
| 3   | i     | 212/215 (99%)   | 199 (94%)  | 12 (6%)  | 1 (0%)   | 24          | 59  |
| All | All   | 7686/7860 (98%) | 7256 (94%) | 420 (6%) | 10 (0%)  | 48          | 79  |

5 of 10 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | K     | 95  | SER  |
| 3   | N     | 95  | SER  |
| 3   | i     | 95  | SER  |
| 3   | f     | 95  | SER  |
| 1   | S     | 309 | ASN  |

### 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 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     | 311/316 (98%) | 307 (99%) | 4 (1%)   | 61          | 78 |
| 1   | B     | 310/316 (98%) | 306 (99%) | 4 (1%)   | 61          | 78 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | C     | 309/316 (98%)   | 305 (99%)  | 4 (1%)   | 61          | 78  |
| 1   | D     | 309/316 (98%)   | 304 (98%)  | 5 (2%)   | 55          | 75  |
| 1   | E     | 309/316 (98%)   | 306 (99%)  | 3 (1%)   | 68          | 80  |
| 1   | P     | 309/316 (98%)   | 304 (98%)  | 5 (2%)   | 55          | 75  |
| 1   | Q     | 309/316 (98%)   | 307 (99%)  | 2 (1%)   | 78          | 84  |
| 1   | R     | 309/316 (98%)   | 307 (99%)  | 2 (1%)   | 78          | 84  |
| 1   | S     | 309/316 (98%)   | 305 (99%)  | 4 (1%)   | 61          | 78  |
| 1   | T     | 309/316 (98%)   | 306 (99%)  | 3 (1%)   | 68          | 80  |
| 2   | F     | 190/193 (98%)   | 188 (99%)  | 2 (1%)   | 65          | 79  |
| 2   | G     | 191/193 (99%)   | 190 (100%) | 1 (0%)   | 81          | 85  |
| 2   | H     | 192/193 (100%)  | 190 (99%)  | 2 (1%)   | 68          | 80  |
| 2   | I     | 191/193 (99%)   | 190 (100%) | 1 (0%)   | 81          | 85  |
| 2   | J     | 191/193 (99%)   | 187 (98%)  | 4 (2%)   | 47          | 71  |
| 2   | U     | 190/193 (98%)   | 187 (98%)  | 3 (2%)   | 55          | 75  |
| 2   | V     | 193/193 (100%)  | 191 (99%)  | 2 (1%)   | 68          | 80  |
| 2   | W     | 193/193 (100%)  | 193 (100%) | 0        | 100         | 100 |
| 2   | X     | 193/193 (100%)  | 191 (99%)  | 2 (1%)   | 68          | 80  |
| 2   | Y     | 190/193 (98%)   | 188 (99%)  | 2 (1%)   | 65          | 79  |
| 3   | K     | 178/182 (98%)   | 177 (99%)  | 1 (1%)   | 78          | 84  |
| 3   | L     | 179/182 (98%)   | 175 (98%)  | 4 (2%)   | 45          | 71  |
| 3   | M     | 178/182 (98%)   | 174 (98%)  | 4 (2%)   | 45          | 71  |
| 3   | N     | 179/182 (98%)   | 178 (99%)  | 1 (1%)   | 78          | 84  |
| 3   | O     | 179/182 (98%)   | 175 (98%)  | 4 (2%)   | 45          | 71  |
| 3   | Z     | 182/182 (100%)  | 180 (99%)  | 2 (1%)   | 65          | 79  |
| 3   | f     | 182/182 (100%)  | 180 (99%)  | 2 (1%)   | 65          | 79  |
| 3   | g     | 179/182 (98%)   | 175 (98%)  | 4 (2%)   | 45          | 71  |
| 3   | h     | 179/182 (98%)   | 175 (98%)  | 4 (2%)   | 45          | 71  |
| 3   | i     | 181/182 (100%)  | 175 (97%)  | 6 (3%)   | 33          | 65  |
| All | All   | 6803/6910 (98%) | 6716 (99%) | 87 (1%)  | 61          | 78  |

5 of 87 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | X     | 45  | LEU  |
| 3   | h     | 149 | VAL  |
| 2   | Y     | 27  | TYR  |
| 3   | g     | 75  | LEU  |
| 3   | i     | 118 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 259 | GLN  |
| 3   | i     | 170 | GLN  |
| 1   | Q     | 299 | HIS  |
| 3   | h     | 39  | GLN  |
| 3   | M     | 172 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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 |
| 5   | POV  | A     | 402 | -    | 22,22,51     | 1.11 | 1 (4%)   | 27,29,59    | 1.19 | 2 (7%)   |
| 4   | NAG  | A     | 401 | 1    | 14,14,15     | 0.29 | 0        | 17,19,21    | 1.02 | 1 (5%)   |
| 4   | NAG  | B     | 402 | 1    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.80 | 0        |
| 4   | NAG  | Q     | 402 | 1    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.63 | 0        |
| 8   | LMT  | D     | 403 | -    | 24,24,36     | 1.08 | 2 (8%)   | 35,35,47    | 1.15 | 2 (5%)   |
| 7   | GOL  | B     | 401 | -    | 5,5,5        | 0.37 | 0        | 5,5,5       | 0.29 | 0        |
| 8   | LMT  | B     | 403 | -    | 24,24,36     | 1.02 | 2 (8%)   | 35,35,47    | 1.43 | 5 (14%)  |
| 5   | POV  | R     | 401 | -    | 33,33,51     | 1.18 | 2 (6%)   | 39,41,59    | 1.14 | 3 (7%)   |
| 5   | POV  | Q     | 401 | -    | 45,45,51     | 1.03 | 2 (4%)   | 51,53,59    | 1.05 | 3 (5%)   |
| 4   | NAG  | D     | 402 | 1    | 14,14,15     | 0.35 | 0        | 17,19,21    | 1.32 | 1 (5%)   |
| 4   | NAG  | C     | 401 | 1    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.86 | 1 (5%)   |
| 4   | NAG  | T     | 402 | 1    | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.77 | 1 (5%)   |
| 8   | LMT  | T     | 403 | -    | 24,24,36     | 1.04 | 2 (8%)   | 35,35,47    | 1.25 | 5 (14%)  |
| 5   | POV  | D     | 401 | -    | 25,25,51     | 1.36 | 2 (8%)   | 31,33,59    | 1.32 | 4 (12%)  |
| 4   | NAG  | P     | 401 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.71 | 0        |
| 8   | LMT  | C     | 402 | -    | 24,24,36     | 1.10 | 2 (8%)   | 35,35,47    | 1.12 | 4 (11%)  |
| 4   | NAG  | E     | 401 | 1    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.59 | 0        |
| 5   | POV  | R     | 402 | -    | 34,34,51     | 1.15 | 2 (5%)   | 37,39,59    | 1.33 | 5 (13%)  |
| 8   | LMT  | P     | 402 | -    | 24,24,36     | 1.04 | 2 (8%)   | 35,35,47    | 1.18 | 2 (5%)   |
| 4   | NAG  | S     | 401 | 1    | 14,14,15     | 0.35 | 0        | 17,19,21    | 1.32 | 1 (5%)   |
| 5   | POV  | P     | 403 | -    | 41,41,51     | 1.07 | 2 (4%)   | 47,49,59    | 1.12 | 4 (8%)   |
| 5   | POV  | T     | 401 | -    | 42,42,51     | 1.04 | 2 (4%)   | 48,50,59    | 1.14 | 4 (8%)   |
| 8   | LMT  | E     | 402 | -    | 24,24,36     | 1.04 | 2 (8%)   | 35,35,47    | 1.15 | 3 (8%)   |
| 8   | LMT  | S     | 402 | -    | 24,24,36     | 1.05 | 2 (8%)   | 35,35,47    | 1.23 | 2 (5%)   |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | POV  | A     | 402 | -    | -       | 4/25/25/55 | -       |
| 4   | NAG  | A     | 401 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 4   | NAG  | B     | 402 | 1    | -       | 0/6/23/26  | 0/1/1/1 |
| 4   | NAG  | Q     | 402 | 1    | -       | 0/6/23/26  | 0/1/1/1 |
| 8   | LMT  | D     | 403 | -    | -       | 4/8/48/61  | 0/2/2/2 |
| 7   | GOL  | B     | 401 | -    | -       | 2/4/4/4    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 8   | LMT  | B     | 403 | -    | -       | 4/8/48/61   | 0/2/2/2 |
| 5   | POV  | R     | 401 | -    | -       | 17/37/37/55 | -       |
| 5   | POV  | Q     | 401 | -    | -       | 14/49/49/55 | -       |
| 4   | NAG  | D     | 402 | 1    | -       | 3/6/23/26   | 0/1/1/1 |
| 4   | NAG  | C     | 401 | 1    | -       | 5/6/23/26   | 0/1/1/1 |
| 4   | NAG  | T     | 402 | 1    | -       | 3/6/23/26   | 0/1/1/1 |
| 8   | LMT  | T     | 403 | -    | -       | 2/8/48/61   | 0/2/2/2 |
| 5   | POV  | D     | 401 | -    | -       | 10/29/29/55 | -       |
| 4   | NAG  | P     | 401 | 1    | -       | 4/6/23/26   | 0/1/1/1 |
| 8   | LMT  | C     | 402 | -    | -       | 6/8/48/61   | 0/2/2/2 |
| 4   | NAG  | E     | 401 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 5   | POV  | R     | 402 | -    | -       | 12/36/36/55 | -       |
| 8   | LMT  | P     | 402 | -    | -       | 1/8/48/61   | 0/2/2/2 |
| 4   | NAG  | S     | 401 | 1    | -       | 0/6/23/26   | 0/1/1/1 |
| 5   | POV  | P     | 403 | -    | -       | 12/45/45/55 | -       |
| 5   | POV  | T     | 401 | -    | -       | 16/46/46/55 | -       |
| 8   | LMT  | E     | 402 | -    | -       | 3/8/48/61   | 0/2/2/2 |
| 8   | LMT  | S     | 402 | -    | -       | 1/8/48/61   | 0/2/2/2 |

The worst 5 of 27 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | D     | 401 | POV  | O31-C31 | 4.48 | 1.46        | 1.33     |
| 5   | P     | 403 | POV  | O31-C31 | 4.35 | 1.46        | 1.33     |
| 5   | Q     | 401 | POV  | O31-C31 | 4.33 | 1.46        | 1.33     |
| 5   | R     | 401 | POV  | O31-C31 | 4.26 | 1.45        | 1.33     |
| 5   | T     | 401 | POV  | O31-C31 | 4.22 | 1.45        | 1.33     |

The worst 5 of 53 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | S     | 401 | NAG  | C1-O5-C5    | 4.58  | 118.32      | 112.19   |
| 4   | D     | 402 | NAG  | C1-O5-C5    | -4.40 | 106.29      | 112.19   |
| 5   | R     | 402 | POV  | O21-C21-C22 | 4.30  | 120.79      | 111.48   |
| 5   | T     | 401 | POV  | O21-C21-C22 | 4.18  | 120.53      | 111.48   |
| 5   | A     | 402 | POV  | O21-C21-C22 | 4.07  | 120.28      | 111.48   |

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

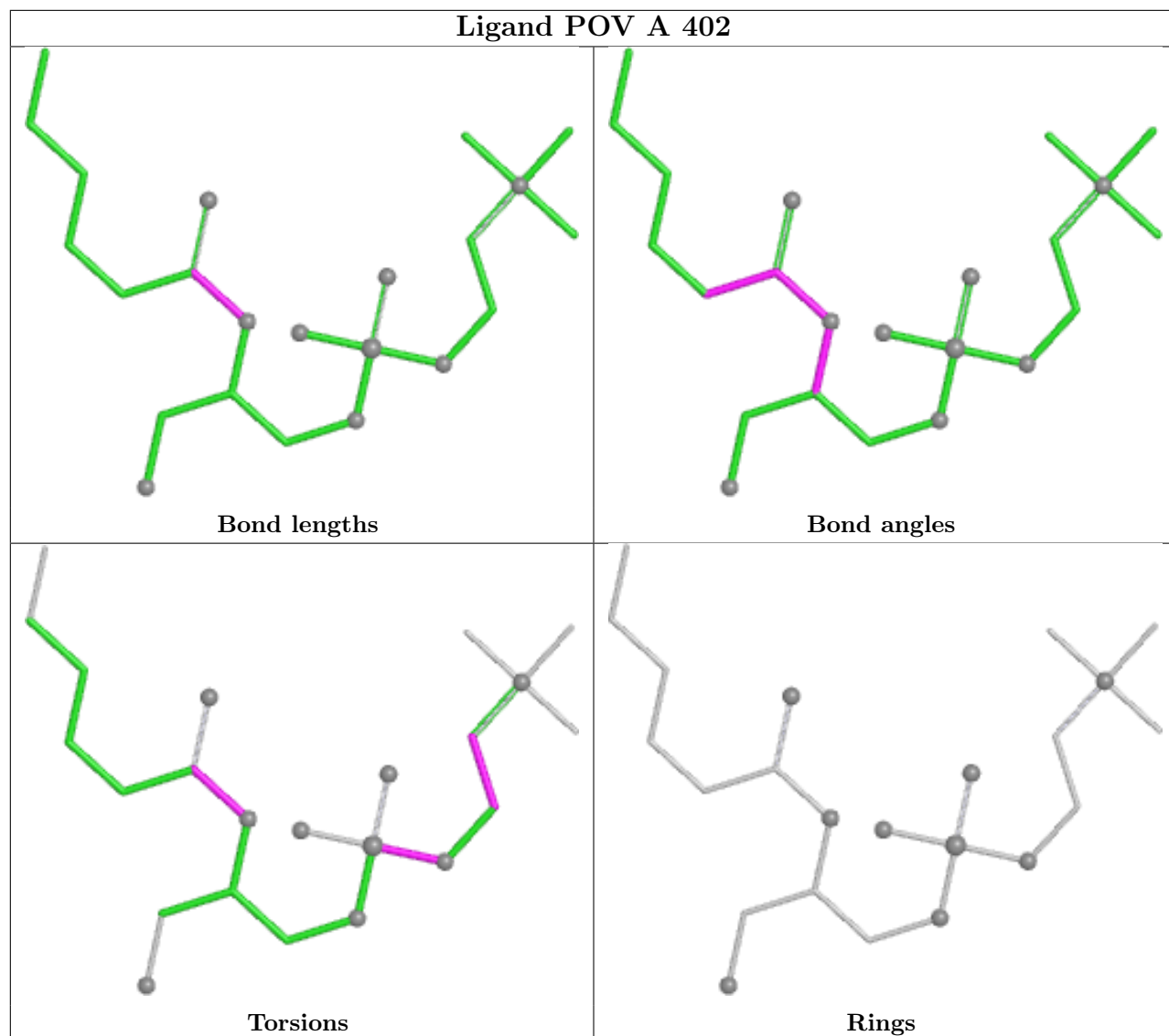
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | C     | 401 | NAG  | C8-C7-N2-C2 |
| 4   | C     | 401 | NAG  | O7-C7-N2-C2 |
| 4   | D     | 402 | NAG  | C8-C7-N2-C2 |
| 4   | D     | 402 | NAG  | O7-C7-N2-C2 |
| 4   | T     | 402 | NAG  | C8-C7-N2-C2 |

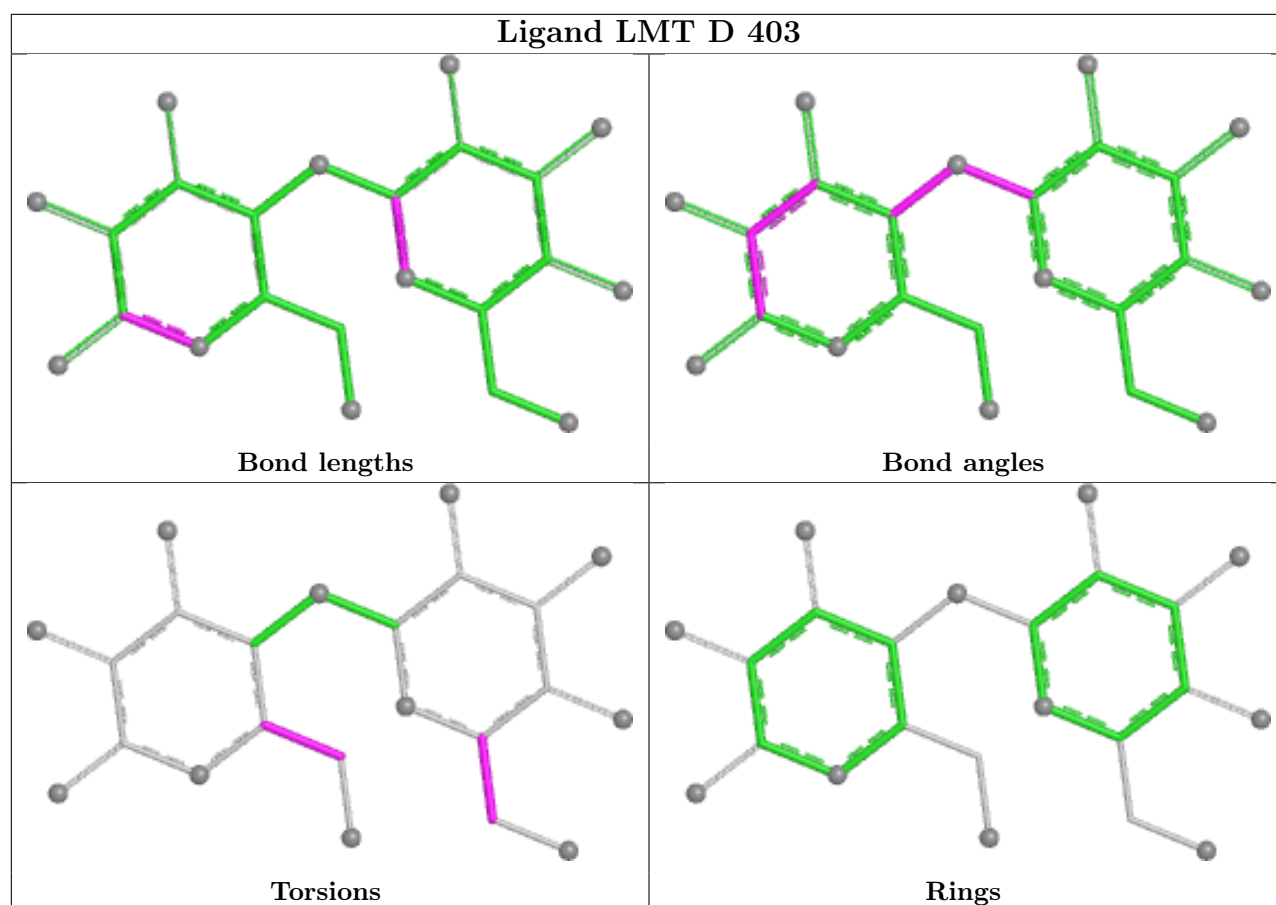
There are no ring outliers.

11 monomers are involved in 29 short contacts:

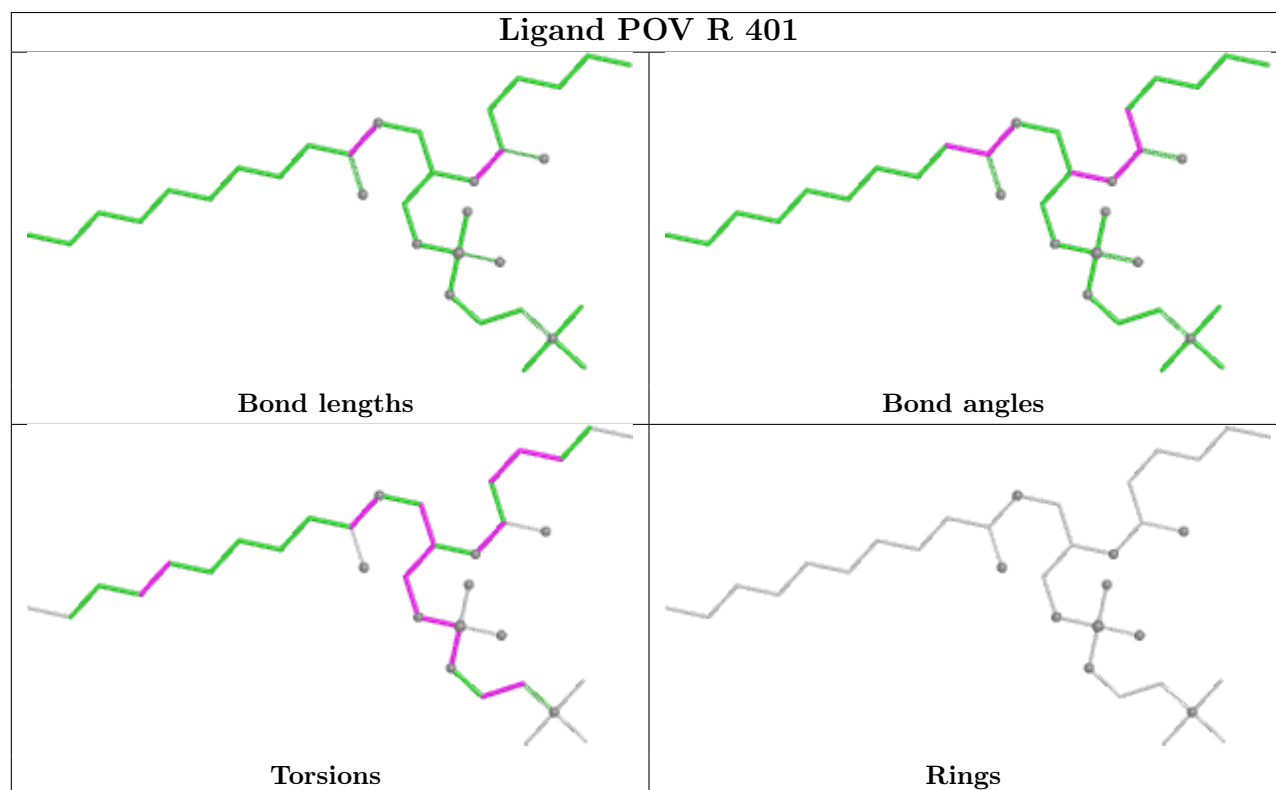
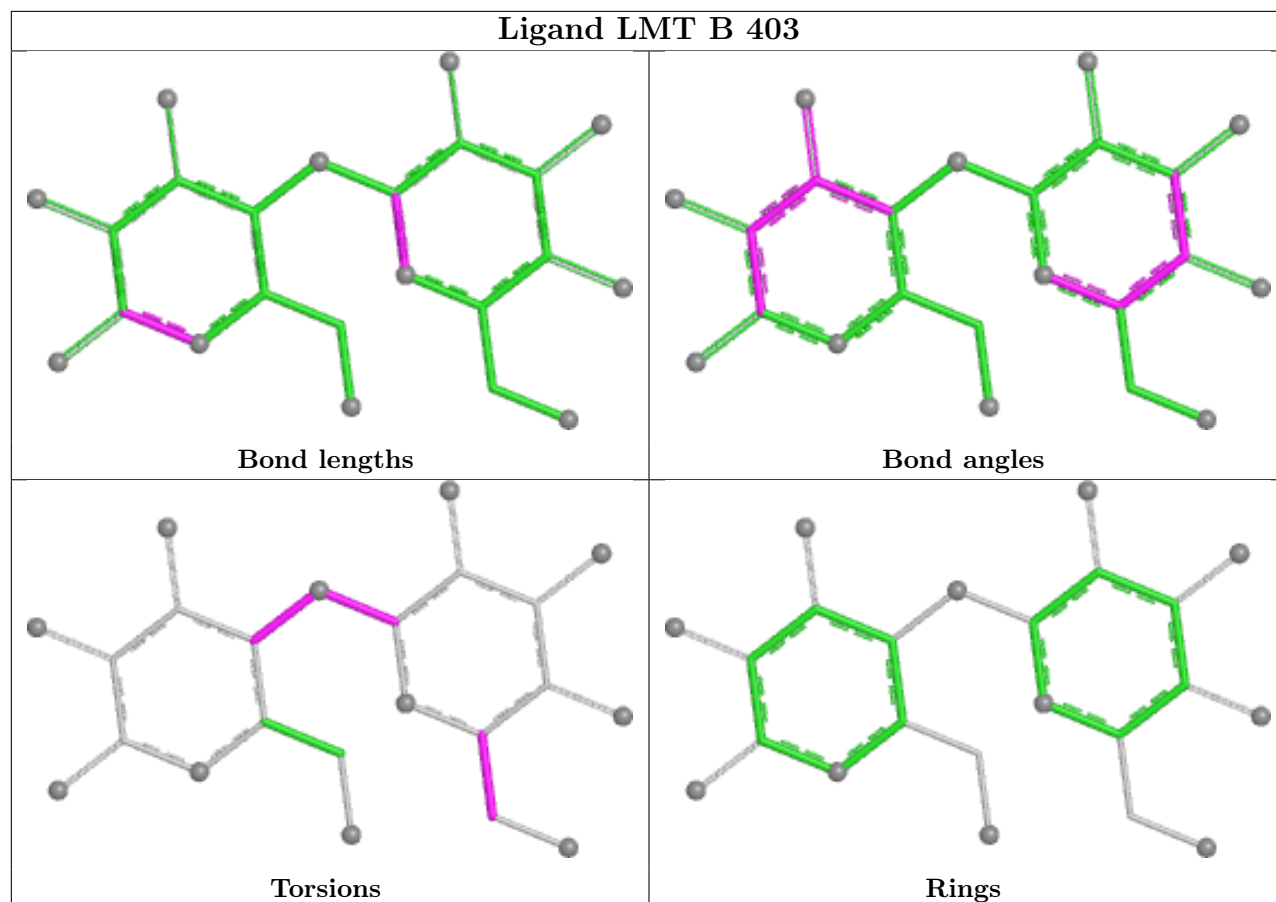
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 402 | POV  | 1       | 0            |
| 8   | D     | 403 | LMT  | 1       | 0            |
| 5   | R     | 401 | POV  | 4       | 0            |
| 5   | Q     | 401 | POV  | 6       | 0            |
| 8   | T     | 403 | LMT  | 1       | 0            |
| 5   | D     | 401 | POV  | 5       | 0            |
| 5   | R     | 402 | POV  | 2       | 0            |
| 4   | S     | 401 | NAG  | 1       | 0            |
| 5   | P     | 403 | POV  | 4       | 0            |
| 5   | T     | 401 | POV  | 3       | 0            |
| 8   | S     | 402 | LMT  | 1       | 0            |

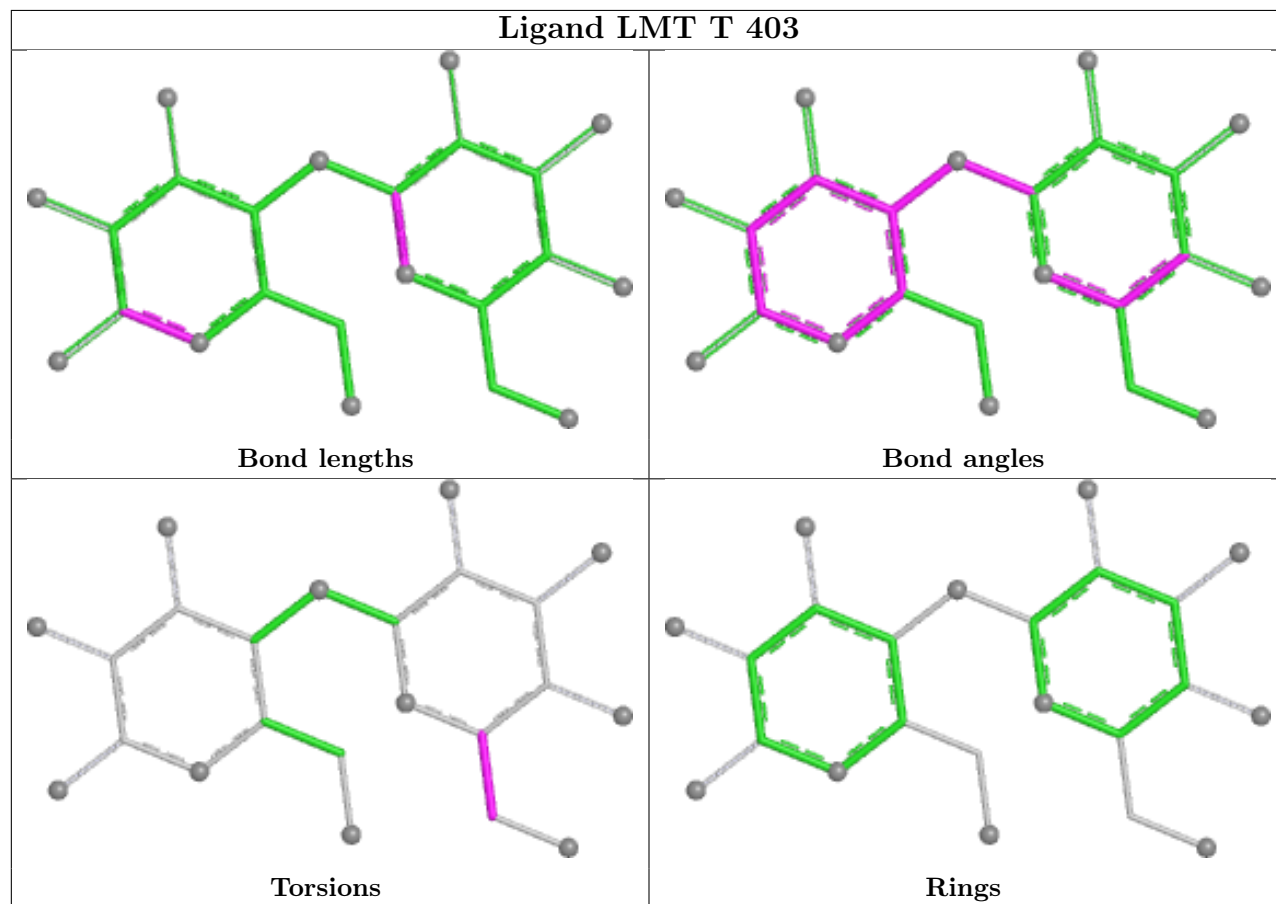
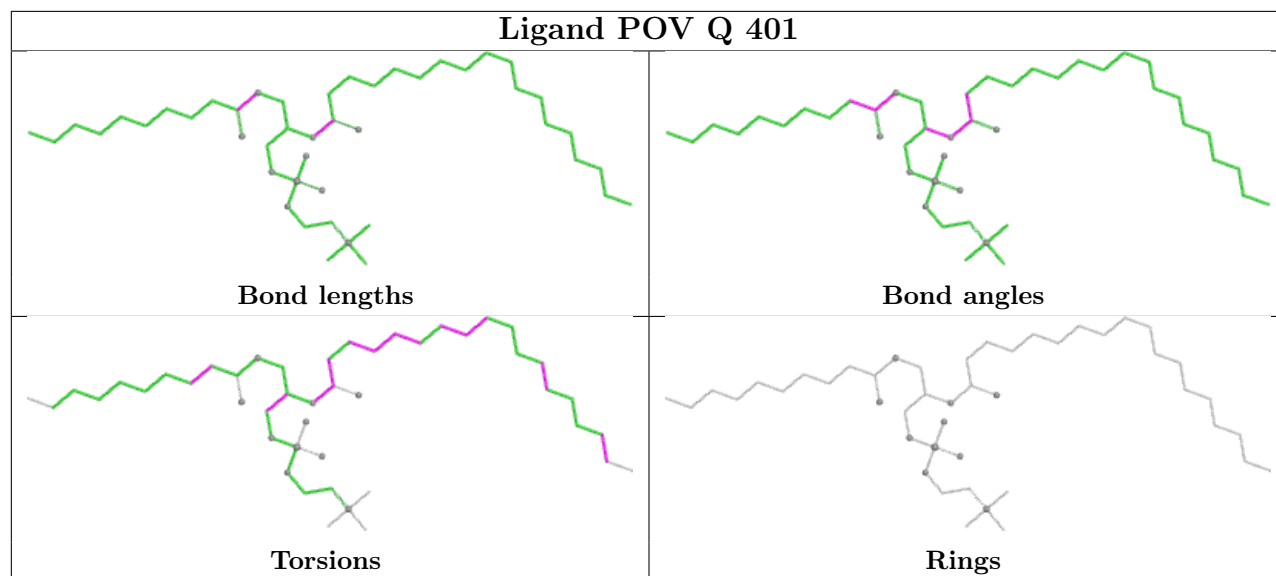
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

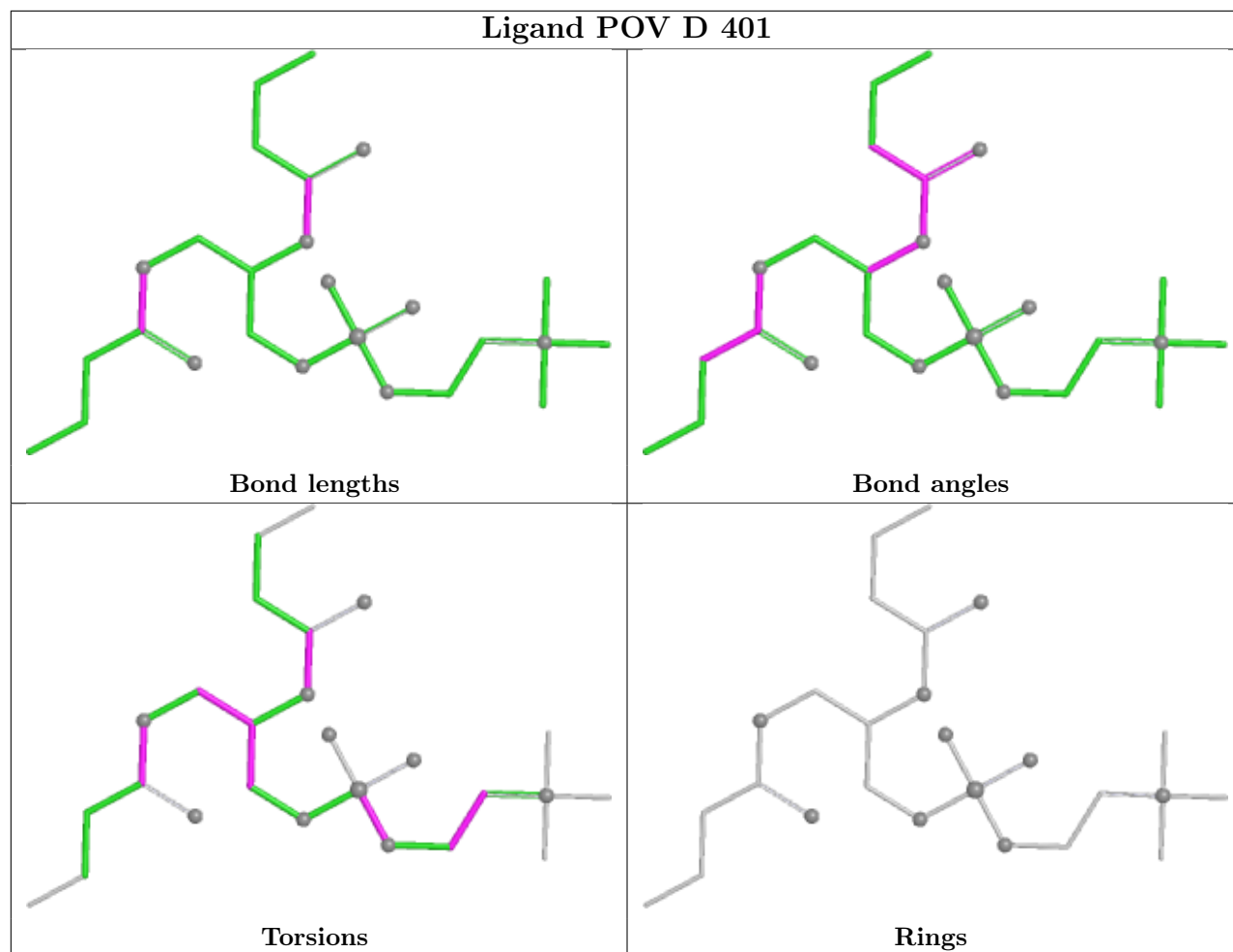


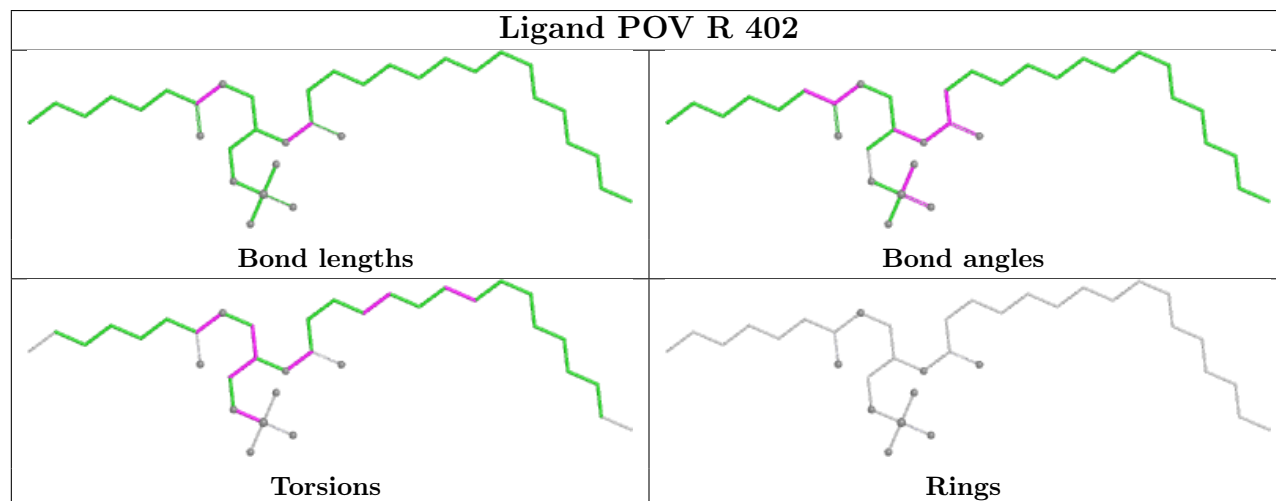
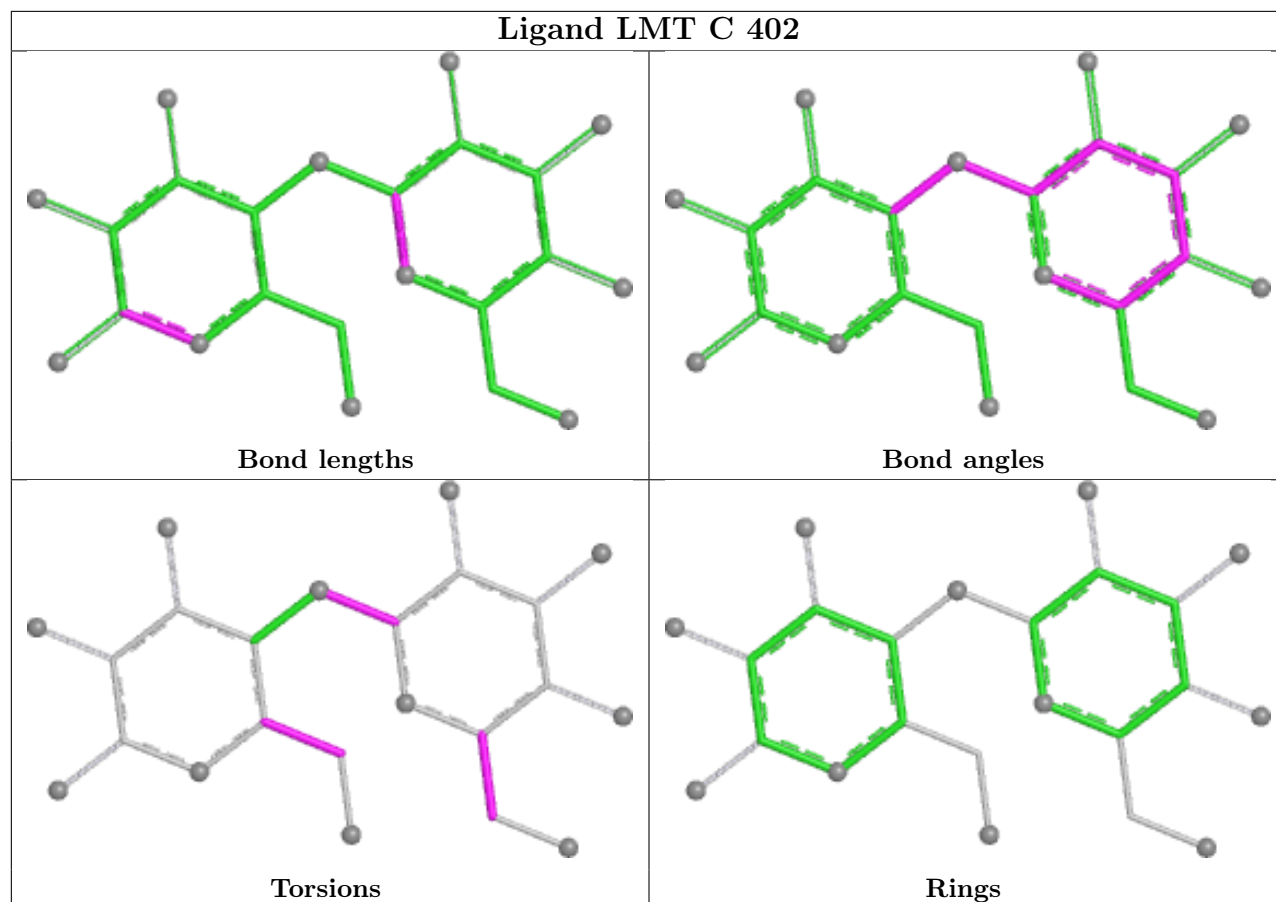


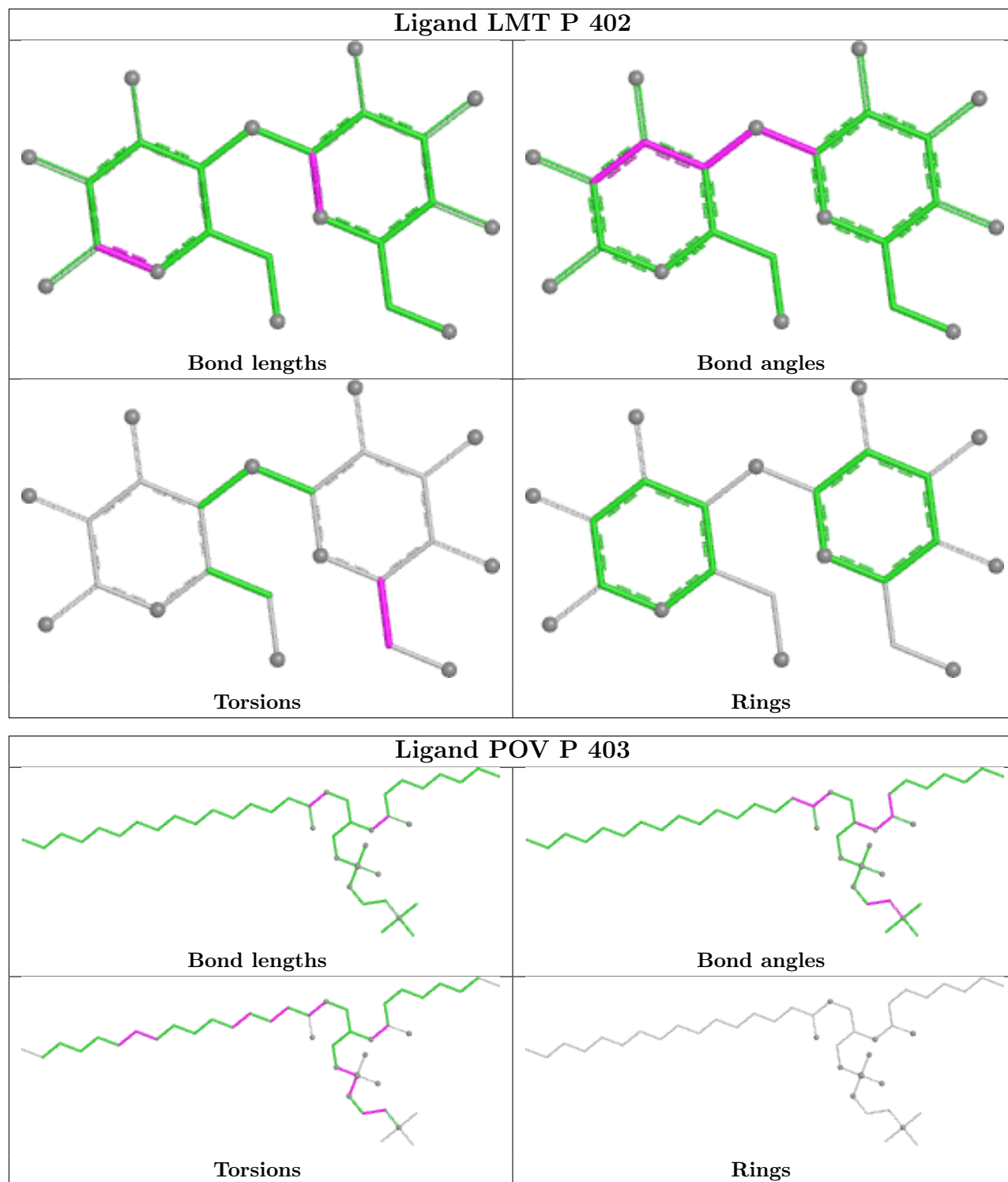


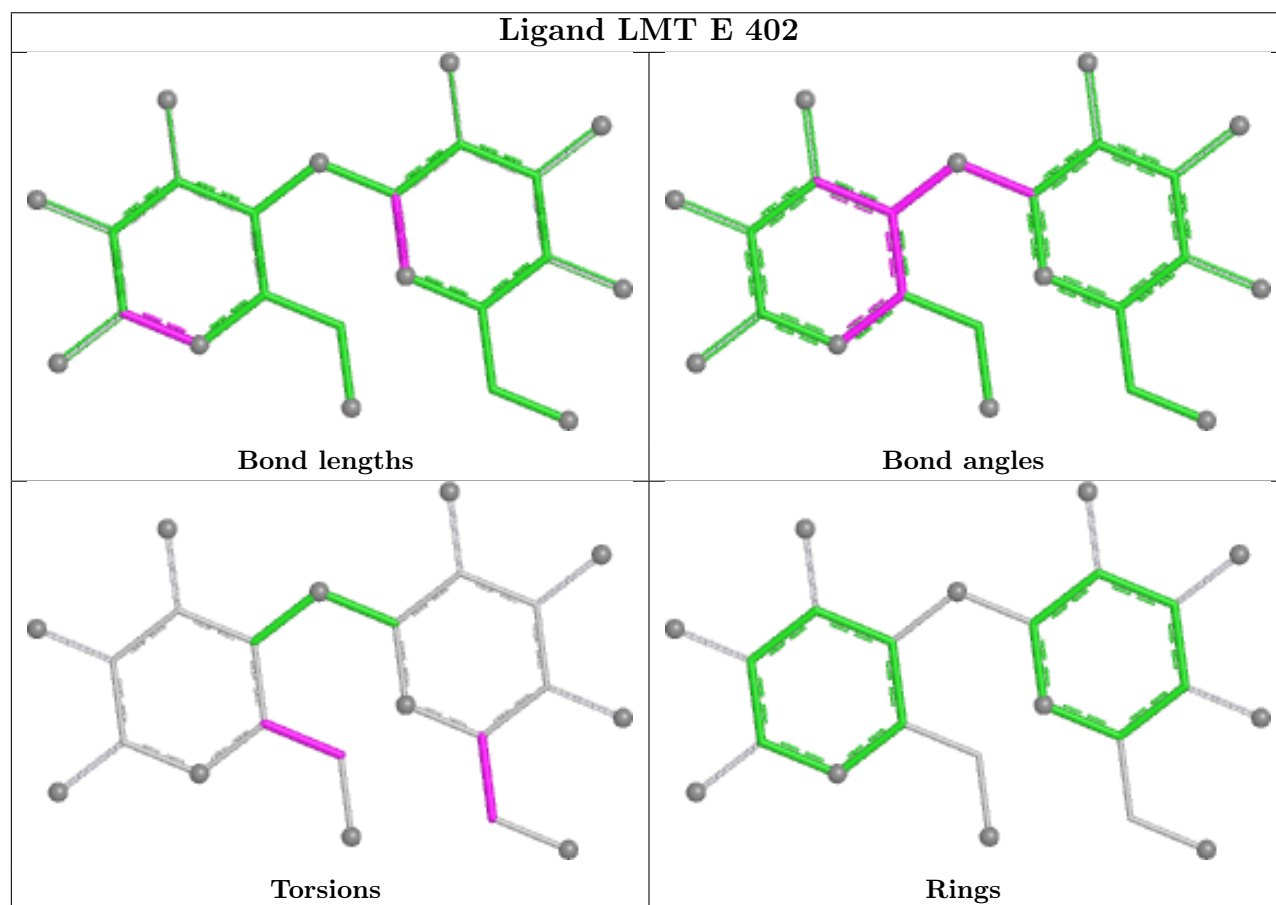
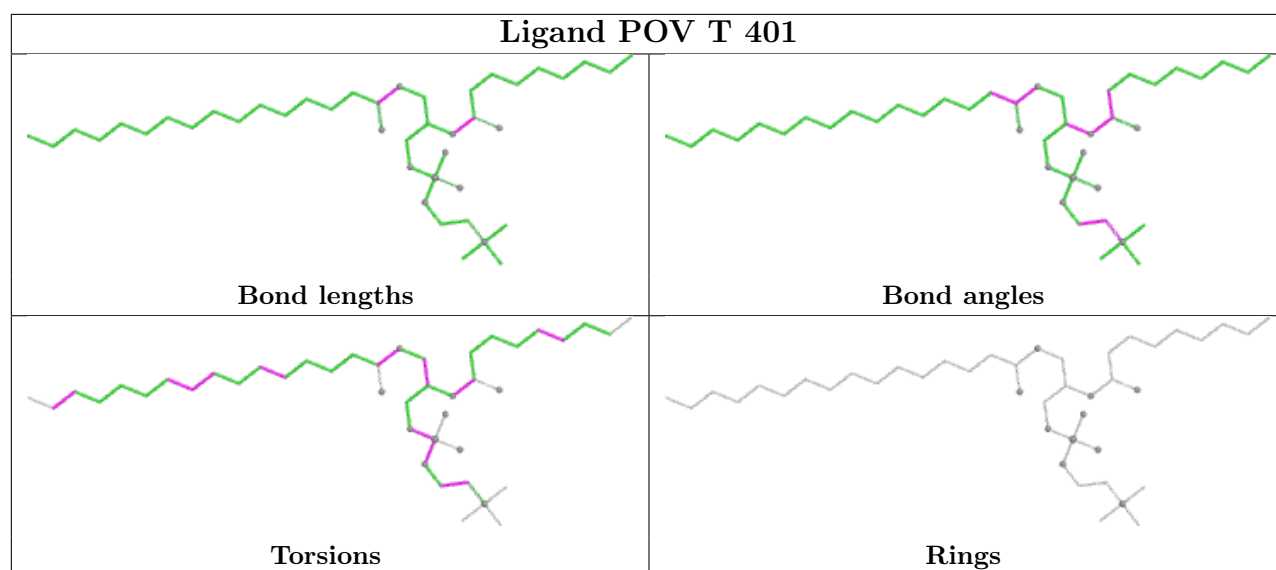


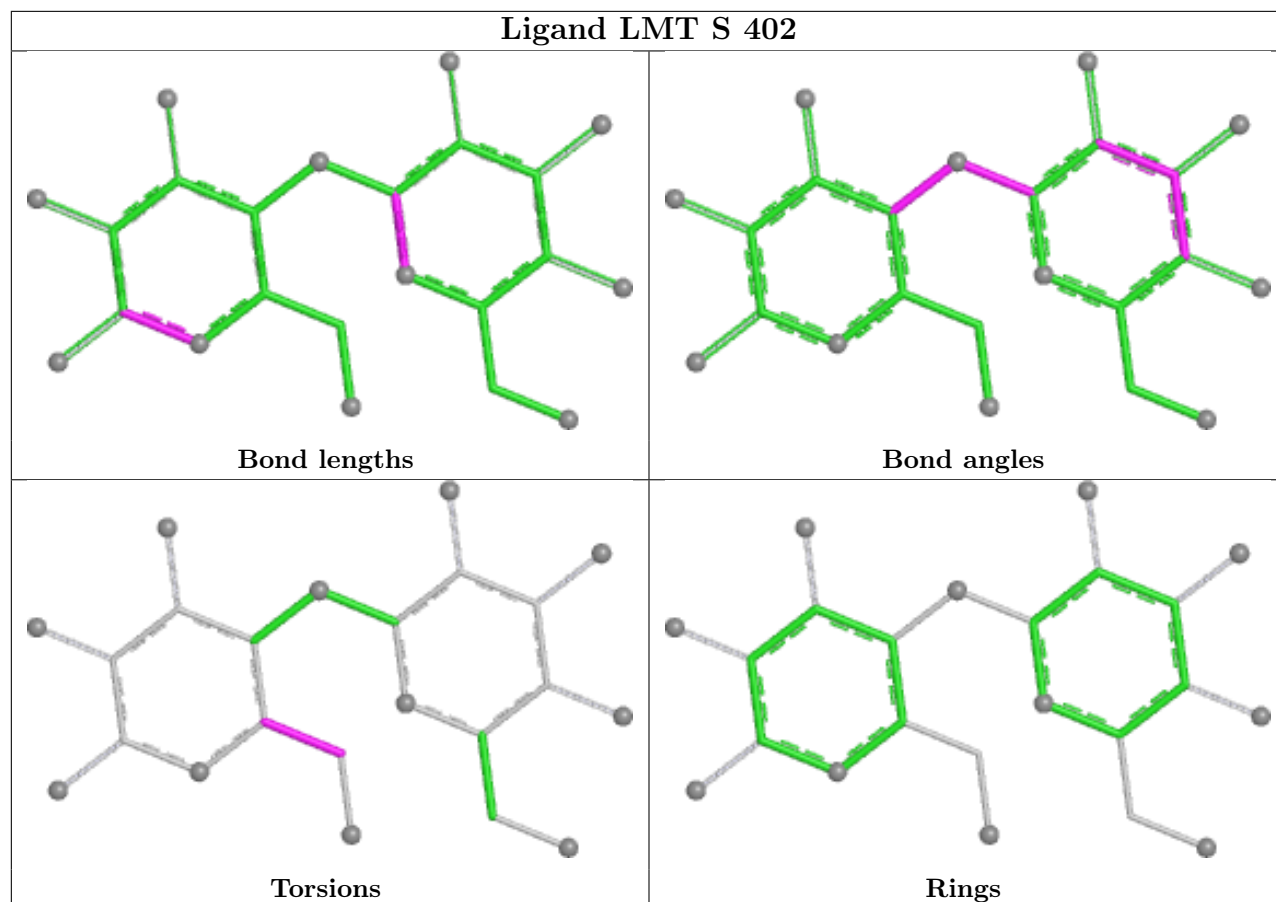












## 5.7 Other polymers [i](#)

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<sup>th</sup> 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(Å²)          | Q<0.9 |
|-----|-------|----------------|--------|----------|----|----|-------------------|-------|
| 1   | A     | 342/347 (98%)  | 0.46   | 32 (9%)  | 14 | 9  | 56, 102, 165, 226 | 0     |
| 1   | B     | 341/347 (98%)  | 0.37   | 15 (4%)  | 39 | 24 | 58, 109, 175, 270 | 0     |
| 1   | C     | 340/347 (97%)  | 0.42   | 21 (6%)  | 26 | 17 | 58, 106, 185, 251 | 0     |
| 1   | D     | 340/347 (97%)  | 0.40   | 17 (5%)  | 34 | 22 | 54, 106, 170, 263 | 0     |
| 1   | E     | 340/347 (97%)  | 0.35   | 16 (4%)  | 36 | 23 | 57, 105, 170, 230 | 0     |
| 1   | P     | 340/347 (97%)  | 0.40   | 19 (5%)  | 30 | 19 | 51, 93, 156, 239  | 0     |
| 1   | Q     | 340/347 (97%)  | 0.39   | 14 (4%)  | 41 | 25 | 58, 99, 167, 242  | 0     |
| 1   | R     | 340/347 (97%)  | 0.32   | 10 (2%)  | 53 | 35 | 58, 97, 158, 274  | 0     |
| 1   | S     | 340/347 (97%)  | 0.32   | 13 (3%)  | 44 | 27 | 53, 89, 144, 247  | 0     |
| 1   | T     | 340/347 (97%)  | 0.31   | 20 (5%)  | 28 | 18 | 49, 88, 151, 210  | 0     |
| 2   | F     | 221/224 (98%)  | 0.35   | 12 (5%)  | 31 | 20 | 68, 113, 202, 265 | 0     |
| 2   | G     | 222/224 (99%)  | 0.65   | 14 (6%)  | 26 | 17 | 75, 142, 230, 309 | 0     |
| 2   | H     | 223/224 (99%)  | 0.35   | 12 (5%)  | 31 | 20 | 52, 100, 158, 275 | 0     |
| 2   | I     | 222/224 (99%)  | 0.27   | 6 (2%)   | 56 | 36 | 63, 105, 192, 239 | 0     |
| 2   | J     | 222/224 (99%)  | 0.67   | 26 (11%) | 9  | 6  | 64, 146, 281, 313 | 0     |
| 2   | U     | 221/224 (98%)  | 0.49   | 8 (3%)   | 46 | 28 | 75, 131, 220, 317 | 0     |
| 2   | V     | 224/224 (100%) | 0.27   | 7 (3%)   | 51 | 32 | 70, 117, 169, 269 | 0     |
| 2   | W     | 224/224 (100%) | 0.24   | 10 (4%)  | 38 | 24 | 68, 102, 155, 257 | 0     |
| 2   | X     | 224/224 (100%) | 0.37   | 12 (5%)  | 31 | 20 | 57, 98, 169, 249  | 0     |
| 2   | Y     | 221/224 (98%)  | 0.37   | 6 (2%)   | 56 | 36 | 64, 127, 195, 277 | 0     |
| 3   | K     | 210/215 (97%)  | 0.49   | 14 (6%)  | 24 | 15 | 59, 114, 222, 295 | 0     |
| 3   | L     | 211/215 (98%)  | 0.25   | 12 (5%)  | 29 | 19 | 49, 91, 170, 224  | 0     |
| 3   | M     | 210/215 (97%)  | 0.34   | 9 (4%)   | 40 | 24 | 69, 130, 248, 270 | 0     |
| 3   | N     | 211/215 (98%)  | 0.28   | 6 (2%)   | 55 | 35 | 66, 116, 158, 200 | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 3   | O     | 211/215 (98%)   | 0.23   | 6 (2%) 55 35   | 65, 108, 143, 157     | 0     |
| 3   | Z     | 215/215 (100%)  | 0.29   | 8 (3%) 45 28   | 71, 120, 160, 199     | 0     |
| 3   | f     | 215/215 (100%)  | 0.31   | 12 (5%) 30 19  | 69, 104, 153, 231     | 0     |
| 3   | g     | 211/215 (98%)   | 0.30   | 10 (4%) 36 23  | 71, 127, 173, 218     | 0     |
| 3   | h     | 211/215 (98%)   | 0.34   | 5 (2%) 59 40   | 75, 137, 177, 249     | 0     |
| 3   | i     | 214/215 (99%)   | 0.08   | 3 (1%) 73 54   | 60, 99, 135, 165      | 0     |
| All | All   | 7746/7860 (98%) | 0.36   | 375 (4%) 35 22 | 49, 107, 191, 317     | 0     |

The worst 5 of 375 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 138 | ALA  | 5.8  |
| 2   | X     | 224 | CYS  | 5.5  |
| 2   | H     | 139 | ALA  | 5.3  |
| 3   | K     | 123 | PRO  | 5.2  |
| 1   | D     | 267 | LEU  | 5.1  |

## 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 ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | NAG  | C     | 401 | 14/15 | 0.45 | 0.17 | 191,210,218,223            | 0     |
| 8   | LMT  | S     | 402 | 23/35 | 0.45 | 0.17 | 169,214,224,235            | 0     |
| 8   | LMT  | E     | 402 | 23/35 | 0.46 | 0.16 | 218,239,254,257            | 0     |
| 4   | NAG  | S     | 401 | 14/15 | 0.48 | 0.17 | 153,184,189,195            | 0     |

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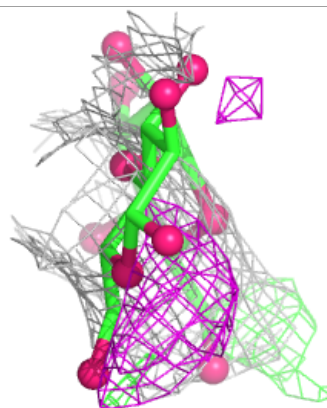
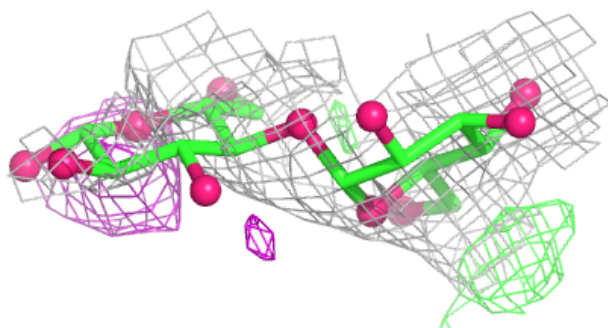
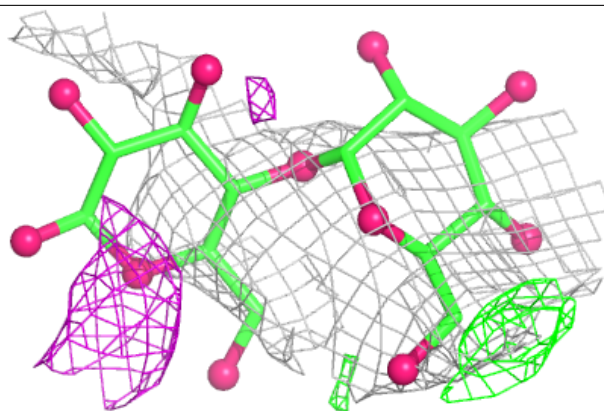
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 8   | LMT  | T     | 403 | 23/35 | 0.50 | 0.17 | 156,202,217,222             | 0     |
| 4   | NAG  | T     | 402 | 14/15 | 0.54 | 0.14 | 153,200,210,211             | 0     |
| 4   | NAG  | P     | 401 | 14/15 | 0.56 | 0.11 | 133,182,192,201             | 0     |
| 4   | NAG  | B     | 402 | 14/15 | 0.56 | 0.14 | 139,168,176,177             | 0     |
| 4   | NAG  | Q     | 402 | 14/15 | 0.58 | 0.13 | 146,184,202,207             | 0     |
| 4   | NAG  | E     | 401 | 14/15 | 0.58 | 0.15 | 157,190,206,212             | 0     |
| 7   | GOL  | B     | 401 | 6/6   | 0.59 | 0.22 | 115,145,151,167             | 0     |
| 8   | LMT  | P     | 402 | 23/35 | 0.61 | 0.16 | 221,221,221,221             | 0     |
| 4   | NAG  | D     | 402 | 14/15 | 0.63 | 0.16 | 153,197,214,221             | 0     |
| 8   | LMT  | C     | 402 | 23/35 | 0.64 | 0.15 | 179,179,179,179             | 0     |
| 4   | NAG  | A     | 401 | 14/15 | 0.69 | 0.14 | 137,181,192,196             | 0     |
| 8   | LMT  | B     | 403 | 23/35 | 0.70 | 0.14 | 176,217,235,242             | 0     |
| 8   | LMT  | D     | 403 | 23/35 | 0.71 | 0.14 | 196,218,239,247             | 0     |
| 5   | POV  | A     | 402 | 23/52 | 0.78 | 0.30 | 137,177,208,241             | 0     |
| 5   | POV  | R     | 401 | 34/52 | 0.81 | 0.29 | 99,146,200,535              | 0     |
| 5   | POV  | D     | 401 | 26/52 | 0.86 | 0.32 | 125,176,201,334             | 0     |
| 5   | POV  | T     | 401 | 43/52 | 0.88 | 0.24 | 77,129,177,205              | 0     |
| 5   | POV  | Q     | 401 | 46/52 | 0.88 | 0.25 | 108,149,198,237             | 0     |
| 5   | POV  | P     | 403 | 42/52 | 0.88 | 0.25 | 82,125,179,206              | 0     |
| 5   | POV  | R     | 402 | 35/52 | 0.90 | 0.23 | 96,123,186,208              | 0     |
| 6   | CL   | A     | 403 | 1/1   | 0.94 | 0.07 | 119,119,119,119             | 0     |
| 6   | CL   | P     | 404 | 1/1   | 0.95 | 0.21 | 90,90,90,90                 | 0     |

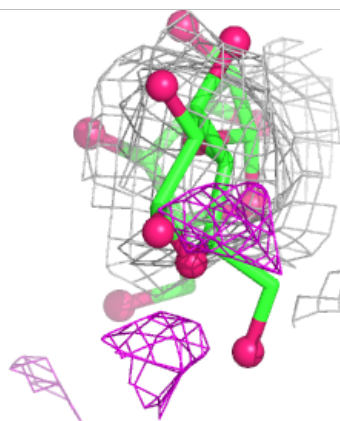
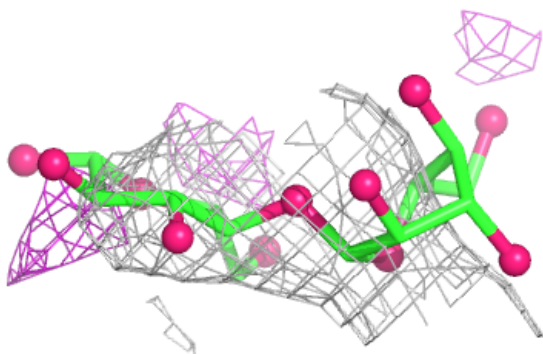
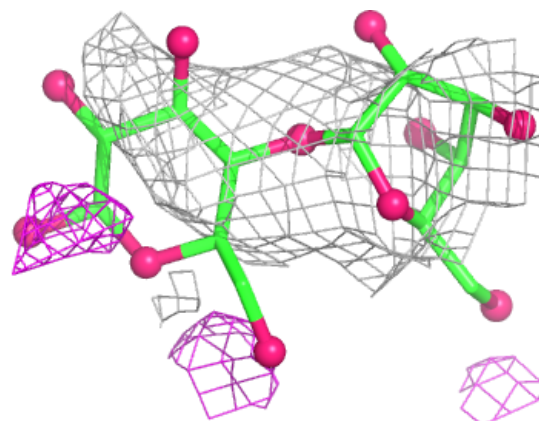
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMT S 402:**

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

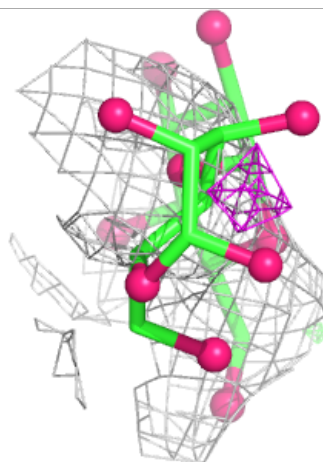
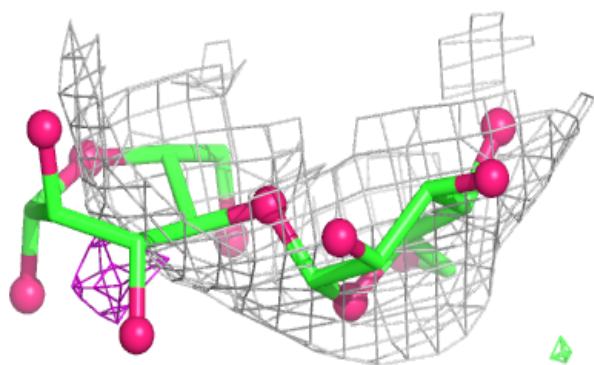
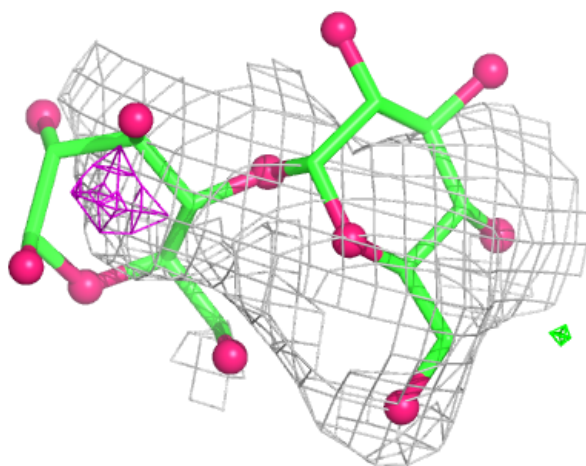
**Electron density around LMT E 402:**

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



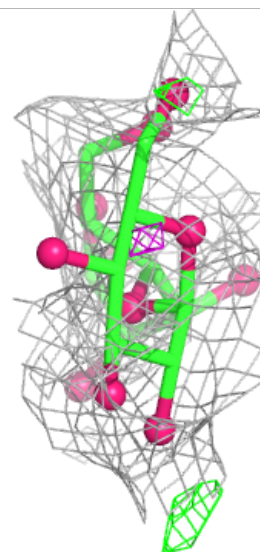
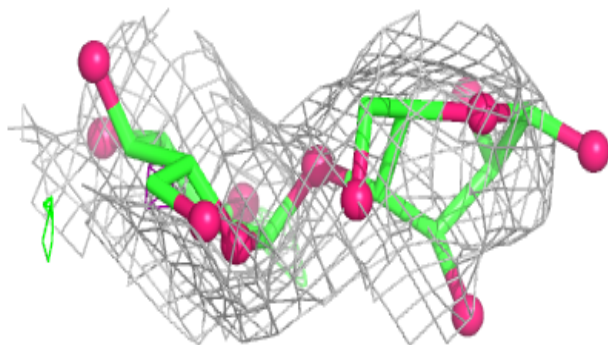
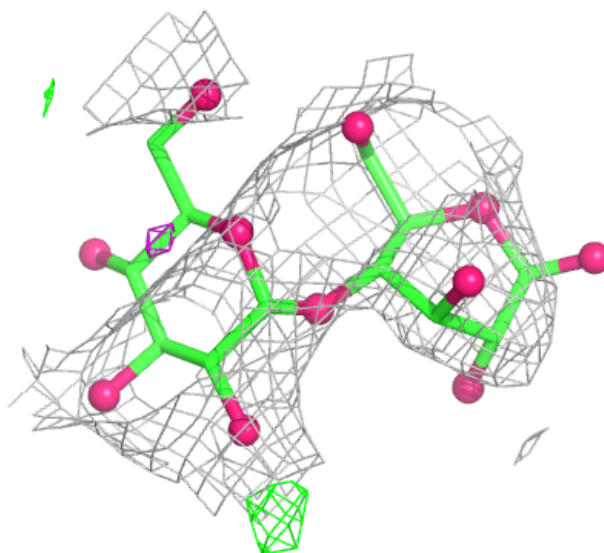
**Electron density around LMT T 403:**

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



**Electron density around LMT P 402:**

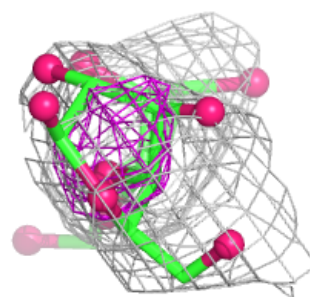
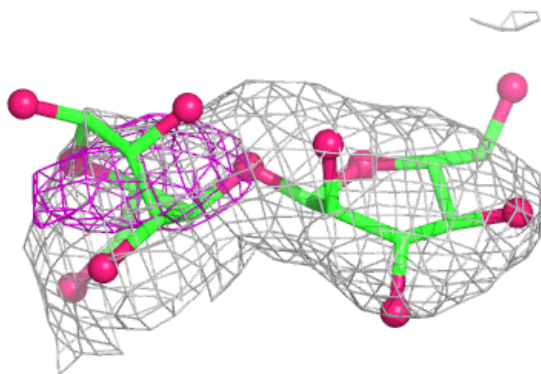
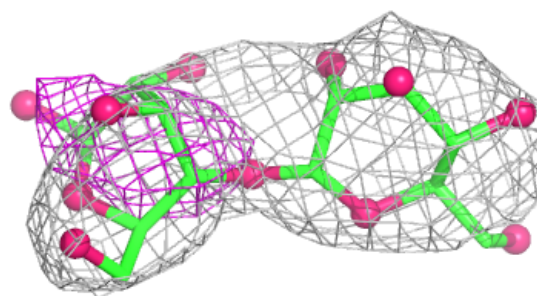
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



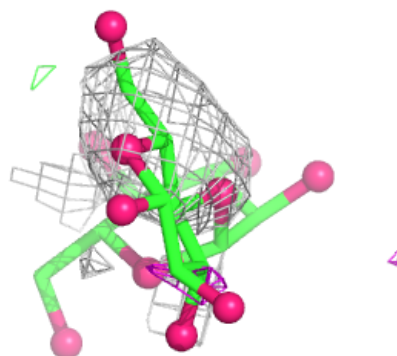
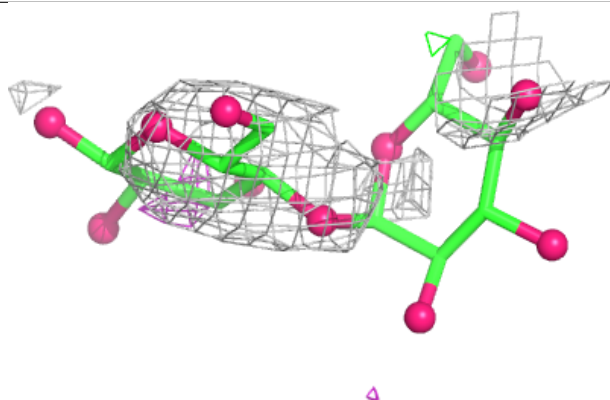
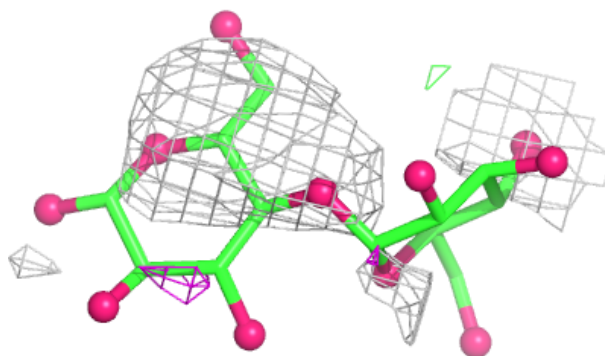


**Electron density around LMT C 402:**

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

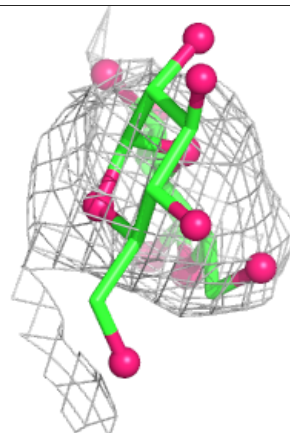
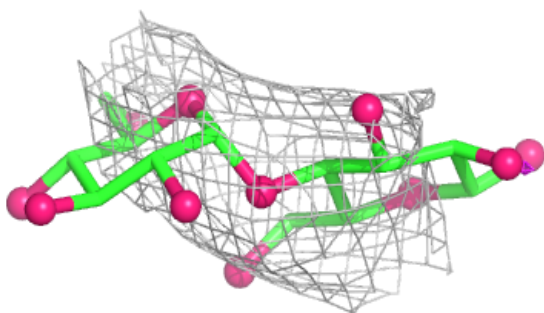
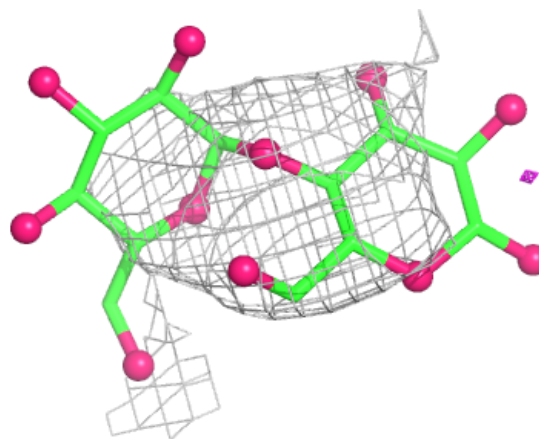
**Electron density around LMT B 403:**

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

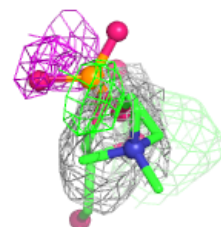
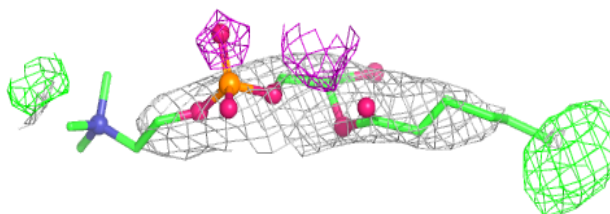
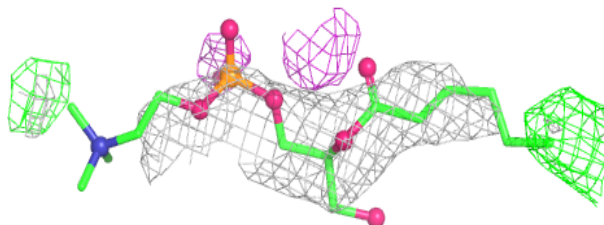


**Electron density around LMT D 403:**

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

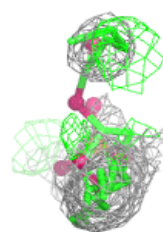
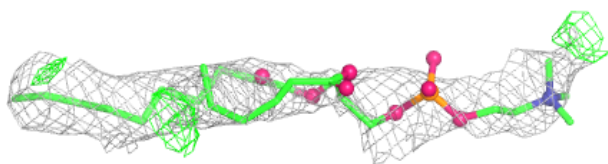
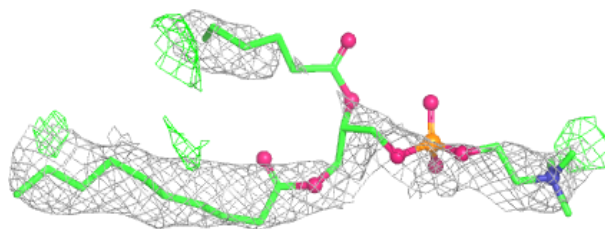
**Electron density around POV A 402:**

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

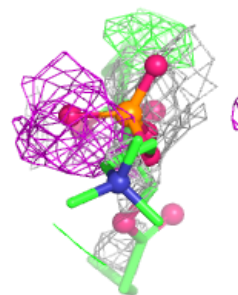
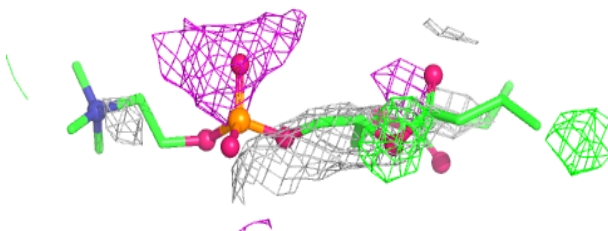
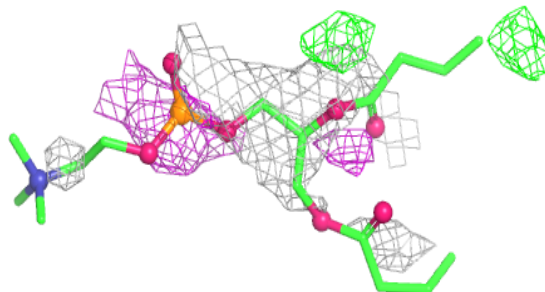


**Electron density around POV R 401:**

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

**Electron density around POV D 401:**

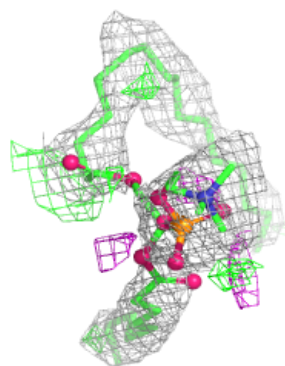
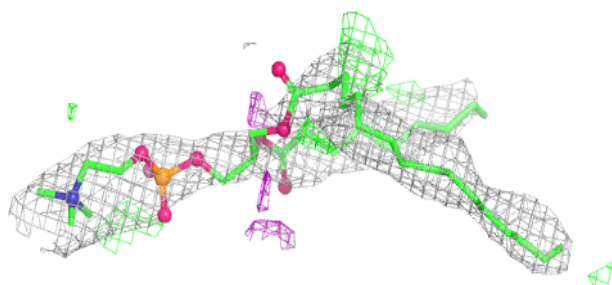
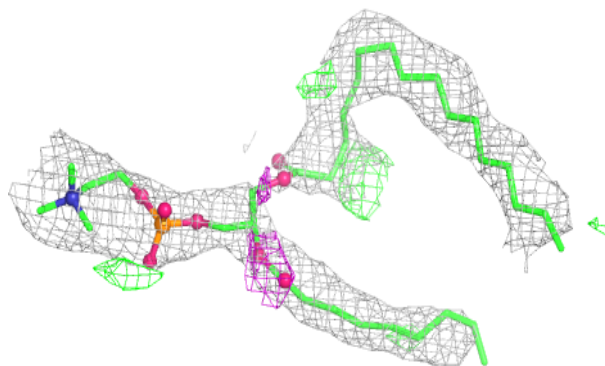
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



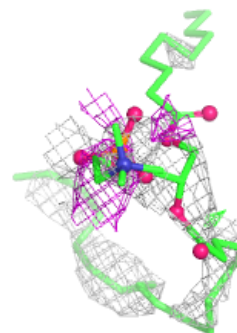
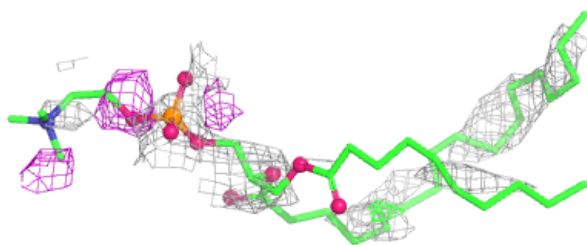
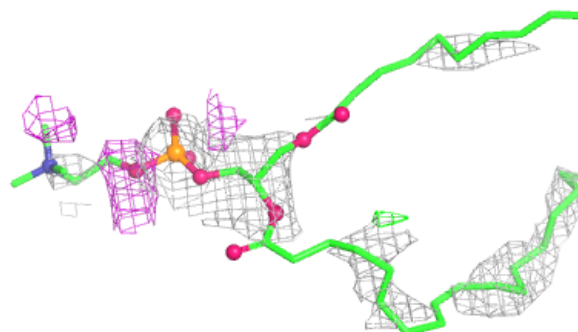


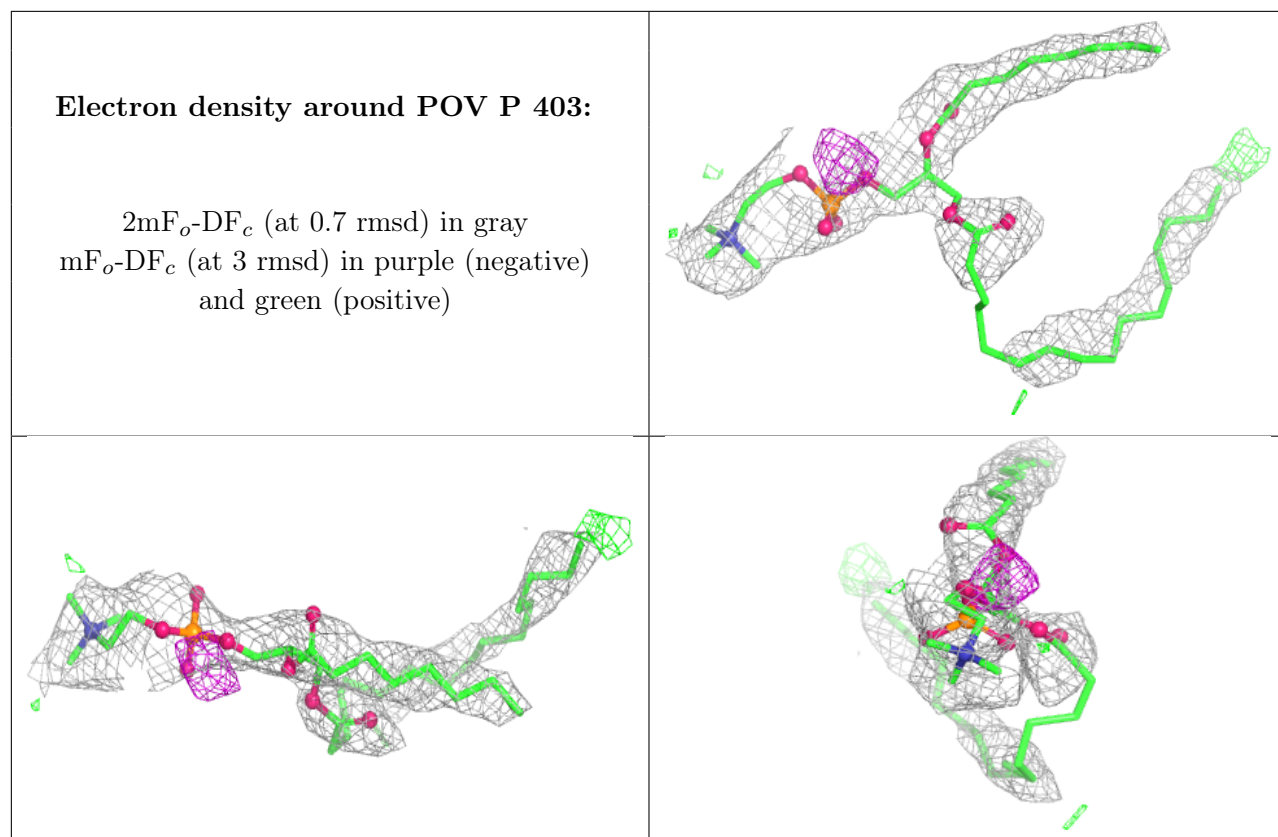
**Electron density around POV T 401:**

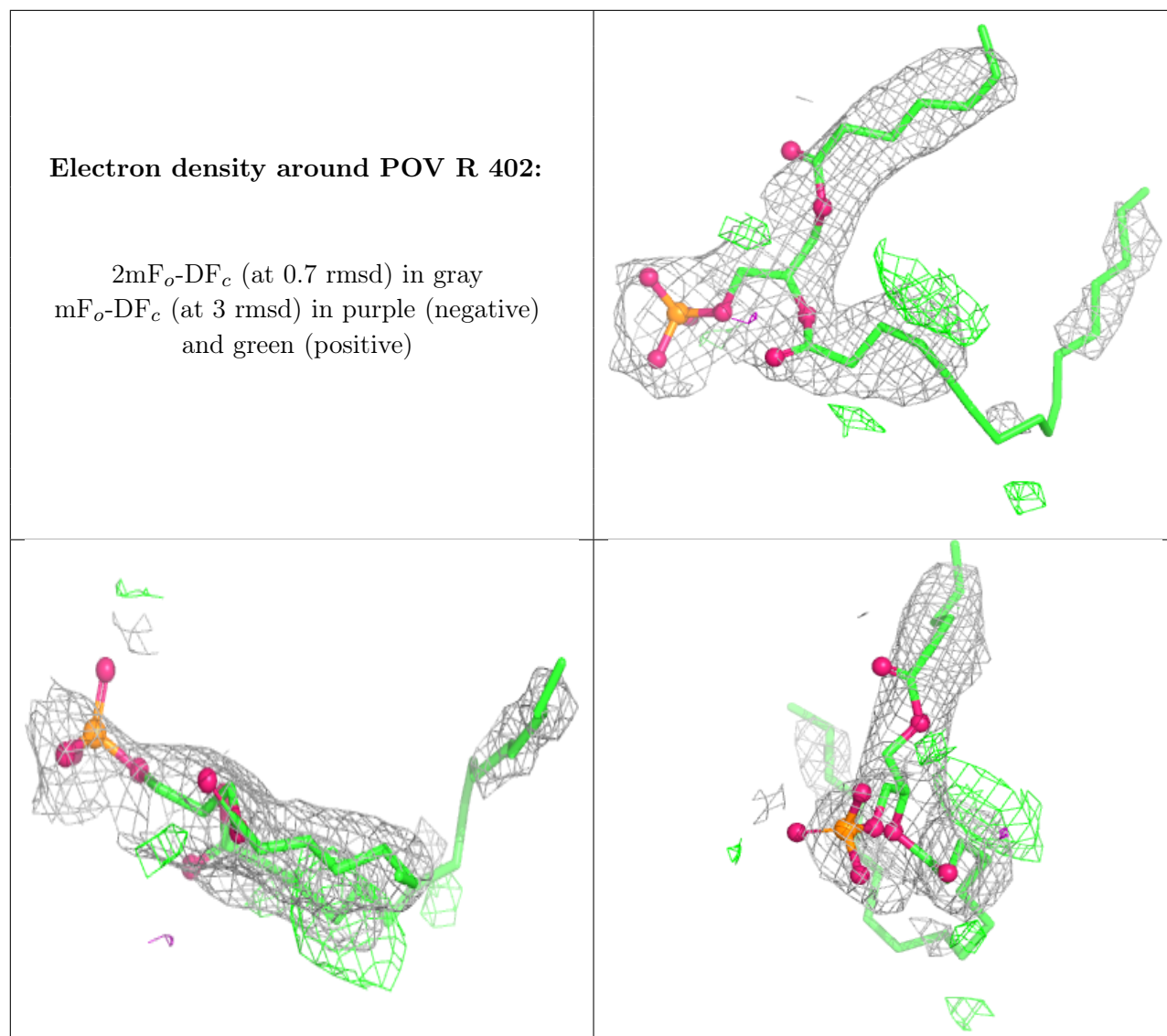
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around POV Q 401:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.