



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 7OJP / pdb\_00007ojp  
Title : Crystal structure of Pseudomonas aeruginosa LpxA in complex with compound 1  
Authors : Ryan, M.D.; Parkes, A.L.; Southey, M.; Andersen, O.A.; Zahn, M.; Barker, J.; DeJonge, B.L.M.  
Deposited on : 2021-05-17  
Resolution : 2.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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                                                             |

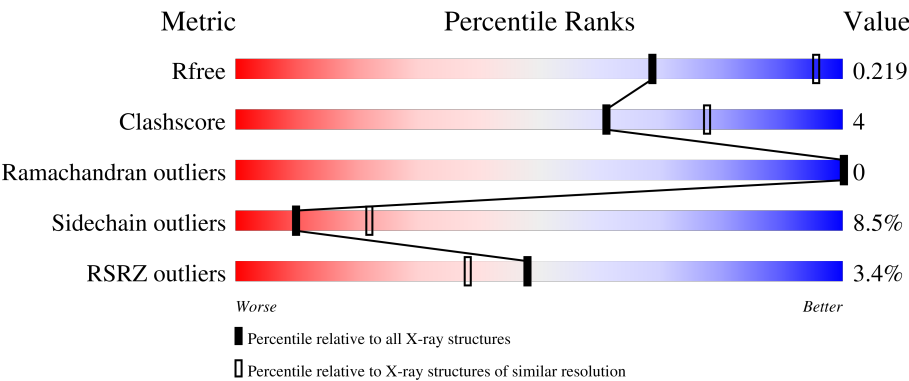
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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 <sub>free</sub>     | 180053                      | 1520 (2.86-2.82)                                      |
| Clashscore            | 190562                      | 1559 (2.86-2.82)                                      |
| Ramachandran outliers | 187476                      | 1517 (2.86-2.82)                                      |
| Sidechain outliers    | 187428                      | 1518 (2.86-2.82)                                      |
| RSRZ outliers         | 180081                      | 1521 (2.86-2.82)                                      |

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     | 261    | <div><div>3%</div><div><div></div><div>84%</div><div>9%</div><div></div><div></div></div><div></div></div>   |
| 1   | B     | 261    | <div><div>3%</div><div><div></div><div>85%</div><div>9%</div><div></div><div></div></div><div></div></div>   |
| 1   | C     | 261    | <div><div>2%</div><div><div></div><div>84%</div><div>9%</div><div>5%</div><div></div></div><div></div></div> |
| 1   | D     | 261    | <div><div>3%</div><div><div></div><div>81%</div><div>13%</div><div></div><div></div></div><div></div></div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 261    |                  |
| 1   | F     | 261    |                  |
| 1   | G     | 261    |                  |
| 1   | H     | 261    |                  |
| 1   | I     | 261    |                  |
| 1   | J     | 261    |                  |
| 1   | K     | 261    |                  |
| 1   | L     | 261    |                  |
| 1   | M     | 261    |                  |
| 1   | N     | 261    |                  |
| 1   | O     | 261    |                  |
| 1   | P     | 261    |                  |
| 1   | Q     | 261    |                  |
| 1   | R     | 261    |                  |
| 1   | S     | 261    |                  |
| 1   | T     | 261    |                  |
| 1   | U     | 261    |                  |
| 1   | V     | 261    |                  |
| 1   | W     | 261    |                  |
| 1   | X     | 261    |                  |
| 1   | Y     | 261    |                  |
| 1   | Z     | 261    |                  |
| 1   | a     | 261    |                  |
| 1   | b     | 261    |                  |
| 1   | c     | 261    |                  |

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| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | d     | 261    | <div><div></div><div>3%</div><div>84%</div><div>11%</div><div></div><div></div></div> |



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 60728 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 Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | B     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | C     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | D     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | E     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | F     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | G     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | H     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | I     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | J     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | K     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | L     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | M     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | N     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | O     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | P     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Q     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | R     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | S     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | T     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | U     | 259      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1992  | 1246 | 370 | 369 | 7 |         |         |       |
| 1   | V     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | W     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | X     | 259      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2003  | 1252 | 374 | 370 | 7 |         |         |       |
| 1   | Y     | 258      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1982  | 1240 | 367 | 368 | 7 |         |         |       |
| 1   | Z     | 261      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2002  | 1251 | 372 | 372 | 7 |         |         |       |
| 1   | a     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | b     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | c     | 257      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1974  | 1235 | 366 | 367 | 6 |         |         |       |
| 1   | d     | 261      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2002  | 1251 | 372 | 372 | 7 |         |         |       |

There are 90 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| A     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| A     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| B     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| B     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| B     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| C     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| C     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| C     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| D     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| D     | -1      | SER      | -      | expression tag | UNP A6V1E4 |

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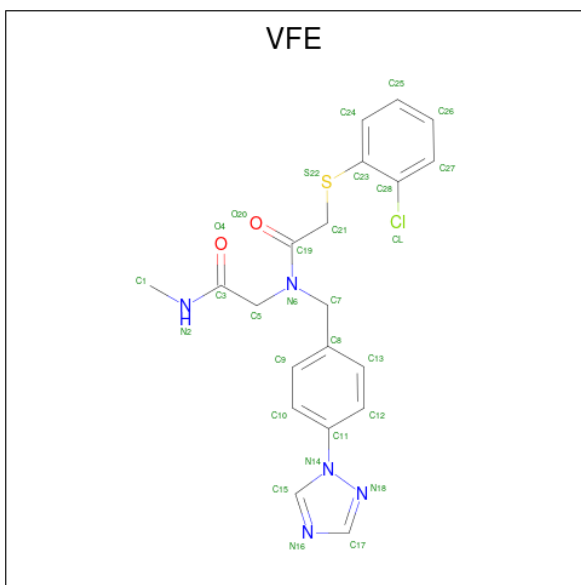
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| E     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| E     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| E     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| F     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| F     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| F     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| G     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| G     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| G     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| H     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| H     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| H     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| I     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| I     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| I     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| J     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| J     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| J     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| K     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| K     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| K     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| L     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| L     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| L     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| M     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| M     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| M     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| N     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| N     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| N     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| O     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| O     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| O     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| P     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| P     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| P     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| Q     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| Q     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| Q     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| R     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| R     | -1      | SER      | -      | expression tag | UNP A6V1E4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| R     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| S     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| S     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| S     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| T     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| T     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| T     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| U     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| U     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| U     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| V     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| V     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| V     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| W     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| W     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| W     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| X     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| X     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| X     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| Y     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| Y     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| Y     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| Z     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| Z     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| Z     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| a     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| a     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| a     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| b     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| b     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| b     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| c     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| c     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| c     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |
| d     | -2      | GLY      | -      | expression tag | UNP A6V1E4 |
| d     | -1      | SER      | -      | expression tag | UNP A6V1E4 |
| d     | 0       | HIS      | -      | expression tag | UNP A6V1E4 |

- Molecule 2 is 2-[2-(2-chlorophenyl)sulfanylethanoyl-[[4-(1,2,4-triazol-1-yl)phenyl]methyl]amino]-N-methyl-ethanamide (CCD ID: VFE) (formula: C<sub>20</sub>H<sub>20</sub>ClN<sub>5</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|--------|---------|---------|
| 2   | A     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | B     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | C     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | D     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | E     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | F     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | G     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | H     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | I     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | J     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | K     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | L     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | M     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | N     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|--------|---------|---------|
| 2   | O     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | P     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | Q     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | R     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | S     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | T     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | U     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | V     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | W     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | X     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | Y     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | Z     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | a     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | b     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | c     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |
| 2   | d     | 1        | Total<br>29 | C<br>20 | Cl<br>1 | N<br>5 | O<br>2 | S<br>1 | 0       | 0       |

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | A     | 13       | Total O<br>13 13 | 0       | 0       |
| 4   | B     | 19       | Total O<br>19 19 | 0       | 0       |
| 4   | C     | 21       | Total O<br>21 21 | 0       | 0       |
| 4   | D     | 23       | Total O<br>23 23 | 0       | 0       |
| 4   | E     | 16       | Total O<br>16 16 | 0       | 0       |
| 4   | F     | 12       | Total O<br>12 12 | 0       | 0       |
| 4   | G     | 2        | Total O<br>2 2   | 0       | 0       |
| 4   | H     | 7        | Total O<br>7 7   | 0       | 0       |
| 4   | I     | 9        | Total O<br>9 9   | 0       | 0       |
| 4   | J     | 6        | Total O<br>6 6   | 0       | 0       |
| 4   | K     | 9        | Total O<br>9 9   | 0       | 0       |
| 4   | L     | 8        | Total O<br>8 8   | 0       | 0       |
| 4   | M     | 14       | Total O<br>14 14 | 0       | 0       |
| 4   | N     | 8        | Total O<br>8 8   | 0       | 0       |
| 4   | O     | 15       | Total O<br>15 15 | 0       | 0       |
| 4   | P     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | Q     | 11       | Total O<br>11 11 | 0       | 0       |
| 4   | R     | 10       | Total O<br>10 10 | 0       | 0       |
| 4   | S     | 15       | Total O<br>15 15 | 0       | 0       |
| 4   | T     | 17       | Total O<br>17 17 | 0       | 0       |
| 4   | U     | 19       | Total O<br>19 19 | 0       | 0       |
| 4   | V     | 13       | Total O<br>13 13 | 0       | 0       |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | W     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | X     | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 4   | Y     | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 4   | Z     | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 4   | a     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 4   | b     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 4   | c     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 4   | d     | 23       | Total<br>23 | O<br>23 | 0       | 0       |

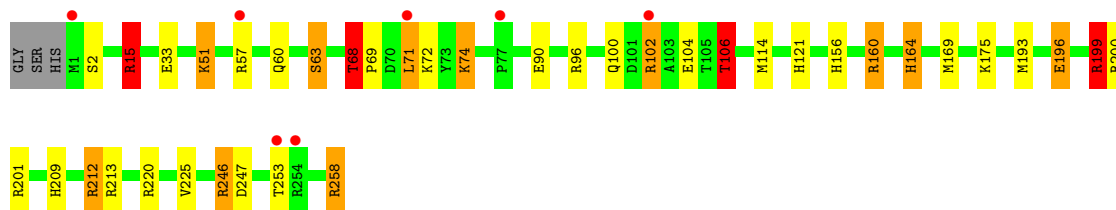


### 3 Residue-property plots [i](#)

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.

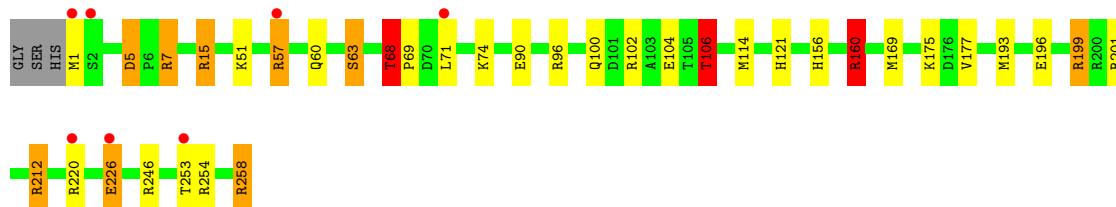
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain A: 



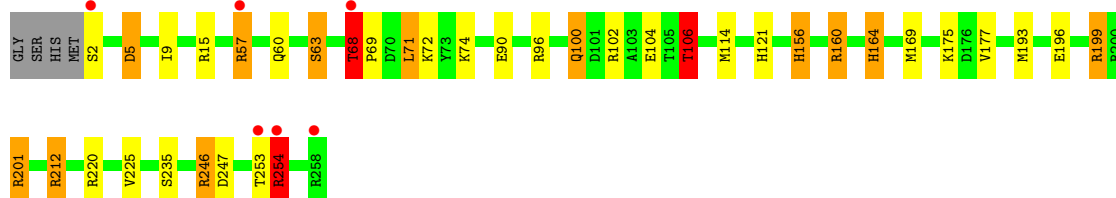
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain B: 



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

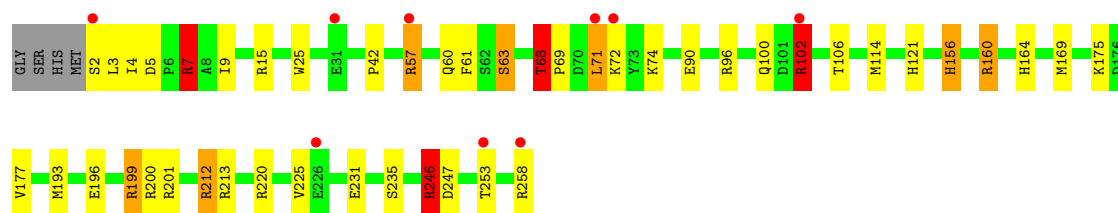
Chain C: 



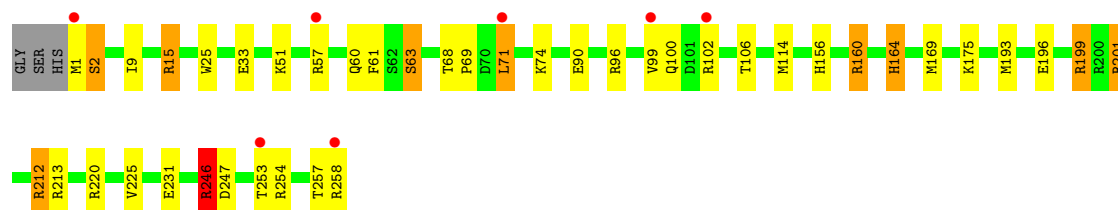
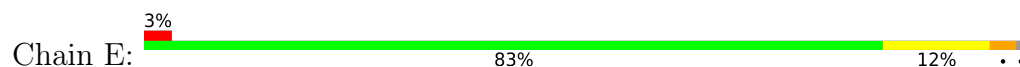
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain D: 

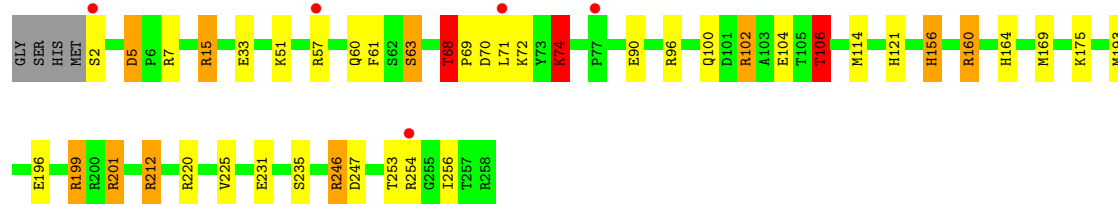
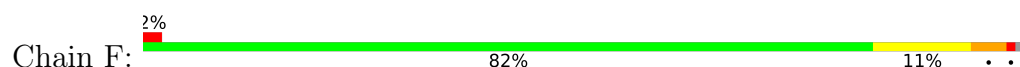




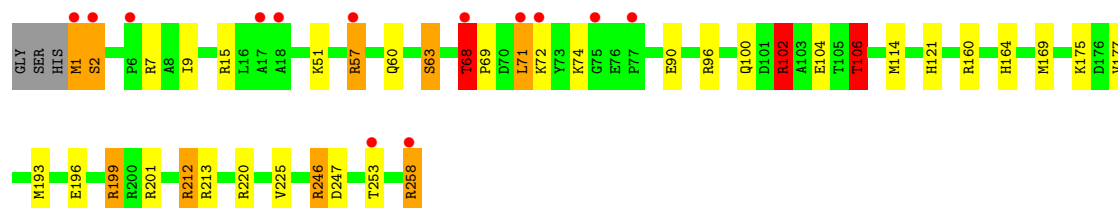
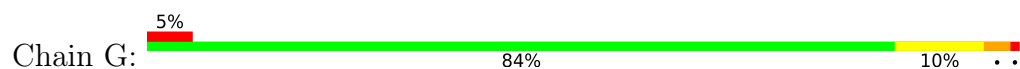
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



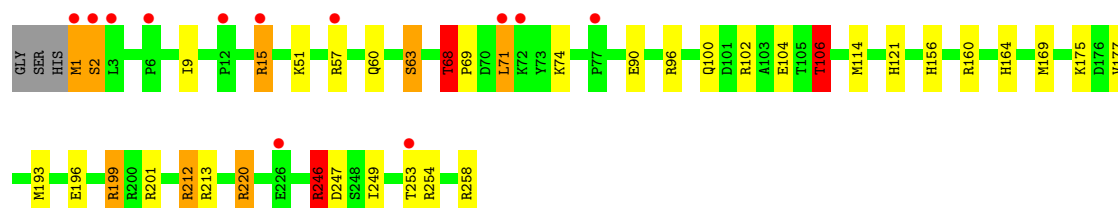
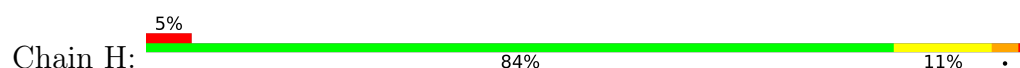
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

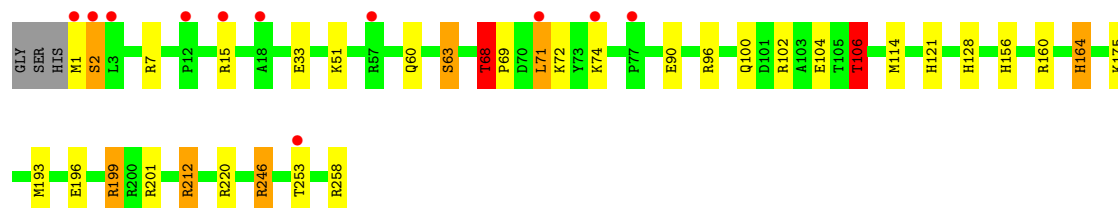


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



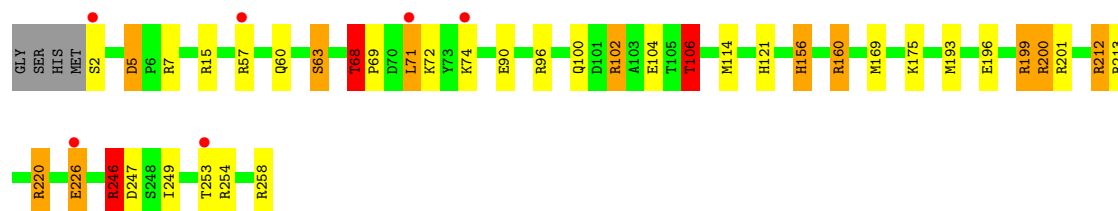
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain I:  4% 85% 10% ..



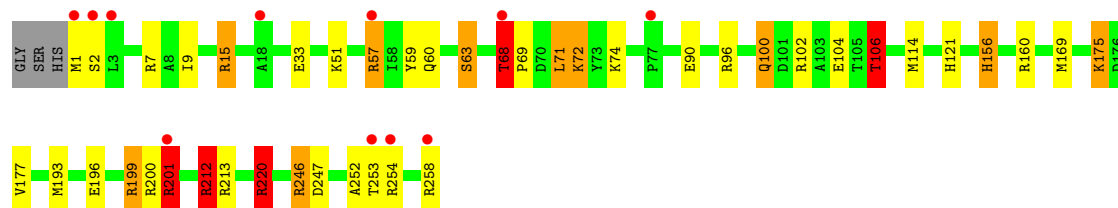
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain J:  2% 84% 10% ..



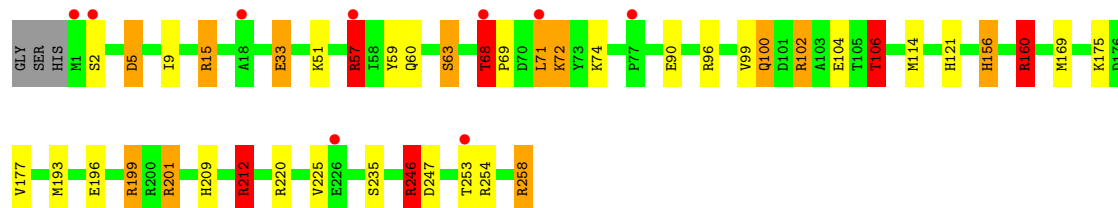
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain K:  4% 82% 11% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

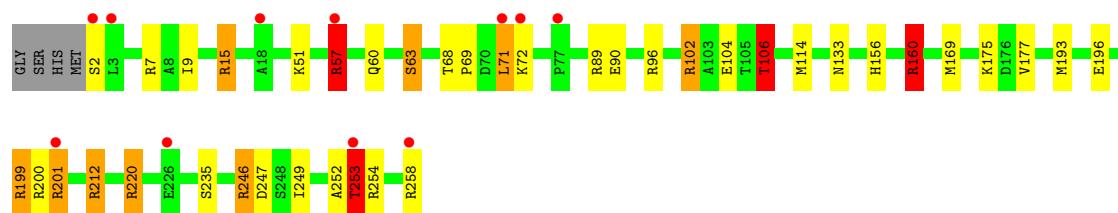
Chain L:  3% 82% 10% 5% ..



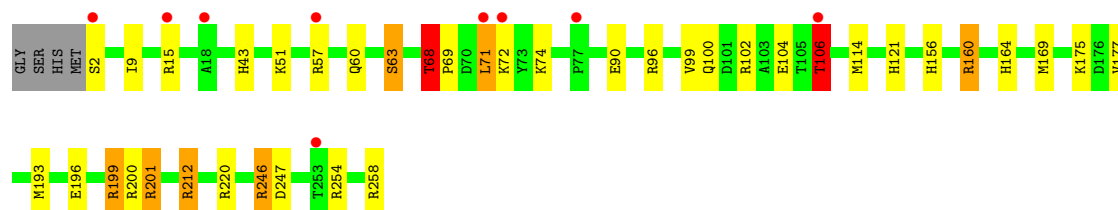
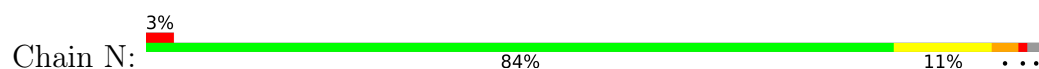
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain M:  4% 83% 10% ..

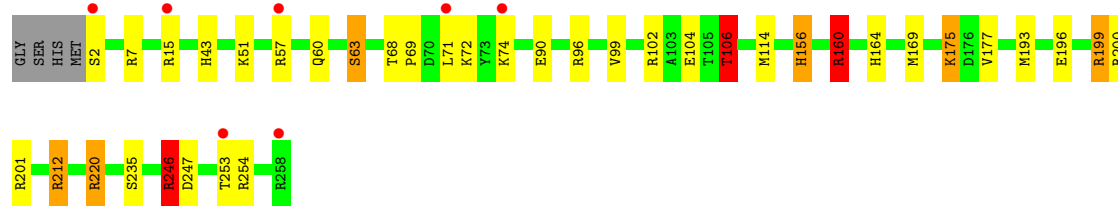
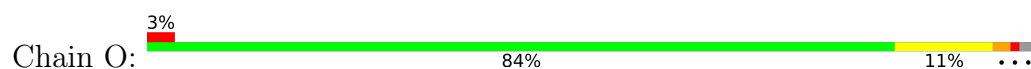




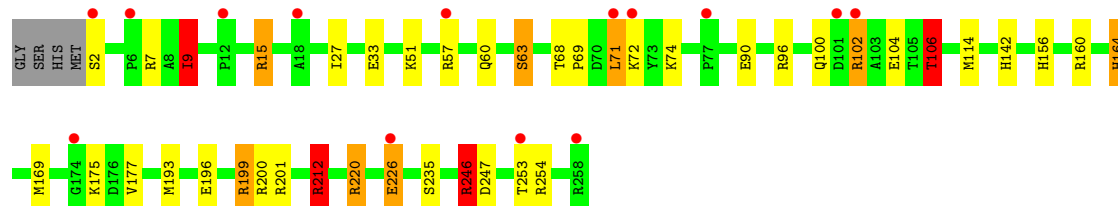
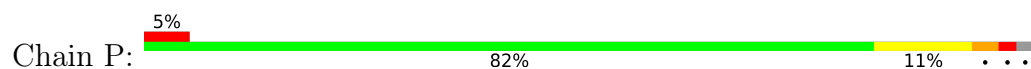
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



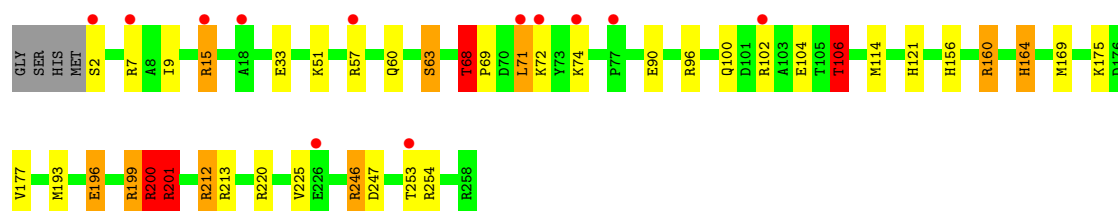
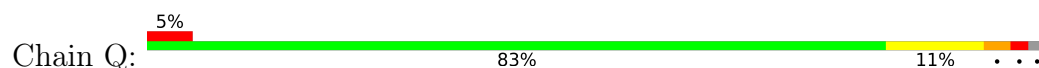
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

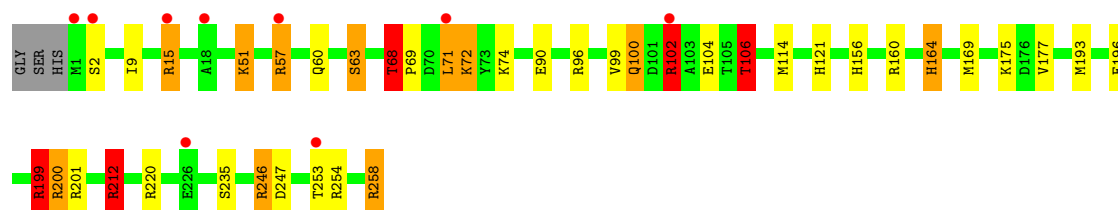


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain R:  3% 84% 9% . . .



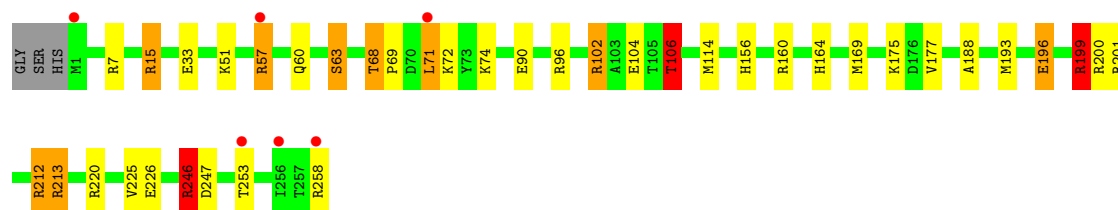
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain S:  2% 83% 12% . . .



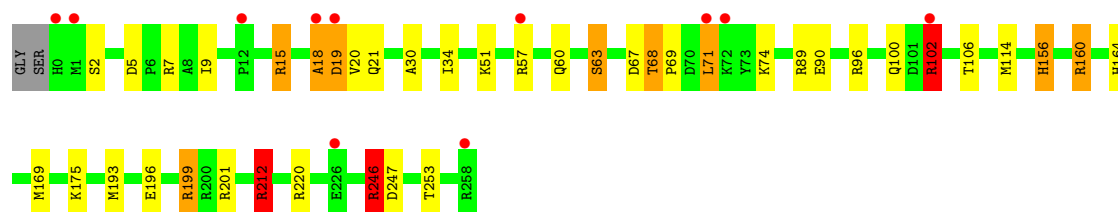
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain T:  2% 84% 10% . . .



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

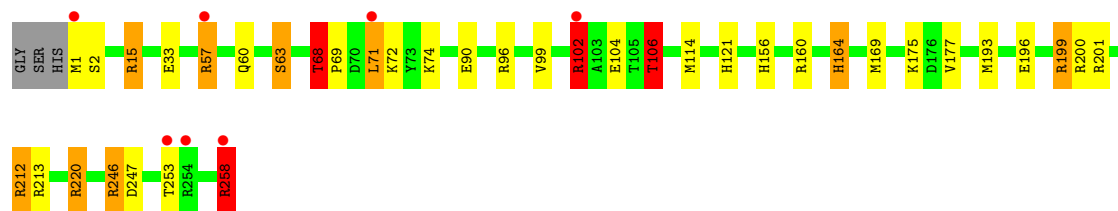
Chain U:  4% 84% 11% . . .



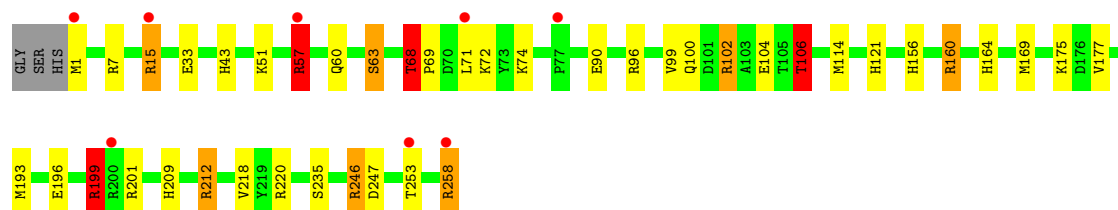
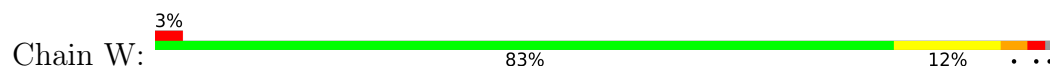
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain V:  3% 84% 10% . . .

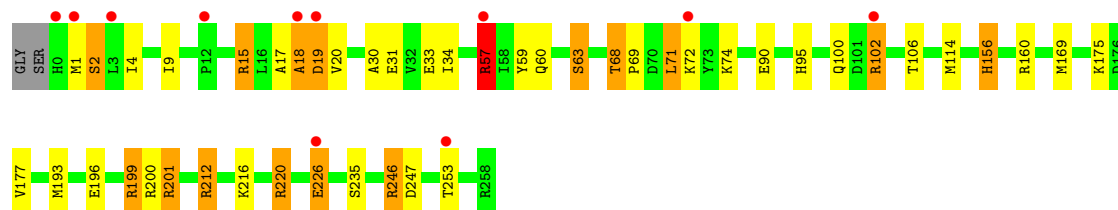
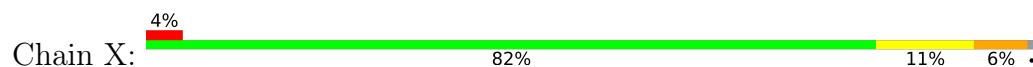




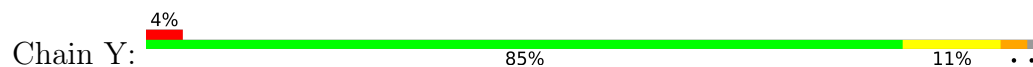
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



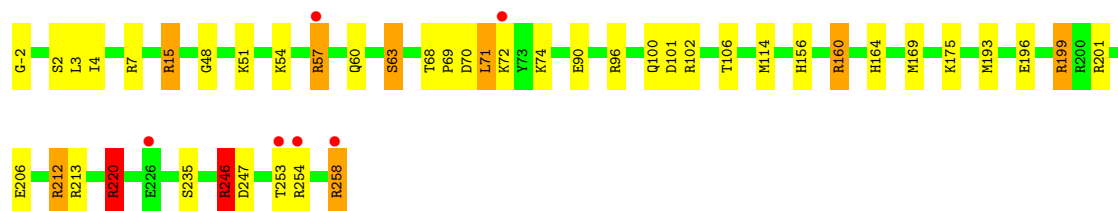
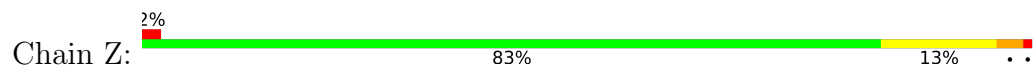
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

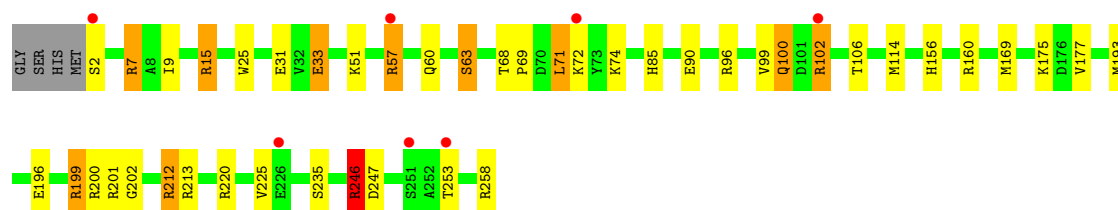


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



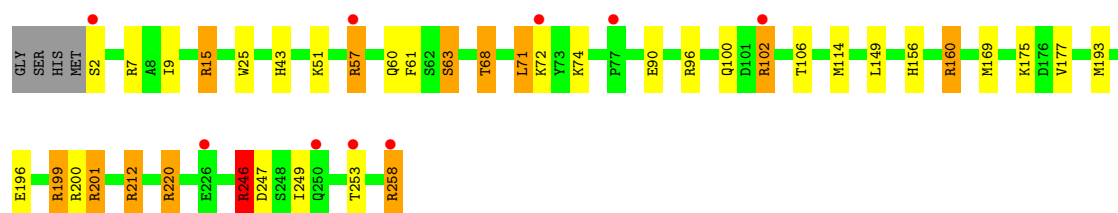
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain a: 



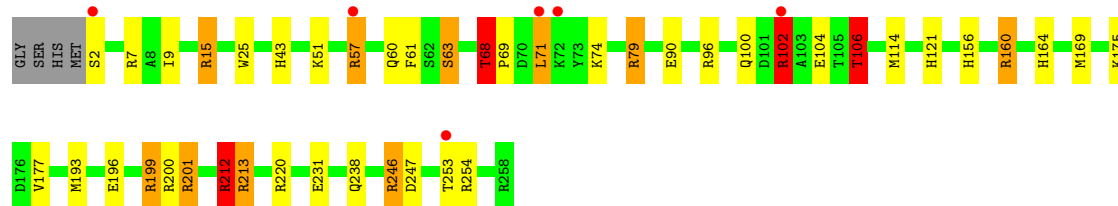
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain b: 



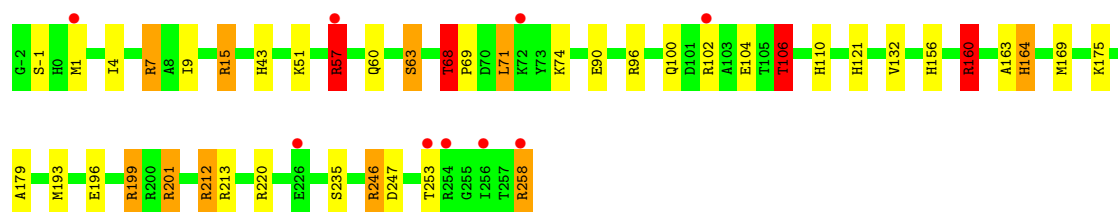
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain c: 



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain d: 



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 245.63Å 367.55Å 370.68Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 105.72 – 2.84<br>105.72 – 2.84                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (105.72-2.84)<br>99.4 (105.72-2.84)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.49 (at 2.86Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0222                                             | Depositor        |
| R, $R_{free}$                                                           | 0.203 , 0.216<br>0.206 , 0.219                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 19383 reflections (5.01%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 45.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.393                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 37.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 60728                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 51.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: MG, VFE

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     | 1.10         | 2/2027 (0.1%)    | 1.10        | 11/2748 (0.4%)   |
| 1   | B     | 1.15         | 2/2027 (0.1%)    | 1.17        | 9/2748 (0.3%)    |
| 1   | C     | 1.16         | 4/2019 (0.2%)    | 1.12        | 7/2738 (0.3%)    |
| 1   | D     | 1.11         | 5/2019 (0.2%)    | 1.13        | 10/2738 (0.4%)   |
| 1   | E     | 1.09         | 2/2027 (0.1%)    | 1.10        | 6/2748 (0.2%)    |
| 1   | F     | 1.10         | 4/2019 (0.2%)    | 1.09        | 8/2738 (0.3%)    |
| 1   | G     | 1.04         | 1/2027 (0.0%)    | 1.08        | 7/2748 (0.3%)    |
| 1   | H     | 1.02         | 1/2027 (0.0%)    | 1.13        | 10/2748 (0.4%)   |
| 1   | I     | 1.09         | 2/2027 (0.1%)    | 1.15        | 12/2748 (0.4%)   |
| 1   | J     | 1.06         | 4/2019 (0.2%)    | 1.11        | 10/2738 (0.4%)   |
| 1   | K     | 1.02         | 3/2027 (0.1%)    | 1.09        | 8/2748 (0.3%)    |
| 1   | L     | 1.07         | 5/2027 (0.2%)    | 1.11        | 10/2748 (0.4%)   |
| 1   | M     | 1.08         | 3/2019 (0.1%)    | 1.14        | 13/2738 (0.5%)   |
| 1   | N     | 1.02         | 1/2019 (0.0%)    | 1.06        | 7/2738 (0.3%)    |
| 1   | O     | 1.04         | 3/2019 (0.1%)    | 1.09        | 9/2738 (0.3%)    |
| 1   | P     | 1.04         | 4/2019 (0.2%)    | 1.09        | 7/2738 (0.3%)    |
| 1   | Q     | 1.03         | 3/2019 (0.1%)    | 1.09        | 11/2738 (0.4%)   |
| 1   | R     | 1.04         | 2/2027 (0.1%)    | 1.08        | 7/2748 (0.3%)    |
| 1   | S     | 1.05         | 1/2027 (0.0%)    | 1.10        | 7/2748 (0.3%)    |
| 1   | T     | 1.08         | 3/2027 (0.1%)    | 1.08        | 8/2748 (0.3%)    |
| 1   | U     | 1.26         | 6/2038 (0.3%)    | 1.22        | 16/2763 (0.6%)   |
| 1   | V     | 1.06         | 2/2027 (0.1%)    | 1.10        | 11/2748 (0.4%)   |
| 1   | W     | 1.11         | 4/2027 (0.2%)    | 1.13        | 13/2748 (0.5%)   |
| 1   | X     | 1.27         | 10/2049 (0.5%)   | 1.24        | 17/2777 (0.6%)   |
| 1   | Y     | 1.09         | 2/2027 (0.1%)    | 1.16        | 16/2748 (0.6%)   |
| 1   | Z     | 1.19         | 4/2048 (0.2%)    | 1.13        | 8/2776 (0.3%)    |
| 1   | a     | 1.15         | 7/2019 (0.3%)    | 1.12        | 8/2738 (0.3%)    |
| 1   | b     | 1.14         | 2/2019 (0.1%)    | 1.13        | 10/2738 (0.4%)   |
| 1   | c     | 1.05         | 2/2019 (0.1%)    | 1.14        | 13/2738 (0.5%)   |
| 1   | d     | 1.18         | 7/2048 (0.3%)    | 1.14        | 10/2776 (0.4%)   |
| All | All   | 1.10         | 101/60789 (0.2%) | 1.12        | 299/82420 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 12                  |
| 1   | B     | 0                   | 11                  |
| 1   | C     | 0                   | 10                  |
| 1   | D     | 0                   | 12                  |
| 1   | E     | 0                   | 9                   |
| 1   | F     | 0                   | 10                  |
| 1   | G     | 0                   | 10                  |
| 1   | H     | 0                   | 11                  |
| 1   | I     | 0                   | 7                   |
| 1   | J     | 0                   | 12                  |
| 1   | K     | 0                   | 13                  |
| 1   | L     | 0                   | 11                  |
| 1   | M     | 0                   | 11                  |
| 1   | N     | 0                   | 10                  |
| 1   | O     | 0                   | 10                  |
| 1   | P     | 0                   | 10                  |
| 1   | Q     | 0                   | 10                  |
| 1   | R     | 0                   | 9                   |
| 1   | S     | 0                   | 12                  |
| 1   | T     | 0                   | 10                  |
| 1   | U     | 0                   | 11                  |
| 1   | V     | 0                   | 10                  |
| 1   | W     | 0                   | 10                  |
| 1   | X     | 0                   | 9                   |
| 1   | Y     | 0                   | 6                   |
| 1   | Z     | 0                   | 11                  |
| 1   | a     | 0                   | 12                  |
| 1   | b     | 0                   | 11                  |
| 1   | c     | 0                   | 10                  |
| 1   | d     | 0                   | 10                  |
| All | All   | 0                   | 310                 |

All (101) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | X     | 19  | ASP  | N-CA  | 12.28 | 1.64        | 1.46     |
| 1   | U     | 19  | ASP  | N-CA  | 10.38 | 1.59        | 1.46     |
| 1   | X     | 18  | ALA  | C-O   | 9.68  | 1.36        | 1.24     |
| 1   | U     | 18  | ALA  | C-O   | 8.93  | 1.34        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | a     | 33  | GLU  | CD-OE2  | 8.68  | 1.41        | 1.25     |
| 1   | U     | 30  | ALA  | C-O     | -8.30 | 1.14        | 1.23     |
| 1   | Z     | 2   | SER  | C-O     | 8.25  | 1.35        | 1.23     |
| 1   | O     | 164 | HIS  | CE1-NE2 | 8.07  | 1.40        | 1.32     |
| 1   | X     | 20  | VAL  | C-O     | -7.63 | 1.15        | 1.24     |
| 1   | X     | 18  | ALA  | N-CA    | -7.38 | 1.36        | 1.46     |
| 1   | Z     | 164 | HIS  | CE1-NE2 | 7.38  | 1.40        | 1.32     |
| 1   | d     | 43  | HIS  | CE1-NE2 | 7.37  | 1.40        | 1.32     |
| 1   | d     | 164 | HIS  | CE1-NE2 | 6.97  | 1.39        | 1.32     |
| 1   | J     | 2   | SER  | C-O     | -6.95 | 1.09        | 1.23     |
| 1   | Q     | 164 | HIS  | CE1-NE2 | 6.94  | 1.39        | 1.32     |
| 1   | Y     | 43  | HIS  | CE1-NE2 | 6.87  | 1.39        | 1.32     |
| 1   | X     | 156 | HIS  | CE1-NE2 | 6.60  | 1.39        | 1.32     |
| 1   | X     | 34  | ILE  | C-O     | -6.58 | 1.17        | 1.24     |
| 1   | E     | 164 | HIS  | CE1-NE2 | 6.57  | 1.39        | 1.32     |
| 1   | U     | 20  | VAL  | C-O     | -6.56 | 1.16        | 1.24     |
| 1   | K     | 201 | ARG  | NE-CZ   | 6.56  | 1.40        | 1.33     |
| 1   | C     | 5   | ASP  | CG-OD1  | -6.51 | 1.12        | 1.25     |
| 1   | R     | 164 | HIS  | CE1-NE2 | 6.48  | 1.39        | 1.32     |
| 1   | C     | 164 | HIS  | CE1-NE2 | 6.46  | 1.39        | 1.32     |
| 1   | I     | 128 | HIS  | CG-ND1  | 6.45  | 1.45        | 1.38     |
| 1   | M     | 2   | SER  | C-O     | -6.44 | 1.10        | 1.23     |
| 1   | P     | 164 | HIS  | CE1-NE2 | 6.42  | 1.39        | 1.32     |
| 1   | A     | 164 | HIS  | CE1-NE2 | 6.42  | 1.39        | 1.32     |
| 1   | U     | 34  | ILE  | C-O     | -6.42 | 1.17        | 1.24     |
| 1   | b     | 43  | HIS  | CE1-NE2 | 6.35  | 1.38        | 1.32     |
| 1   | c     | 43  | HIS  | CE1-NE2 | 6.32  | 1.38        | 1.32     |
| 1   | T     | 164 | HIS  | CE1-NE2 | 6.28  | 1.38        | 1.32     |
| 1   | d     | 7   | ARG  | NE-CZ   | -6.26 | 1.26        | 1.33     |
| 1   | O     | 156 | HIS  | CE1-NE2 | 6.21  | 1.38        | 1.32     |
| 1   | S     | 177 | VAL  | N-CA    | -6.10 | 1.40        | 1.46     |
| 1   | D     | 102 | ARG  | CD-NE   | 6.02  | 1.54        | 1.46     |
| 1   | X     | 30  | ALA  | C-O     | -6.02 | 1.16        | 1.23     |
| 1   | G     | 177 | VAL  | N-CA    | -5.96 | 1.40        | 1.46     |
| 1   | b     | 177 | VAL  | N-CA    | -5.94 | 1.41        | 1.46     |
| 1   | U     | 156 | HIS  | CE1-NE2 | 5.88  | 1.38        | 1.32     |
| 1   | a     | 15  | ARG  | NE-CZ   | 5.86  | 1.39        | 1.33     |
| 1   | P     | 142 | HIS  | CE1-NE2 | 5.84  | 1.38        | 1.32     |
| 1   | P     | 177 | VAL  | N-CA    | -5.84 | 1.41        | 1.46     |
| 1   | a     | 7   | ARG  | NE-CZ   | 5.77  | 1.39        | 1.33     |
| 1   | R     | 177 | VAL  | N-CA    | -5.76 | 1.41        | 1.46     |
| 1   | K     | 156 | HIS  | CE1-NE2 | 5.72  | 1.38        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | Q     | 200 | ARG  | C-O     | -5.70 | 1.17        | 1.24     |
| 1   | X     | 95  | HIS  | CE1-NE2 | 5.69  | 1.38        | 1.32     |
| 1   | M     | 177 | VAL  | N-CA    | -5.66 | 1.41        | 1.46     |
| 1   | D     | 177 | VAL  | N-CA    | -5.66 | 1.41        | 1.46     |
| 1   | W     | 209 | HIS  | CE1-NE2 | 5.64  | 1.38        | 1.32     |
| 1   | L     | 177 | VAL  | N-CA    | -5.63 | 1.41        | 1.46     |
| 1   | V     | 177 | VAL  | N-CA    | -5.63 | 1.41        | 1.46     |
| 1   | L     | 5   | ASP  | CG-OD1  | -5.60 | 1.14        | 1.25     |
| 1   | a     | 177 | VAL  | N-CA    | -5.57 | 1.41        | 1.46     |
| 1   | I     | 164 | HIS  | CE1-NE2 | 5.53  | 1.38        | 1.32     |
| 1   | P     | 235 | SER  | CA-CB   | -5.49 | 1.44        | 1.53     |
| 1   | M     | 201 | ARG  | NE-CZ   | 5.46  | 1.39        | 1.33     |
| 1   | Z     | 206 | GLU  | CD-OE1  | 5.46  | 1.35        | 1.25     |
| 1   | B     | 5   | ASP  | CG-OD1  | -5.45 | 1.15        | 1.25     |
| 1   | E     | 257 | THR  | N-CA    | -5.45 | 1.39        | 1.46     |
| 1   | Z     | 3   | LEU  | N-CA    | 5.40  | 1.53        | 1.46     |
| 1   | K     | 177 | VAL  | N-CA    | -5.38 | 1.41        | 1.46     |
| 1   | W     | 177 | VAL  | N-CA    | -5.38 | 1.41        | 1.46     |
| 1   | Q     | 177 | VAL  | N-CA    | -5.37 | 1.41        | 1.46     |
| 1   | X     | 2   | SER  | CA-CB   | -5.35 | 1.45        | 1.53     |
| 1   | F     | 235 | SER  | CA-CB   | -5.35 | 1.44        | 1.53     |
| 1   | Y     | 177 | VAL  | N-CA    | -5.34 | 1.41        | 1.46     |
| 1   | A     | 209 | HIS  | CE1-NE2 | 5.34  | 1.37        | 1.32     |
| 1   | F     | 156 | HIS  | CE1-NE2 | 5.33  | 1.37        | 1.32     |
| 1   | H     | 177 | VAL  | N-CA    | -5.33 | 1.41        | 1.46     |
| 1   | D     | 235 | SER  | CA-CB   | -5.30 | 1.44        | 1.53     |
| 1   | F     | 5   | ASP  | CG-OD1  | -5.30 | 1.15        | 1.25     |
| 1   | c     | 177 | VAL  | N-CA    | -5.26 | 1.41        | 1.46     |
| 1   | a     | 202 | GLY  | C-O     | -5.26 | 1.17        | 1.24     |
| 1   | d     | 179 | ALA  | C-O     | -5.25 | 1.17        | 1.23     |
| 1   | L     | 33  | GLU  | CD-OE2  | 5.24  | 1.35        | 1.25     |
| 1   | d     | 235 | SER  | CA-CB   | -5.24 | 1.44        | 1.53     |
| 1   | J     | 5   | ASP  | CG-OD1  | -5.23 | 1.15        | 1.25     |
| 1   | F     | 70  | ASP  | CG-OD2  | 5.21  | 1.35        | 1.25     |
| 1   | D     | 156 | HIS  | CE1-NE2 | 5.21  | 1.37        | 1.32     |
| 1   | d     | 110 | HIS  | CE1-NE2 | 5.20  | 1.37        | 1.32     |
| 1   | N     | 177 | VAL  | N-CA    | -5.19 | 1.41        | 1.46     |
| 1   | L     | 156 | HIS  | CE1-NE2 | 5.18  | 1.37        | 1.32     |
| 1   | W     | 43  | HIS  | CE1-NE2 | 5.17  | 1.37        | 1.32     |
| 1   | C     | 177 | VAL  | N-CA    | -5.17 | 1.41        | 1.46     |
| 1   | T     | 177 | VAL  | N-CA    | -5.16 | 1.41        | 1.46     |
| 1   | J     | 156 | HIS  | CE1-NE2 | 5.14  | 1.37        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | X     | 177 | VAL  | N-CA    | -5.13 | 1.41        | 1.46     |
| 1   | V     | 164 | HIS  | CE1-NE2 | 5.10  | 1.37        | 1.32     |
| 1   | W     | 235 | SER  | CA-CB   | -5.09 | 1.44        | 1.53     |
| 1   | a     | 235 | SER  | CA-CB   | -5.07 | 1.44        | 1.53     |
| 1   | a     | 85  | HIS  | CE1-NE2 | 5.07  | 1.37        | 1.32     |
| 1   | D     | 42  | PRO  | C-O     | -5.04 | 1.17        | 1.23     |
| 1   | B     | 177 | VAL  | N-CA    | -5.03 | 1.41        | 1.46     |
| 1   | O     | 177 | VAL  | N-CA    | -5.03 | 1.41        | 1.46     |
| 1   | C     | 156 | HIS  | CE1-NE2 | 5.02  | 1.37        | 1.32     |
| 1   | L     | 235 | SER  | CA-CB   | -5.02 | 1.44        | 1.53     |
| 1   | d     | 163 | ALA  | C-O     | -5.02 | 1.18        | 1.23     |
| 1   | J     | 200 | ARG  | C-O     | -5.02 | 1.18        | 1.24     |
| 1   | T     | 188 | ALA  | C-O     | -5.01 | 1.17        | 1.23     |

All (299) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | B     | 246 | ARG  | CG-CD-NE  | -17.20 | 74.15       | 112.00   |
| 1   | H     | 199 | ARG  | CG-CD-NE  | -16.49 | 75.72       | 112.00   |
| 1   | I     | 246 | ARG  | CG-CD-NE  | -12.98 | 83.45       | 112.00   |
| 1   | X     | 18  | ALA  | CA-C-N    | 12.34  | 140.51      | 122.74   |
| 1   | X     | 18  | ALA  | C-N-CA    | 12.34  | 140.51      | 122.74   |
| 1   | D     | 102 | ARG  | CG-CD-NE  | 11.95  | 138.30      | 112.00   |
| 1   | W     | 199 | ARG  | NE-CZ-NH2 | 10.74  | 128.87      | 119.20   |
| 1   | X     | 106 | THR  | CA-CB-OG1 | 10.63  | 125.55      | 109.60   |
| 1   | Y     | 160 | ARG  | CB-CG-CD  | 10.57  | 135.61      | 111.30   |
| 1   | D     | 106 | THR  | CA-CB-OG1 | 10.49  | 125.33      | 109.60   |
| 1   | U     | 102 | ARG  | CB-CG-CD  | 9.87   | 133.99      | 111.30   |
| 1   | E     | 106 | THR  | CA-CB-OG1 | 9.80   | 124.30      | 109.60   |
| 1   | Y     | 102 | ARG  | CB-CG-CD  | 9.71   | 133.63      | 111.30   |
| 1   | U     | 18  | ALA  | CA-C-N    | 9.70   | 140.06      | 121.54   |
| 1   | U     | 18  | ALA  | C-N-CA    | 9.70   | 140.06      | 121.54   |
| 1   | S     | 15  | ARG  | CG-CD-NE  | 9.69   | 133.31      | 112.00   |
| 1   | c     | 102 | ARG  | CB-CG-CD  | 9.64   | 133.48      | 111.30   |
| 1   | U     | 106 | THR  | CA-CB-OG1 | 9.60   | 124.01      | 109.60   |
| 1   | Y     | 201 | ARG  | CD-NE-CZ  | 9.52   | 137.72      | 124.40   |
| 1   | H     | 199 | ARG  | NE-CZ-NH1 | -9.46  | 112.04      | 121.50   |
| 1   | Y     | 106 | THR  | CA-CB-OG1 | 9.44   | 123.76      | 109.60   |
| 1   | Q     | 201 | ARG  | NE-CZ-NH1 | -9.16  | 112.34      | 121.50   |
| 1   | b     | 201 | ARG  | CB-CG-CD  | 9.09   | 132.20      | 111.30   |
| 1   | a     | 106 | THR  | CA-CB-OG1 | 9.05   | 123.17      | 109.60   |
| 1   | K     | 220 | ARG  | CB-CG-CD  | 9.04   | 132.09      | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | b     | 106 | THR  | CA-CB-OG1  | 9.02  | 123.12      | 109.60   |
| 1   | V     | 102 | ARG  | CB-CG-CD   | 8.97  | 131.94      | 111.30   |
| 1   | Z     | 106 | THR  | CA-CB-OG1  | 8.59  | 122.48      | 109.60   |
| 1   | J     | 2   | SER  | CA-C-O     | -8.57 | 106.22      | 120.80   |
| 1   | L     | 201 | ARG  | CB-CG-CD   | 8.46  | 130.75      | 111.30   |
| 1   | R     | 102 | ARG  | CB-CG-CD   | 8.37  | 130.55      | 111.30   |
| 1   | M     | 2   | SER  | CA-C-O     | -8.13 | 106.97      | 120.80   |
| 1   | X     | 201 | ARG  | CB-CG-CD   | 8.14  | 130.01      | 111.30   |
| 1   | Y     | 160 | ARG  | CA-CB-CG   | 8.10  | 130.29      | 114.10   |
| 1   | b     | 258 | ARG  | CB-CG-CD   | 7.99  | 129.67      | 111.30   |
| 1   | L     | 160 | ARG  | CB-CG-CD   | 7.98  | 129.65      | 111.30   |
| 1   | O     | 201 | ARG  | CB-CG-CD   | 7.85  | 129.35      | 111.30   |
| 1   | d     | 160 | ARG  | CB-CG-CD   | 7.81  | 129.25      | 111.30   |
| 1   | I     | 128 | HIS  | CB-CG-CD2  | -7.75 | 121.12      | 131.20   |
| 1   | c     | 201 | ARG  | CG-CD-NE   | -7.51 | 95.47       | 112.00   |
| 1   | X     | 18  | ALA  | CA-C-O     | 7.47  | 127.90      | 120.88   |
| 1   | I     | 246 | ARG  | NE-CZ-NH2  | 7.43  | 125.89      | 119.20   |
| 1   | Z     | 201 | ARG  | CB-CG-CD   | 7.32  | 128.14      | 111.30   |
| 1   | T     | 201 | ARG  | CB-CG-CD   | 7.18  | 127.83      | 111.30   |
| 1   | c     | 79  | ARG  | CG-CD-NE   | -7.16 | 96.24       | 112.00   |
| 1   | Y     | 220 | ARG  | NE-CZ-NH2  | -7.11 | 112.80      | 119.20   |
| 1   | c     | 201 | ARG  | CD-NE-CZ   | 7.07  | 134.30      | 124.40   |
| 1   | b     | 220 | ARG  | CB-CG-CD   | 7.01  | 127.42      | 111.30   |
| 1   | M     | 253 | THR  | OG1-CB-CG2 | 6.99  | 123.27      | 109.30   |
| 1   | J     | 226 | GLU  | CB-CG-CD   | 6.98  | 124.47      | 112.60   |
| 1   | X     | 31  | GLU  | CB-CG-CD   | -6.95 | 100.79      | 112.60   |
| 1   | F     | 74  | LYS  | CA-CB-CG   | 6.87  | 127.84      | 114.10   |
| 1   | U     | 19  | ASP  | CA-CB-CG   | -6.86 | 105.74      | 112.60   |
| 1   | M     | 201 | ARG  | CB-CG-CD   | 6.85  | 127.05      | 111.30   |
| 1   | S     | 68  | THR  | CA-CB-CG2  | 6.74  | 121.96      | 110.50   |
| 1   | H     | 199 | ARG  | CD-NE-CZ   | 6.73  | 133.83      | 124.40   |
| 1   | Y     | 68  | THR  | CA-CB-CG2  | 6.71  | 121.91      | 110.50   |
| 1   | b     | 68  | THR  | CA-CB-CG2  | 6.70  | 121.89      | 110.50   |
| 1   | U     | 68  | THR  | CA-CB-CG2  | 6.66  | 121.83      | 110.50   |
| 1   | X     | 2   | SER  | CA-C-O     | 6.62  | 129.09      | 121.47   |
| 1   | d     | 1   | MET  | CA-C-O     | 6.51  | 127.18      | 119.56   |
| 1   | M     | 253 | THR  | CA-CB-OG1  | 6.48  | 119.32      | 109.60   |
| 1   | V     | 68  | THR  | OG1-CB-CG2 | 6.47  | 122.25      | 109.30   |
| 1   | M     | 15  | ARG  | NE-CZ-NH2  | 6.45  | 125.00      | 119.20   |
| 1   | I     | 128 | HIS  | CB-CG-ND1  | 6.43  | 132.34      | 122.70   |
| 1   | W     | 71  | LEU  | CA-C-N     | 6.43  | 129.19      | 120.38   |
| 1   | W     | 71  | LEU  | C-N-CA     | 6.43  | 129.19      | 120.38   |

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| Mol | Chain | Res   | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1   | X     | 68    | THR  | CA-CB-CG2  | 6.42  | 121.41      | 110.50   |
| 1   | Y     | 201   | ARG  | CG-CD-NE   | 6.41  | 126.11      | 112.00   |
| 1   | S     | 71    | LEU  | CA-C-N     | 6.41  | 129.16      | 120.38   |
| 1   | S     | 71    | LEU  | C-N-CA     | 6.41  | 129.16      | 120.38   |
| 1   | E     | 201   | ARG  | CD-NE-CZ   | 6.39  | 133.35      | 124.40   |
| 1   | J     | 226   | GLU  | CA-CB-CG   | 6.38  | 126.87      | 114.10   |
| 1   | A     | 68    | THR  | OG1-CB-CG2 | 6.36  | 122.02      | 109.30   |
| 1   | T     | 68    | THR  | CA-CB-CG2  | 6.36  | 121.31      | 110.50   |
| 1   | c     | 68    | THR  | OG1-CB-CG2 | 6.36  | 122.01      | 109.30   |
| 1   | P     | 226   | GLU  | CA-CB-CG   | 6.33  | 126.77      | 114.10   |
| 1   | Y     | 160   | ARG  | CG-CD-NE   | 6.32  | 125.90      | 112.00   |
| 1   | P     | 71    | LEU  | CA-C-N     | 6.30  | 129.01      | 120.38   |
| 1   | P     | 71    | LEU  | C-N-CA     | 6.30  | 129.01      | 120.38   |
| 1   | A     | 51    | LYS  | CB-CG-CD   | 6.28  | 125.74      | 111.30   |
| 1   | J     | 68    | THR  | OG1-CB-CG2 | 6.25  | 121.80      | 109.30   |
| 1   | Q     | 68    | THR  | OG1-CB-CG2 | 6.24  | 121.78      | 109.30   |
| 1   | D     | 7     | ARG  | CA-CB-CG   | 6.23  | 126.57      | 114.10   |
| 1   | K     | 68    | THR  | OG1-CB-CG2 | 6.23  | 121.75      | 109.30   |
| 1   | C     | 68    | THR  | N-CA-CB    | 6.23  | 119.20      | 110.11   |
| 1   | C     | 68    | THR  | OG1-CB-CG2 | 6.22  | 121.74      | 109.30   |
| 1   | M     | 57[A] | ARG  | CG-CD-NE   | -6.22 | 98.31       | 112.00   |
| 1   | M     | 57[B] | ARG  | CG-CD-NE   | -6.22 | 98.31       | 112.00   |
| 1   | B     | 201   | ARG  | CB-CG-CD   | 6.22  | 125.60      | 111.30   |
| 1   | D     | 68    | THR  | OG1-CB-CG2 | 6.21  | 121.71      | 109.30   |
| 1   | M     | 72    | LYS  | CB-CG-CD   | 6.19  | 125.53      | 111.30   |
| 1   | K     | 201   | ARG  | CB-CG-CD   | 6.16  | 125.47      | 111.30   |
| 1   | V     | 220   | ARG  | CB-CG-CD   | 6.10  | 125.33      | 111.30   |
| 1   | A     | 51    | LYS  | CA-CB-CG   | 6.10  | 126.30      | 114.10   |
| 1   | V     | 258   | ARG  | CB-CG-CD   | 6.10  | 125.33      | 111.30   |
| 1   | O     | 71    | LEU  | CA-C-N     | 6.09  | 128.73      | 120.38   |
| 1   | O     | 71    | LEU  | C-N-CA     | 6.09  | 128.73      | 120.38   |
| 1   | B     | 226   | GLU  | CA-CB-CG   | 6.09  | 126.27      | 114.10   |
| 1   | V     | 220   | ARG  | CA-CB-CG   | 6.09  | 126.27      | 114.10   |
| 1   | R     | 68    | THR  | N-CA-CB    | 6.08  | 119.21      | 110.03   |
| 1   | N     | 68    | THR  | OG1-CB-CG2 | 6.07  | 121.44      | 109.30   |
| 1   | X     | 18    | ALA  | N-CA-C     | -6.07 | 101.66      | 110.64   |
| 1   | L     | 68    | THR  | OG1-CB-CG2 | 6.06  | 121.42      | 109.30   |
| 1   | K     | 68    | THR  | N-CA-CB    | 6.04  | 119.15      | 110.03   |
| 1   | W     | 68    | THR  | N-CA-CB    | 6.04  | 119.15      | 110.03   |
| 1   | Q     | 200   | ARG  | CB-CG-CD   | 6.02  | 125.15      | 111.30   |
| 1   | V     | 71    | LEU  | CA-C-N     | 6.02  | 128.62      | 120.38   |
| 1   | V     | 71    | LEU  | C-N-CA     | 6.02  | 128.62      | 120.38   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 68  | THR  | OG1-CB-CG2 | 6.01  | 121.32      | 109.30   |
| 1   | M     | 160 | ARG  | CB-CG-CD   | 6.00  | 125.11      | 111.30   |
| 1   | G     | 68  | THR  | N-CA-CB    | 6.00  | 118.86      | 110.11   |
| 1   | V     | 68  | THR  | N-CA-CB    | 5.99  | 119.08      | 110.03   |
| 1   | F     | 71  | LEU  | CA-C-N     | 5.98  | 128.57      | 120.38   |
| 1   | F     | 71  | LEU  | C-N-CA     | 5.98  | 128.57      | 120.38   |
| 1   | H     | 68  | THR  | OG1-CB-CG2 | 5.98  | 121.26      | 109.30   |
| 1   | b     | 71  | LEU  | CA-C-N     | 5.97  | 128.56      | 120.38   |
| 1   | b     | 71  | LEU  | C-N-CA     | 5.97  | 128.56      | 120.38   |
| 1   | X     | 19  | ASP  | CA-CB-CG   | -5.96 | 106.64      | 112.60   |
| 1   | H     | 68  | THR  | N-CA-CB    | 5.96  | 118.81      | 110.11   |
| 1   | U     | 15  | ARG  | CA-CB-CG   | -5.96 | 102.18      | 114.10   |
| 1   | F     | 68  | THR  | OG1-CB-CG2 | 5.96  | 121.21      | 109.30   |
| 1   | B     | 68  | THR  | N-CA-CB    | 5.95  | 119.01      | 110.03   |
| 1   | A     | 74  | LYS  | CA-CB-CG   | 5.94  | 125.98      | 114.10   |
| 1   | C     | 106 | THR  | CA-CB-OG1  | -5.94 | 100.69      | 109.60   |
| 1   | R     | 68  | THR  | OG1-CB-CG2 | 5.94  | 121.17      | 109.30   |
| 1   | A     | 71  | LEU  | CA-C-N     | 5.93  | 128.51      | 120.38   |
| 1   | A     | 71  | LEU  | C-N-CA     | 5.93  | 128.51      | 120.38   |
| 1   | B     | 68  | THR  | OG1-CB-CG2 | 5.93  | 121.17      | 109.30   |
| 1   | D     | 68  | THR  | N-CA-CB    | 5.93  | 118.99      | 110.03   |
| 1   | R     | 71  | LEU  | CA-C-N     | 5.93  | 128.51      | 120.38   |
| 1   | R     | 71  | LEU  | C-N-CA     | 5.93  | 128.51      | 120.38   |
| 1   | T     | 68  | THR  | N-CA-CB    | 5.93  | 118.98      | 110.03   |
| 1   | L     | 68  | THR  | N-CA-CB    | 5.92  | 118.98      | 110.03   |
| 1   | W     | 199 | ARG  | NE-CZ-NH1  | -5.92 | 115.58      | 121.50   |
| 1   | d     | 106 | THR  | CA-CB-OG1  | -5.92 | 100.72      | 109.60   |
| 1   | V     | 106 | THR  | CA-CB-OG1  | -5.91 | 100.73      | 109.60   |
| 1   | a     | 71  | LEU  | CA-C-N     | 5.90  | 128.46      | 120.38   |
| 1   | a     | 71  | LEU  | C-N-CA     | 5.90  | 128.46      | 120.38   |
| 1   | A     | 68  | THR  | N-CA-CB    | 5.89  | 118.93      | 110.03   |
| 1   | A     | 258 | ARG  | CG-CD-NE   | 5.89  | 124.97      | 112.00   |
| 1   | X     | 71  | LEU  | CA-C-N     | 5.89  | 128.45      | 120.38   |
| 1   | X     | 71  | LEU  | C-N-CA     | 5.89  | 128.45      | 120.38   |
| 1   | Z     | 71  | LEU  | CA-C-N     | 5.89  | 128.45      | 120.38   |
| 1   | Z     | 71  | LEU  | C-N-CA     | 5.89  | 128.45      | 120.38   |
| 1   | I     | 258 | ARG  | CG-CD-NE   | 5.89  | 124.96      | 112.00   |
| 1   | I     | 68  | THR  | OG1-CB-CG2 | 5.89  | 121.07      | 109.30   |
| 1   | T     | 106 | THR  | CA-CB-OG1  | -5.88 | 100.77      | 109.60   |
| 1   | I     | 68  | THR  | N-CA-CB    | 5.88  | 118.91      | 110.03   |
| 1   | J     | 68  | THR  | N-CA-CB    | 5.87  | 118.89      | 110.03   |
| 1   | d     | 68  | THR  | OG1-CB-CG2 | 5.86  | 121.02      | 109.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | L     | 71  | LEU  | CA-C-N    | 5.85  | 128.39      | 120.38   |
| 1   | L     | 71  | LEU  | C-N-CA    | 5.85  | 128.39      | 120.38   |
| 1   | c     | 68  | THR  | N-CA-CB   | 5.84  | 118.85      | 110.03   |
| 1   | d     | 68  | THR  | N-CA-CB   | 5.83  | 118.84      | 110.03   |
| 1   | G     | 71  | LEU  | CA-C-N    | 5.83  | 128.37      | 120.38   |
| 1   | G     | 71  | LEU  | C-N-CA    | 5.83  | 128.37      | 120.38   |
| 1   | K     | 71  | LEU  | CA-C-N    | 5.83  | 128.37      | 120.38   |
| 1   | K     | 71  | LEU  | C-N-CA    | 5.83  | 128.37      | 120.38   |
| 1   | X     | 68  | THR  | N-CA-CB   | 5.83  | 118.83      | 110.03   |
| 1   | Y     | 201 | ARG  | CB-CG-CD  | 5.82  | 124.69      | 111.30   |
| 1   | U     | 68  | THR  | N-CA-CB   | 5.82  | 118.82      | 110.03   |
| 1   | c     | 106 | THR  | CA-CB-OG1 | -5.82 | 100.87      | 109.60   |
| 1   | d     | 71  | LEU  | CA-C-N    | 5.81  | 128.35      | 120.38   |
| 1   | d     | 71  | LEU  | C-N-CA    | 5.81  | 128.35      | 120.38   |
| 1   | D     | 71  | LEU  | CA-C-N    | 5.80  | 128.33      | 120.38   |
| 1   | D     | 71  | LEU  | C-N-CA    | 5.80  | 128.33      | 120.38   |
| 1   | T     | 71  | LEU  | CA-C-N    | 5.80  | 128.33      | 120.38   |
| 1   | T     | 71  | LEU  | C-N-CA    | 5.80  | 128.33      | 120.38   |
| 1   | C     | 71  | LEU  | CA-C-N    | 5.79  | 128.32      | 120.38   |
| 1   | C     | 71  | LEU  | C-N-CA    | 5.79  | 128.32      | 120.38   |
| 1   | E     | 71  | LEU  | CA-C-N    | 5.79  | 128.31      | 120.38   |
| 1   | E     | 71  | LEU  | C-N-CA    | 5.79  | 128.31      | 120.38   |
| 1   | M     | 71  | LEU  | CA-C-N    | 5.79  | 128.31      | 120.38   |
| 1   | M     | 71  | LEU  | C-N-CA    | 5.79  | 128.31      | 120.38   |
| 1   | V     | 99  | VAL  | CA-CB-CG2 | -5.79 | 100.56      | 110.40   |
| 1   | b     | 68  | THR  | N-CA-CB   | 5.79  | 118.77      | 110.03   |
| 1   | Q     | 68  | THR  | N-CA-CB   | 5.78  | 118.76      | 110.03   |
| 1   | B     | 106 | THR  | CA-CB-OG1 | -5.78 | 100.93      | 109.60   |
| 1   | A     | 106 | THR  | CA-CB-OG1 | -5.77 | 100.94      | 109.60   |
| 1   | N     | 71  | LEU  | CA-C-N    | 5.77  | 128.28      | 120.38   |
| 1   | N     | 71  | LEU  | C-N-CA    | 5.77  | 128.28      | 120.38   |
| 1   | Y     | 71  | LEU  | CA-C-N    | 5.76  | 128.28      | 120.38   |
| 1   | Y     | 71  | LEU  | C-N-CA    | 5.76  | 128.28      | 120.38   |
| 1   | c     | 213 | ARG  | NE-CZ-NH1 | -5.76 | 115.74      | 121.50   |
| 1   | N     | 68  | THR  | N-CA-CB   | 5.75  | 118.72      | 110.03   |
| 1   | H     | 106 | THR  | CA-CB-OG1 | -5.75 | 100.97      | 109.60   |
| 1   | b     | 15  | ARG  | NE-CZ-NH2 | 5.75  | 124.37      | 119.20   |
| 1   | W     | 106 | THR  | CA-CB-OG1 | -5.75 | 100.98      | 109.60   |
| 1   | I     | 106 | THR  | CA-CB-OG1 | -5.74 | 100.99      | 109.60   |
| 1   | F     | 106 | THR  | CA-CB-OG1 | -5.74 | 101.00      | 109.60   |
| 1   | O     | 106 | THR  | CA-CB-OG1 | -5.72 | 101.02      | 109.60   |
| 1   | W     | 99  | VAL  | CA-CB-CG2 | -5.72 | 100.67      | 110.40   |

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| Mol | Chain | Res   | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1   | O     | 99    | VAL  | CA-CB-CG2  | -5.72 | 100.68      | 110.40   |
| 1   | Z     | 201   | ARG  | CD-NE-CZ   | 5.71  | 132.40      | 124.40   |
| 1   | E     | 99    | VAL  | CA-CB-CG2  | -5.70 | 100.70      | 110.40   |
| 1   | I     | 71    | LEU  | CA-C-N     | 5.70  | 128.18      | 120.38   |
| 1   | I     | 71    | LEU  | C-N-CA     | 5.70  | 128.18      | 120.38   |
| 1   | Q     | 71    | LEU  | CA-C-N     | 5.69  | 128.18      | 120.38   |
| 1   | Q     | 71    | LEU  | C-N-CA     | 5.69  | 128.18      | 120.38   |
| 1   | K     | 106   | THR  | CA-CB-OG1  | -5.69 | 101.07      | 109.60   |
| 1   | W     | 68    | THR  | OG1-CB-CG2 | 5.68  | 120.67      | 109.30   |
| 1   | C     | 201   | ARG  | CD-NE-CZ   | 5.68  | 132.35      | 124.40   |
| 1   | Q     | 201   | ARG  | CD-NE-CZ   | 5.68  | 132.35      | 124.40   |
| 1   | B     | 71    | LEU  | CA-C-N     | 5.67  | 128.15      | 120.38   |
| 1   | B     | 71    | LEU  | C-N-CA     | 5.67  | 128.15      | 120.38   |
| 1   | L     | 99    | VAL  | CA-CB-CG2  | -5.67 | 100.76      | 110.40   |
| 1   | U     | 15    | ARG  | CG-CD-NE   | 5.67  | 124.46      | 112.00   |
| 1   | G     | 106   | THR  | CA-CB-OG1  | -5.66 | 101.11      | 109.60   |
| 1   | Y     | 68    | THR  | N-CA-CB    | 5.66  | 118.57      | 110.03   |
| 1   | Q     | 106   | THR  | CA-CB-OG1  | -5.64 | 101.14      | 109.60   |
| 1   | F     | 68    | THR  | N-CA-CB    | 5.62  | 118.52      | 110.03   |
| 1   | J     | 71    | LEU  | CA-C-N     | 5.62  | 128.08      | 120.38   |
| 1   | J     | 71    | LEU  | C-N-CA     | 5.62  | 128.08      | 120.38   |
| 1   | N     | 106   | THR  | CA-CB-OG1  | -5.61 | 101.19      | 109.60   |
| 1   | W     | 57[A] | ARG  | CB-CG-CD   | 5.60  | 124.18      | 111.30   |
| 1   | W     | 57[B] | ARG  | CB-CG-CD   | 5.60  | 124.18      | 111.30   |
| 1   | C     | 254   | ARG  | CG-CD-NE   | 5.60  | 124.32      | 112.00   |
| 1   | M     | 106   | THR  | CA-CB-OG1  | -5.60 | 101.21      | 109.60   |
| 1   | R     | 106   | THR  | CA-CB-OG1  | -5.59 | 101.21      | 109.60   |
| 1   | U     | 102   | ARG  | CG-CD-NE   | 5.59  | 124.31      | 112.00   |
| 1   | P     | 106   | THR  | CA-CB-OG1  | -5.59 | 101.21      | 109.60   |
| 1   | S     | 68    | THR  | N-CA-CB    | 5.59  | 118.47      | 110.03   |
| 1   | L     | 106   | THR  | CA-CB-OG1  | -5.58 | 101.22      | 109.60   |
| 1   | a     | 100   | GLN  | CB-CG-CD   | 5.57  | 122.08      | 112.60   |
| 1   | U     | 7     | ARG  | NE-CZ-NH1  | -5.55 | 115.95      | 121.50   |
| 1   | L     | 201   | ARG  | CD-NE-CZ   | 5.54  | 132.16      | 124.40   |
| 1   | H     | 71    | LEU  | CA-C-N     | 5.54  | 127.97      | 120.38   |
| 1   | H     | 71    | LEU  | C-N-CA     | 5.54  | 127.97      | 120.38   |
| 1   | J     | 106   | THR  | CA-CB-OG1  | -5.54 | 101.30      | 109.60   |
| 1   | S     | 106   | THR  | CA-CB-OG1  | -5.54 | 101.30      | 109.60   |
| 1   | c     | 201   | ARG  | NE-CZ-NH1  | -5.53 | 115.97      | 121.50   |
| 1   | Y     | 102   | ARG  | CG-CD-NE   | 5.51  | 124.13      | 112.00   |
| 1   | c     | 71    | LEU  | CA-C-N     | 5.50  | 127.92      | 120.38   |
| 1   | c     | 71    | LEU  | C-N-CA     | 5.50  | 127.92      | 120.38   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | W     | 235 | SER  | N-CA-CB   | 5.50  | 119.52      | 110.39   |
| 1   | I     | 246 | ARG  | NE-CZ-NH1 | -5.49 | 116.01      | 121.50   |
| 1   | c     | 15  | ARG  | NE-CZ-NH2 | 5.46  | 124.11      | 119.20   |
| 1   | Q     | 200 | ARG  | CD-NE-CZ  | 5.44  | 132.01      | 124.40   |
| 1   | U     | 2   | SER  | CA-C-O    | 5.41  | 127.69      | 121.47   |
| 1   | D     | 102 | ARG  | NE-CZ-NH2 | 5.39  | 124.05      | 119.20   |
| 1   | X     | 15  | ARG  | CA-CB-CG  | -5.35 | 103.41      | 114.10   |
| 1   | d     | 15  | ARG  | NE-CZ-NH2 | 5.34  | 124.01      | 119.20   |
| 1   | U     | 71  | LEU  | CA-C-N    | 5.34  | 127.69      | 120.38   |
| 1   | U     | 71  | LEU  | C-N-CA    | 5.34  | 127.69      | 120.38   |
| 1   | U     | 15  | ARG  | CB-CG-CD  | 5.31  | 123.52      | 111.30   |
| 1   | O     | 72  | LYS  | CB-CG-CD  | 5.29  | 123.47      | 111.30   |
| 1   | P     | 212 | ARG  | CG-CD-NE  | -5.29 | 100.37      | 112.00   |
| 1   | d     | 201 | ARG  | CD-NE-CZ  | 5.28  | 131.79      | 124.40   |
| 1   | J     | 100 | GLN  | CB-CG-CD  | 5.27  | 121.56      | 112.60   |
| 1   | X     | 226 | GLU  | CA-CB-CG  | 5.27  | 124.65      | 114.10   |
| 1   | P     | 68  | THR  | CA-CB-OG1 | 5.26  | 117.49      | 109.60   |
| 1   | M     | 68  | THR  | CA-CB-OG1 | 5.26  | 117.48      | 109.60   |
| 1   | S     | 1   | MET  | CB-CA-C   | 5.25  | 120.08      | 110.10   |
| 1   | Z     | 15  | ARG  | NE-CZ-NH2 | 5.25  | 123.92      | 119.20   |
| 1   | L     | 235 | SER  | N-CA-CB   | 5.24  | 119.09      | 110.39   |
| 1   | T     | 72  | LYS  | CB-CG-CD  | 5.24  | 123.36      | 111.30   |
| 1   | Z     | 68  | THR  | CA-CB-OG1 | 5.24  | 117.46      | 109.60   |
| 1   | F     | 201 | ARG  | CD-NE-CZ  | 5.23  | 131.72      | 124.40   |
| 1   | G     | 100 | GLN  | CB-CG-CD  | 5.22  | 121.48      | 112.60   |
| 1   | R     | 15  | ARG  | NE-CZ-NH2 | 5.22  | 123.90      | 119.20   |
| 1   | D     | 100 | GLN  | CB-CG-CD  | 5.22  | 121.47      | 112.60   |
| 1   | O     | 201 | ARG  | CD-NE-CZ  | 5.22  | 131.70      | 124.40   |
| 1   | Y     | 102 | ARG  | CA-CB-CG  | 5.21  | 124.52      | 114.10   |
| 1   | b     | 100 | GLN  | CB-CG-CD  | 5.21  | 121.45      | 112.60   |
| 1   | X     | 100 | GLN  | CB-CG-CD  | 5.20  | 121.44      | 112.60   |
| 1   | G     | 102 | ARG  | CB-CG-CD  | 5.20  | 123.26      | 111.30   |
| 1   | I     | 100 | GLN  | CB-CG-CD  | 5.20  | 121.44      | 112.60   |
| 1   | U     | 67  | ASP  | CA-CB-CG  | 5.20  | 117.80      | 112.60   |
| 1   | P     | 9   | ILE  | CA-CB-CG1 | 5.19  | 119.22      | 110.40   |
| 1   | Y     | 100 | GLN  | CB-CG-CD  | 5.19  | 121.42      | 112.60   |
| 1   | E     | 68  | THR  | CA-CB-OG1 | 5.18  | 117.37      | 109.60   |
| 1   | V     | 102 | ARG  | CA-CB-CG  | 5.18  | 124.45      | 114.10   |
| 1   | a     | 201 | ARG  | CD-NE-CZ  | 5.15  | 131.62      | 124.40   |
| 1   | O     | 68  | THR  | CA-CB-OG1 | 5.14  | 117.32      | 109.60   |
| 1   | A     | 100 | GLN  | CB-CG-CD  | 5.14  | 121.33      | 112.60   |
| 1   | W     | 102 | ARG  | CB-CG-CD  | 5.14  | 123.11      | 111.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | N     | 100 | GLN  | CB-CG-CD  | 5.13  | 121.33      | 112.60   |
| 1   | W     | 160 | ARG  | NE-CZ-NH2 | 5.13  | 123.82      | 119.20   |
| 1   | a     | 68  | THR  | CA-CB-OG1 | 5.12  | 117.28      | 109.60   |
| 1   | a     | 235 | SER  | N-CA-CB   | 5.12  | 118.89      | 110.39   |
| 1   | K     | 253 | THR  | CA-CB-OG1 | 5.12  | 117.28      | 109.60   |
| 1   | Q     | 201 | ARG  | NE-CZ-NH2 | 5.11  | 123.80      | 119.20   |
| 1   | F     | 235 | SER  | N-CA-CB   | 5.11  | 118.19      | 110.28   |
| 1   | A     | 74  | LYS  | CB-CA-C   | -5.10 | 103.22      | 111.28   |
| 1   | O     | 160 | ARG  | CB-CG-CD  | 5.10  | 123.04      | 111.30   |
| 1   | D     | 235 | SER  | N-CA-CB   | 5.09  | 118.17      | 110.28   |
| 1   | X     | 216 | LYS  | CG-CD-CE  | 5.08  | 122.99      | 111.30   |
| 1   | T     | 102 | ARG  | CB-CG-CD  | 5.08  | 122.98      | 111.30   |
| 1   | B     | 201 | ARG  | CD-NE-CZ  | 5.07  | 131.49      | 124.40   |
| 1   | H     | 220 | ARG  | NE-CZ-NH2 | 5.05  | 123.75      | 119.20   |
| 1   | a     | 100 | GLN  | CG-CD-NE2 | 5.05  | 123.98      | 116.40   |
| 1   | c     | 212 | ARG  | CG-CD-NE  | -5.05 | 100.89      | 112.00   |
| 1   | d     | 1   | MET  | CG-SD-CE  | 5.05  | 112.01      | 100.90   |
| 1   | Z     | 54  | LYS  | CG-CD-CE  | 5.03  | 122.87      | 111.30   |
| 1   | N     | 201 | ARG  | CD-NE-CZ  | 5.02  | 131.43      | 124.40   |
| 1   | H     | 15  | ARG  | NE-CZ-NH2 | 5.01  | 123.71      | 119.20   |
| 1   | J     | 201 | ARG  | CB-CG-CD  | 5.00  | 122.81      | 111.30   |
| 1   | Q     | 100 | GLN  | CB-CG-CD  | 5.00  | 121.11      | 112.60   |

There are no chirality outliers.

All (310) planarity outliers are listed below:

| Mol | Chain | Res   | Type | Group     |
|-----|-------|-------|------|-----------|
| 1   | A     | 102   | ARG  | Sidechain |
| 1   | A     | 15    | ARG  | Sidechain |
| 1   | A     | 160   | ARG  | Sidechain |
| 1   | A     | 199   | ARG  | Sidechain |
| 1   | A     | 200   | ARG  | Sidechain |
| 1   | A     | 212   | ARG  | Sidechain |
| 1   | A     | 213   | ARG  | Sidechain |
| 1   | A     | 220   | ARG  | Sidechain |
| 1   | A     | 258   | ARG  | Sidechain |
| 1   | A     | 57[A] | ARG  | Sidechain |
| 1   | A     | 57[B] | ARG  | Sidechain |
| 1   | A     | 96    | ARG  | Sidechain |
| 1   | B     | 102   | ARG  | Sidechain |
| 1   | B     | 15    | ARG  | Sidechain |
| 1   | B     | 160   | ARG  | Sidechain |

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| Mol | Chain | Res   | Type | Group     |
|-----|-------|-------|------|-----------|
| 1   | B     | 199   | ARG  | Sidechain |
| 1   | B     | 212   | ARG  | Sidechain |
| 1   | B     | 220   | ARG  | Sidechain |
| 1   | B     | 5     | ASP  | Sidechain |
| 1   | B     | 57[A] | ARG  | Sidechain |
| 1   | B     | 57[B] | ARG  | Sidechain |
| 1   | B     | 7     | ARG  | Sidechain |
| 1   | B     | 96    | ARG  | Sidechain |
| 1   | C     | 102   | ARG  | Sidechain |
| 1   | C     | 160   | ARG  | Sidechain |
| 1   | C     | 199   | ARG  | Sidechain |
| 1   | C     | 212   | ARG  | Sidechain |
| 1   | C     | 220   | ARG  | Sidechain |
| 1   | C     | 254   | ARG  | Sidechain |
| 1   | C     | 5     | ASP  | Sidechain |
| 1   | C     | 57[A] | ARG  | Sidechain |
| 1   | C     | 57[B] | ARG  | Sidechain |
| 1   | C     | 96    | ARG  | Sidechain |
| 1   | D     | 102   | ARG  | Sidechain |
| 1   | D     | 160   | ARG  | Sidechain |
| 1   | D     | 199   | ARG  | Sidechain |
| 1   | D     | 200   | ARG  | Sidechain |
| 1   | D     | 212   | ARG  | Sidechain |
| 1   | D     | 213   | ARG  | Sidechain |
| 1   | D     | 220   | ARG  | Sidechain |
| 1   | D     | 246   | ARG  | Sidechain |
| 1   | D     | 57[A] | ARG  | Sidechain |
| 1   | D     | 57[B] | ARG  | Sidechain |
| 1   | D     | 7     | ARG  | Sidechain |
| 1   | D     | 96    | ARG  | Sidechain |
| 1   | E     | 102   | ARG  | Sidechain |
| 1   | E     | 15    | ARG  | Sidechain |
| 1   | E     | 160   | ARG  | Sidechain |
| 1   | E     | 199   | ARG  | Sidechain |
| 1   | E     | 212   | ARG  | Sidechain |
| 1   | E     | 213   | ARG  | Sidechain |
| 1   | E     | 220   | ARG  | Sidechain |
| 1   | E     | 246   | ARG  | Sidechain |
| 1   | E     | 96    | ARG  | Sidechain |
| 1   | F     | 102   | ARG  | Sidechain |
| 1   | F     | 15    | ARG  | Sidechain |
| 1   | F     | 160   | ARG  | Sidechain |

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| Mol | Chain | Res   | Type | Group     |
|-----|-------|-------|------|-----------|
| 1   | F     | 199   | ARG  | Sidechain |
| 1   | F     | 212   | ARG  | Sidechain |
| 1   | F     | 220   | ARG  | Sidechain |
| 1   | F     | 5     | ASP  | Sidechain |
| 1   | F     | 57[A] | ARG  | Sidechain |
| 1   | F     | 57[B] | ARG  | Sidechain |
| 1   | F     | 96    | ARG  | Sidechain |
| 1   | G     | 1     | MET  | Peptide   |
| 1   | G     | 102   | ARG  | Sidechain |
| 1   | G     | 160   | ARG  | Sidechain |
| 1   | G     | 199   | ARG  | Sidechain |
| 1   | G     | 212   | ARG  | Sidechain |
| 1   | G     | 213   | ARG  | Sidechain |
| 1   | G     | 220   | ARG  | Sidechain |
| 1   | G     | 57[A] | ARG  | Sidechain |
| 1   | G     | 57[B] | ARG  | Sidechain |
| 1   | G     | 96    | ARG  | Sidechain |
| 1   | H     | 1     | MET  | Peptide   |
| 1   | H     | 102   | ARG  | Sidechain |
| 1   | H     | 160   | ARG  | Sidechain |
| 1   | H     | 199   | ARG  | Sidechain |
| 1   | H     | 212   | ARG  | Sidechain |
| 1   | H     | 213   | ARG  | Sidechain |
| 1   | H     | 220   | ARG  | Sidechain |
| 1   | H     | 246   | ARG  | Sidechain |
| 1   | H     | 57[A] | ARG  | Sidechain |
| 1   | H     | 57[B] | ARG  | Sidechain |
| 1   | H     | 96    | ARG  | Sidechain |
| 1   | I     | 102   | ARG  | Sidechain |
| 1   | I     | 160   | ARG  | Sidechain |
| 1   | I     | 199   | ARG  | Sidechain |
| 1   | I     | 212   | ARG  | Sidechain |
| 1   | I     | 220   | ARG  | Sidechain |
| 1   | I     | 246   | ARG  | Sidechain |
| 1   | I     | 96    | ARG  | Sidechain |
| 1   | J     | 102   | ARG  | Sidechain |
| 1   | J     | 160   | ARG  | Sidechain |
| 1   | J     | 199   | ARG  | Sidechain |
| 1   | J     | 200   | ARG  | Sidechain |
| 1   | J     | 212   | ARG  | Sidechain |
| 1   | J     | 213   | ARG  | Sidechain |
| 1   | J     | 220   | ARG  | Sidechain |

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| Mol | Chain | Res   | Type | Group     |
|-----|-------|-------|------|-----------|
| 1   | J     | 246   | ARG  | Sidechain |
| 1   | J     | 5     | ASP  | Sidechain |
| 1   | J     | 57[A] | ARG  | Sidechain |
| 1   | J     | 57[B] | ARG  | Sidechain |
| 1   | J     | 96    | ARG  | Sidechain |
| 1   | K     | 102   | ARG  | Sidechain |
| 1   | K     | 15    | ARG  | Sidechain |
| 1   | K     | 160   | ARG  | Sidechain |
| 1   | K     | 199   | ARG  | Sidechain |
| 1   | K     | 200   | ARG  | Sidechain |
| 1   | K     | 201   | ARG  | Sidechain |
| 1   | K     | 212   | ARG  | Sidechain |
| 1   | K     | 213   | ARG  | Sidechain |
| 1   | K     | 220   | ARG  | Sidechain |
| 1   | K     | 252   | ALA  | Peptide   |
| 1   | K     | 57[A] | ARG  | Sidechain |
| 1   | K     | 57[B] | ARG  | Sidechain |
| 1   | K     | 96    | ARG  | Sidechain |
| 1   | L     | 102   | ARG  | Sidechain |
| 1   | L     | 15    | ARG  | Sidechain |
| 1   | L     | 160   | ARG  | Sidechain |
| 1   | L     | 199   | ARG  | Sidechain |
| 1   | L     | 212   | ARG  | Sidechain |
| 1   | L     | 220   | ARG  | Sidechain |
| 1   | L     | 246   | ARG  | Sidechain |
| 1   | L     | 5     | ASP  | Sidechain |
| 1   | L     | 57[A] | ARG  | Sidechain |
| 1   | L     | 57[B] | ARG  | Sidechain |
| 1   | L     | 96    | ARG  | Sidechain |
| 1   | M     | 102   | ARG  | Sidechain |
| 1   | M     | 160   | ARG  | Sidechain |
| 1   | M     | 199   | ARG  | Sidechain |
| 1   | M     | 200   | ARG  | Sidechain |
| 1   | M     | 212   | ARG  | Sidechain |
| 1   | M     | 220   | ARG  | Sidechain |
| 1   | M     | 252   | ALA  | Peptide   |
| 1   | M     | 258   | ARG  | Sidechain |
| 1   | M     | 57[A] | ARG  | Sidechain |
| 1   | M     | 57[B] | ARG  | Sidechain |
| 1   | M     | 96    | ARG  | Sidechain |
| 1   | N     | 102   | ARG  | Sidechain |
| 1   | N     | 160   | ARG  | Sidechain |

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| Mol | Chain | Res   | Type | Group     |
|-----|-------|-------|------|-----------|
| 1   | N     | 199   | ARG  | Sidechain |
| 1   | N     | 200   | ARG  | Sidechain |
| 1   | N     | 212   | ARG  | Sidechain |
| 1   | N     | 220   | ARG  | Sidechain |
| 1   | N     | 258   | ARG  | Sidechain |
| 1   | N     | 57[A] | ARG  | Sidechain |
| 1   | N     | 57[B] | ARG  | Sidechain |
| 1   | N     | 96    | ARG  | Sidechain |
| 1   | O     | 102   | ARG  | Sidechain |
| 1   | O     | 160   | ARG  | Sidechain |
| 1   | O     | 199   | ARG  | Sidechain |
| 1   | O     | 200   | ARG  | Sidechain |
| 1   | O     | 212   | ARG  | Sidechain |
| 1   | O     | 220   | ARG  | Sidechain |
| 1   | O     | 246   | ARG  | Sidechain |
| 1   | O     | 57[A] | ARG  | Sidechain |
| 1   | O     | 57[B] | ARG  | Sidechain |
| 1   | O     | 96    | ARG  | Sidechain |
| 1   | P     | 102   | ARG  | Sidechain |
| 1   | P     | 160   | ARG  | Sidechain |
| 1   | P     | 199   | ARG  | Sidechain |
| 1   | P     | 200   | ARG  | Sidechain |
| 1   | P     | 212   | ARG  | Sidechain |
| 1   | P     | 220   | ARG  | Sidechain |
| 1   | P     | 246   | ARG  | Sidechain |
| 1   | P     | 57[A] | ARG  | Sidechain |
| 1   | P     | 57[B] | ARG  | Sidechain |
| 1   | P     | 96    | ARG  | Sidechain |
| 1   | Q     | 102   | ARG  | Sidechain |
| 1   | Q     | 15    | ARG  | Sidechain |
| 1   | Q     | 160   | ARG  | Sidechain |
| 1   | Q     | 199   | ARG  | Sidechain |
| 1   | Q     | 200   | ARG  | Sidechain |
| 1   | Q     | 201   | ARG  | Sidechain |
| 1   | Q     | 212   | ARG  | Sidechain |
| 1   | Q     | 213   | ARG  | Sidechain |
| 1   | Q     | 220   | ARG  | Sidechain |
| 1   | Q     | 96    | ARG  | Sidechain |
| 1   | R     | 102   | ARG  | Sidechain |
| 1   | R     | 160   | ARG  | Sidechain |
| 1   | R     | 199   | ARG  | Sidechain |
| 1   | R     | 200   | ARG  | Sidechain |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 1          | R            | 212        | ARG         | Sidechain    |
| 1          | R            | 220        | ARG         | Sidechain    |
| 1          | R            | 57[A]      | ARG         | Sidechain    |
| 1          | R            | 57[B]      | ARG         | Sidechain    |
| 1          | R            | 96         | ARG         | Sidechain    |
| 1          | S            | 102        | ARG         | Sidechain    |
| 1          | S            | 15         | ARG         | Sidechain    |
| 1          | S            | 160        | ARG         | Sidechain    |
| 1          | S            | 199        | ARG         | Sidechain    |
| 1          | S            | 200        | ARG         | Sidechain    |
| 1          | S            | 212        | ARG         | Sidechain    |
| 1          | S            | 213        | ARG         | Sidechain    |
| 1          | S            | 220        | ARG         | Sidechain    |
| 1          | S            | 246        | ARG         | Sidechain    |
| 1          | S            | 57[A]      | ARG         | Sidechain    |
| 1          | S            | 57[B]      | ARG         | Sidechain    |
| 1          | S            | 96         | ARG         | Sidechain    |
| 1          | T            | 102        | ARG         | Sidechain    |
| 1          | T            | 160        | ARG         | Sidechain    |
| 1          | T            | 199        | ARG         | Sidechain    |
| 1          | T            | 200        | ARG         | Sidechain    |
| 1          | T            | 212        | ARG         | Sidechain    |
| 1          | T            | 220        | ARG         | Sidechain    |
| 1          | T            | 246        | ARG         | Sidechain    |
| 1          | T            | 57[A]      | ARG         | Sidechain    |
| 1          | T            | 57[B]      | ARG         | Sidechain    |
| 1          | T            | 96         | ARG         | Sidechain    |
| 1          | U            | 102        | ARG         | Sidechain    |
| 1          | U            | 15         | ARG         | Sidechain    |
| 1          | U            | 160        | ARG         | Sidechain    |
| 1          | U            | 199        | ARG         | Sidechain    |
| 1          | U            | 212        | ARG         | Sidechain    |
| 1          | U            | 220        | ARG         | Sidechain    |
| 1          | U            | 246        | ARG         | Sidechain    |
| 1          | U            | 5          | ASP         | Sidechain    |
| 1          | U            | 57[A]      | ARG         | Sidechain    |
| 1          | U            | 57[B]      | ARG         | Sidechain    |
| 1          | U            | 96         | ARG         | Sidechain    |
| 1          | V            | 102        | ARG         | Sidechain    |
| 1          | V            | 160        | ARG         | Sidechain    |
| 1          | V            | 199        | ARG         | Sidechain    |
| 1          | V            | 200        | ARG         | Sidechain    |

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| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 1   | V     | 212    | ARG  | Sidechain |
| 1   | V     | 213    | ARG  | Sidechain |
| 1   | V     | 220    | ARG  | Sidechain |
| 1   | V     | 57[A]  | ARG  | Sidechain |
| 1   | V     | 57[B]  | ARG  | Sidechain |
| 1   | V     | 96     | ARG  | Sidechain |
| 1   | W     | 1      | MET  | Peptide   |
| 1   | W     | 102    | ARG  | Sidechain |
| 1   | W     | 15     | ARG  | Sidechain |
| 1   | W     | 199    | ARG  | Sidechain |
| 1   | W     | 212    | ARG  | Sidechain |
| 1   | W     | 220    | ARG  | Sidechain |
| 1   | W     | 258    | ARG  | Sidechain |
| 1   | W     | 57[A]  | ARG  | Sidechain |
| 1   | W     | 57[B]  | ARG  | Sidechain |
| 1   | W     | 96     | ARG  | Sidechain |
| 1   | X     | 102[A] | ARG  | Sidechain |
| 1   | X     | 160    | ARG  | Sidechain |
| 1   | X     | 17     | ALA  | Peptide   |
| 1   | X     | 199    | ARG  | Sidechain |
| 1   | X     | 200    | ARG  | Sidechain |
| 1   | X     | 212    | ARG  | Sidechain |
| 1   | X     | 220    | ARG  | Sidechain |
| 1   | X     | 57[A]  | ARG  | Sidechain |
| 1   | X     | 57[B]  | ARG  | Sidechain |
| 1   | Y     | 102    | ARG  | Sidechain |
| 1   | Y     | 199    | ARG  | Sidechain |
| 1   | Y     | 200    | ARG  | Sidechain |
| 1   | Y     | 212    | ARG  | Sidechain |
| 1   | Y     | 220    | ARG  | Sidechain |
| 1   | Y     | 96     | ARG  | Sidechain |
| 1   | Z     | 102    | ARG  | Sidechain |
| 1   | Z     | 160    | ARG  | Sidechain |
| 1   | Z     | 199    | ARG  | Sidechain |
| 1   | Z     | 212    | ARG  | Sidechain |
| 1   | Z     | 213    | ARG  | Sidechain |
| 1   | Z     | 220    | ARG  | Sidechain |
| 1   | Z     | 246    | ARG  | Sidechain |
| 1   | Z     | 258    | ARG  | Sidechain |
| 1   | Z     | 57[A]  | ARG  | Sidechain |
| 1   | Z     | 57[B]  | ARG  | Sidechain |
| 1   | Z     | 96     | ARG  | Sidechain |

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| Mol | Chain | Res   | Type | Group     |
|-----|-------|-------|------|-----------|
| 1   | a     | 102   | ARG  | Sidechain |
| 1   | a     | 160   | ARG  | Sidechain |
| 1   | a     | 199   | ARG  | Sidechain |
| 1   | a     | 200   | ARG  | Sidechain |
| 1   | a     | 212   | ARG  | Sidechain |
| 1   | a     | 213   | ARG  | Sidechain |
| 1   | a     | 220   | ARG  | Sidechain |
| 1   | a     | 246   | ARG  | Sidechain |
| 1   | a     | 258   | ARG  | Sidechain |
| 1   | a     | 57[A] | ARG  | Sidechain |
| 1   | a     | 57[B] | ARG  | Sidechain |
| 1   | a     | 96    | ARG  | Sidechain |
| 1   | b     | 102   | ARG  | Sidechain |
| 1   | b     | 160   | ARG  | Sidechain |
| 1   | b     | 199   | ARG  | Sidechain |
| 1   | b     | 200   | ARG  | Sidechain |
| 1   | b     | 212   | ARG  | Sidechain |
| 1   | b     | 220   | ARG  | Sidechain |
| 1   | b     | 246   | ARG  | Sidechain |
| 1   | b     | 258   | ARG  | Sidechain |
| 1   | b     | 57[A] | ARG  | Sidechain |
| 1   | b     | 57[B] | ARG  | Sidechain |
| 1   | b     | 96    | ARG  | Sidechain |
| 1   | c     | 102   | ARG  | Sidechain |
| 1   | c     | 160   | ARG  | Sidechain |
| 1   | c     | 199   | ARG  | Sidechain |
| 1   | c     | 200   | ARG  | Sidechain |
| 1   | c     | 212   | ARG  | Sidechain |
| 1   | c     | 213   | ARG  | Sidechain |
| 1   | c     | 220   | ARG  | Sidechain |
| 1   | c     | 57[A] | ARG  | Sidechain |
| 1   | c     | 57[B] | ARG  | Sidechain |
| 1   | c     | 96    | ARG  | Sidechain |
| 1   | d     | 102   | ARG  | Sidechain |
| 1   | d     | 160   | ARG  | Sidechain |
| 1   | d     | 199   | ARG  | Sidechain |
| 1   | d     | 212   | ARG  | Sidechain |
| 1   | d     | 213   | ARG  | Sidechain |
| 1   | d     | 220   | ARG  | Sidechain |
| 1   | d     | 258   | ARG  | Sidechain |
| 1   | d     | 57[A] | ARG  | Sidechain |
| 1   | d     | 57[B] | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | d     | 96  | ARG  | Sidechain |

## 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     | 1982  | 0        | 1960     | 20      | 0            |
| 1   | B     | 1982  | 0        | 1960     | 14      | 0            |
| 1   | C     | 1974  | 0        | 1948     | 24      | 0            |
| 1   | D     | 1974  | 0        | 1948     | 30      | 0            |
| 1   | E     | 1982  | 0        | 1960     | 24      | 0            |
| 1   | F     | 1974  | 0        | 1948     | 27      | 0            |
| 1   | G     | 1982  | 0        | 1960     | 21      | 0            |
| 1   | H     | 1982  | 0        | 1960     | 22      | 0            |
| 1   | I     | 1982  | 0        | 1960     | 13      | 0            |
| 1   | J     | 1974  | 0        | 1948     | 21      | 0            |
| 1   | K     | 1982  | 0        | 1960     | 23      | 0            |
| 1   | L     | 1982  | 0        | 1960     | 29      | 0            |
| 1   | M     | 1974  | 0        | 1948     | 23      | 0            |
| 1   | N     | 1974  | 0        | 1948     | 20      | 0            |
| 1   | O     | 1974  | 0        | 1948     | 19      | 0            |
| 1   | P     | 1974  | 0        | 1948     | 22      | 0            |
| 1   | Q     | 1974  | 0        | 1948     | 27      | 0            |
| 1   | R     | 1982  | 0        | 1960     | 30      | 0            |
| 1   | S     | 1982  | 0        | 1960     | 20      | 0            |
| 1   | T     | 1982  | 0        | 1960     | 16      | 0            |
| 1   | U     | 1992  | 0        | 1967     | 18      | 0            |
| 1   | V     | 1982  | 0        | 1960     | 21      | 0            |
| 1   | W     | 1982  | 0        | 1960     | 19      | 0            |
| 1   | X     | 2003  | 0        | 1979     | 20      | 0            |
| 1   | Y     | 1982  | 0        | 1960     | 16      | 0            |
| 1   | Z     | 2002  | 0        | 1975     | 28      | 0            |
| 1   | a     | 1974  | 0        | 1948     | 25      | 0            |
| 1   | b     | 1974  | 0        | 1948     | 17      | 0            |
| 1   | c     | 1974  | 0        | 1948     | 27      | 0            |
| 1   | d     | 2002  | 0        | 1975     | 25      | 0            |
| 2   | A     | 29    | 0        | 0        | 0       | 0            |
| 2   | B     | 29    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | C     | 29    | 0        | 0        | 1       | 0            |
| 2   | D     | 29    | 0        | 0        | 0       | 0            |
| 2   | E     | 29    | 0        | 0        | 0       | 0            |
| 2   | F     | 29    | 0        | 0        | 1       | 0            |
| 2   | G     | 29    | 0        | 0        | 0       | 0            |
| 2   | H     | 29    | 0        | 0        | 0       | 0            |
| 2   | I     | 29    | 0        | 0        | 0       | 0            |
| 2   | J     | 29    | 0        | 0        | 0       | 0            |
| 2   | K     | 29    | 0        | 0        | 0       | 0            |
| 2   | L     | 29    | 0        | 0        | 0       | 0            |
| 2   | M     | 29    | 0        | 0        | 1       | 0            |
| 2   | N     | 29    | 0        | 0        | 0       | 0            |
| 2   | O     | 29    | 0        | 0        | 0       | 0            |
| 2   | P     | 29    | 0        | 0        | 0       | 0            |
| 2   | Q     | 29    | 0        | 0        | 0       | 0            |
| 2   | R     | 29    | 0        | 0        | 0       | 0            |
| 2   | S     | 29    | 0        | 0        | 0       | 0            |
| 2   | T     | 29    | 0        | 0        | 0       | 0            |
| 2   | U     | 29    | 0        | 0        | 1       | 0            |
| 2   | V     | 29    | 0        | 0        | 0       | 0            |
| 2   | W     | 29    | 0        | 0        | 0       | 0            |
| 2   | X     | 29    | 0        | 0        | 1       | 0            |
| 2   | Y     | 29    | 0        | 0        | 1       | 0            |
| 2   | Z     | 29    | 0        | 0        | 0       | 0            |
| 2   | a     | 29    | 0        | 0        | 0       | 0            |
| 2   | b     | 29    | 0        | 0        | 0       | 0            |
| 2   | c     | 29    | 0        | 0        | 0       | 0            |
| 2   | d     | 29    | 0        | 0        | 1       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 13    | 0        | 0        | 0       | 0            |
| 4   | B     | 19    | 0        | 0        | 1       | 0            |
| 4   | C     | 21    | 0        | 0        | 2       | 0            |
| 4   | D     | 23    | 0        | 0        | 1       | 0            |
| 4   | E     | 16    | 0        | 0        | 0       | 0            |
| 4   | F     | 12    | 0        | 0        | 0       | 0            |
| 4   | G     | 2     | 0        | 0        | 0       | 0            |
| 4   | H     | 7     | 0        | 0        | 2       | 0            |
| 4   | I     | 9     | 0        | 0        | 0       | 0            |
| 4   | J     | 6     | 0        | 0        | 3       | 0            |
| 4   | K     | 9     | 0        | 0        | 0       | 0            |
| 4   | L     | 8     | 0        | 0        | 1       | 0            |
| 4   | M     | 14    | 0        | 0        | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | N     | 8     | 0        | 0        | 0       | 0            |
| 4   | O     | 15    | 0        | 0        | 2       | 0            |
| 4   | P     | 5     | 0        | 0        | 3       | 0            |
| 4   | Q     | 11    | 0        | 0        | 0       | 0            |
| 4   | R     | 10    | 0        | 0        | 3       | 0            |
| 4   | S     | 15    | 0        | 0        | 2       | 0            |
| 4   | T     | 17    | 0        | 0        | 0       | 0            |
| 4   | U     | 19    | 0        | 0        | 1       | 0            |
| 4   | V     | 13    | 0        | 0        | 1       | 0            |
| 4   | W     | 12    | 0        | 0        | 0       | 0            |
| 4   | X     | 19    | 0        | 0        | 3       | 0            |
| 4   | Y     | 24    | 0        | 0        | 0       | 0            |
| 4   | Z     | 23    | 0        | 0        | 5       | 0            |
| 4   | a     | 26    | 0        | 0        | 0       | 0            |
| 4   | b     | 14    | 0        | 0        | 0       | 0            |
| 4   | c     | 9     | 0        | 0        | 0       | 0            |
| 4   | d     | 23    | 0        | 0        | 2       | 0            |
| All | All   | 60728 | 0        | 58712    | 503     | 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 4.

All (503) 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:X:246:ARG:HG2  | 1:X:246:ARG:HH11 | 1.30                     | 0.97              |
| 1:G:246:ARG:HG2  | 1:G:246:ARG:HH11 | 1.30                     | 0.96              |
| 1:K:246:ARG:HH11 | 1:K:246:ARG:HG2  | 1.30                     | 0.96              |
| 1:a:246:ARG:HH11 | 1:a:246:ARG:HG2  | 1.28                     | 0.96              |
| 1:L:246:ARG:HG2  | 1:L:246:ARG:HH11 | 1.30                     | 0.96              |
| 1:O:246:ARG:HG2  | 1:O:246:ARG:HH11 | 1.30                     | 0.96              |
| 1:Z:169:MET:HE2  | 1:a:156:HIS:CD2  | 2.00                     | 0.96              |
| 1:D:246:ARG:HG2  | 1:D:246:ARG:HH11 | 1.29                     | 0.96              |
| 1:R:246:ARG:HH11 | 1:R:246:ARG:HG2  | 1.30                     | 0.95              |
| 1:b:246:ARG:HG2  | 1:b:246:ARG:HH11 | 1.30                     | 0.95              |
| 1:N:246:ARG:HG2  | 1:N:246:ARG:HH11 | 1.30                     | 0.95              |
| 1:Q:246:ARG:HG2  | 1:Q:246:ARG:HH11 | 1.29                     | 0.95              |
| 1:V:246:ARG:HG2  | 1:V:246:ARG:HH11 | 1.30                     | 0.95              |
| 1:C:246:ARG:HH11 | 1:C:246:ARG:HG2  | 1.30                     | 0.95              |
| 1:H:246:ARG:HH11 | 1:H:246:ARG:HG2  | 1.30                     | 0.95              |
| 1:M:246:ARG:HH11 | 1:M:246:ARG:HG2  | 1.30                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:246:ARG:HH11 | 1:c:246:ARG:HG2  | 1.31                     | 0.94              |
| 1:F:246:ARG:HH11 | 1:F:246:ARG:HG2  | 1.31                     | 0.94              |
| 1:d:246:ARG:HG2  | 1:d:246:ARG:HH11 | 1.31                     | 0.94              |
| 1:A:246:ARG:HH11 | 1:A:246:ARG:HG2  | 1.29                     | 0.94              |
| 1:E:246:ARG:HG2  | 1:E:246:ARG:HH11 | 1.31                     | 0.94              |
| 1:Y:246:ARG:HH11 | 1:Y:246:ARG:HG2  | 1.31                     | 0.93              |
| 1:Z:246:ARG:HG2  | 1:Z:246:ARG:HH11 | 1.30                     | 0.93              |
| 1:J:246:ARG:HG2  | 1:J:246:ARG:HH11 | 1.30                     | 0.93              |
| 1:W:246:ARG:HH11 | 1:W:246:ARG:HG2  | 1.30                     | 0.93              |
| 1:S:246:ARG:HG2  | 1:S:246:ARG:HH11 | 1.31                     | 0.93              |
| 1:T:246:ARG:HH11 | 1:T:246:ARG:HG2  | 1.30                     | 0.93              |
| 1:A:156:HIS:CD2  | 1:C:169:MET:HE2  | 2.04                     | 0.93              |
| 1:U:246:ARG:HG2  | 1:U:246:ARG:HH11 | 1.30                     | 0.92              |
| 1:P:246:ARG:HG2  | 1:P:246:ARG:HH11 | 1.30                     | 0.92              |
| 1:F:254:ARG:HH11 | 1:L:160:ARG:HD3  | 1.39                     | 0.88              |
| 1:b:156:HIS:CD2  | 1:d:169:MET:HE2  | 2.08                     | 0.87              |
| 1:b:169:MET:HE2  | 1:c:156:HIS:CD2  | 2.09                     | 0.86              |
| 1:Q:169:MET:HE2  | 1:R:156:HIS:CD2  | 2.11                     | 0.84              |
| 1:M:169:MET:HE2  | 1:N:156:HIS:CD2  | 2.13                     | 0.83              |
| 1:T:114:MET:HE3  | 1:U:69:PRO:HG2   | 1.58                     | 0.83              |
| 1:D:7:ARG:HH21   | 1:D:7:ARG:CG     | 1.92                     | 0.82              |
| 1:F:160:ARG:HD2  | 1:L:254:ARG:HH11 | 1.41                     | 0.82              |
| 1:N:254:ARG:HH11 | 1:Q:160:ARG:HD2  | 1.41                     | 0.82              |
| 1:Y:169:MET:HE2  | 1:Z:156:HIS:CD2  | 2.14                     | 0.82              |
| 1:Y:9:ILE:HD11   | 1:a:7:ARG:CZ     | 2.10                     | 0.82              |
| 1:W:114:MET:HE3  | 1:X:69:PRO:HG2   | 1.64                     | 0.79              |
| 1:D:169:MET:HE2  | 1:E:156:HIS:CD2  | 2.18                     | 0.79              |
| 1:P:156:HIS:CD2  | 1:R:169:MET:HE2  | 2.17                     | 0.79              |
| 1:J:114:MET:HE3  | 1:K:69:PRO:HG2   | 1.67                     | 0.77              |
| 1:U:160:ARG:NH2  | 4:U:301:HOH:O    | 2.18                     | 0.76              |
| 1:V:156:HIS:CD2  | 1:X:169:MET:HE2  | 2.19                     | 0.76              |
| 1:D:69:PRO:HG2   | 1:F:114:MET:HE3  | 1.68                     | 0.75              |
| 1:P:69:PRO:HG2   | 1:R:114:MET:HE3  | 1.68                     | 0.75              |
| 1:F:254:ARG:NH1  | 1:L:160:ARG:HD3  | 2.01                     | 0.75              |
| 1:N:68:THR:HG21  | 1:N:121:HIS:ND1  | 2.02                     | 0.74              |
| 1:F:68:THR:HG21  | 1:F:121:HIS:ND1  | 2.03                     | 0.74              |
| 1:G:68:THR:HG21  | 1:G:121:HIS:ND1  | 2.03                     | 0.74              |
| 1:J:68:THR:HG21  | 1:J:121:HIS:ND1  | 2.03                     | 0.74              |
| 1:R:68:THR:HG21  | 1:R:121:HIS:ND1  | 2.02                     | 0.74              |
| 1:V:258:ARG:HG3  | 1:V:258:ARG:HH11 | 1.53                     | 0.74              |
| 1:D:68:THR:HG21  | 1:D:121:HIS:ND1  | 2.03                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:K:68:THR:HG21   | 1:K:121:HIS:ND1    | 2.03                     | 0.74              |
| 1:W:68:THR:HG21   | 1:W:121:HIS:ND1    | 2.03                     | 0.74              |
| 1:C:68:THR:HG21   | 1:C:121:HIS:ND1    | 2.03                     | 0.73              |
| 1:L:68:THR:HG21   | 1:L:121:HIS:ND1    | 2.03                     | 0.73              |
| 1:B:68:THR:HG21   | 1:B:121:HIS:ND1    | 2.03                     | 0.73              |
| 1:I:68:THR:HG21   | 1:I:121:HIS:ND1    | 2.03                     | 0.73              |
| 1:Q:68:THR:HG21   | 1:Q:121:HIS:ND1    | 2.02                     | 0.73              |
| 1:d:68:THR:HG21   | 1:d:121:HIS:ND1    | 2.03                     | 0.73              |
| 1:V:68:THR:HG21   | 1:V:121:HIS:ND1    | 2.03                     | 0.73              |
| 1:H:68:THR:HG21   | 1:H:121:HIS:ND1    | 2.02                     | 0.73              |
| 1:A:68:THR:HG21   | 1:A:121:HIS:ND1    | 2.03                     | 0.73              |
| 1:M:102:ARG:NH2   | 1:Z:101:ASP:O      | 2.21                     | 0.73              |
| 1:Z:114:MET:HE3   | 1:a:69:PRO:HG2     | 1.70                     | 0.73              |
| 1:c:68:THR:HG21   | 1:c:121:HIS:ND1    | 2.03                     | 0.73              |
| 1:K:114:MET:HE3   | 1:L:69:PRO:HG2     | 1.71                     | 0.72              |
| 1:E:160:ARG:HD2   | 1:S:254:ARG:HH11   | 1.52                     | 0.72              |
| 1:b:114:MET:HE3   | 1:c:69:PRO:HG2     | 1.70                     | 0.72              |
| 1:D:160:ARG:HD2   | 1:P:254:ARG:HH11   | 1.54                     | 0.72              |
| 1:Y:156:HIS:CD2   | 1:a:169:MET:HE2    | 2.24                     | 0.72              |
| 1:E:15:ARG:NH2    | 1:E:33:GLU:OE2     | 2.23                     | 0.72              |
| 1:D:114:MET:HE3   | 1:E:69:PRO:HG2     | 1.72                     | 0.71              |
| 1:K:169:MET:HE2   | 1:L:156:HIS:CD2    | 2.25                     | 0.70              |
| 1:V:169:MET:HE2   | 1:W:156:HIS:CD2    | 2.26                     | 0.70              |
| 1:J:254:ARG:HH11  | 1:c:160:ARG:HD2    | 1.55                     | 0.70              |
| 1:N:160:ARG:HD2   | 1:Q:254:ARG:HH11   | 1.56                     | 0.70              |
| 1:Z:235:SER:CB    | 4:Z:1110:HOH:O     | 2.40                     | 0.70              |
| 1:Z:235:SER:HB3   | 4:Z:1110:HOH:O     | 1.91                     | 0.69              |
| 1:E:169:MET:HE2   | 1:F:156:HIS:CD2    | 2.26                     | 0.69              |
| 1:C:254:ARG:HH11  | 1:C:254:ARG:HB3    | 1.57                     | 0.68              |
| 1:X:220:ARG:NH2   | 4:X:1101:HOH:O     | 2.27                     | 0.68              |
| 1:H:169:MET:HE2   | 1:I:156:HIS:CD2    | 2.28                     | 0.67              |
| 1:K:15:ARG:NH2    | 1:K:33:GLU:OE2     | 2.26                     | 0.67              |
| 1:Q:15:ARG:NH2    | 1:Q:33:GLU:OE2     | 2.28                     | 0.67              |
| 1:X:57[B]:ARG:HG3 | 1:X:57[B]:ARG:HH21 | 1.60                     | 0.66              |
| 1:Y:69:PRO:HG2    | 1:a:114:MET:HE3    | 1.76                     | 0.66              |
| 1:d:246:ARG:HH11  | 1:d:246:ARG:CG     | 2.08                     | 0.66              |
| 1:M:69:PRO:HG2    | 1:O:114:MET:HE3    | 1.77                     | 0.66              |
| 1:S:69:PRO:HG2    | 1:U:114:MET:HE3    | 1.76                     | 0.66              |
| 1:I:15:ARG:NH2    | 1:I:33:GLU:OE2     | 2.29                     | 0.66              |
| 1:O:246:ARG:HH11  | 1:O:246:ARG:CG     | 2.08                     | 0.66              |
| 1:S:114:MET:HE3   | 1:T:69:PRO:HG2     | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:156:HIS:CD2  | 1:L:169:MET:HE2  | 2.31                     | 0.66              |
| 1:V:69:PRO:HG2   | 1:X:114:MET:HE3  | 1.77                     | 0.66              |
| 1:D:156:HIS:CD2  | 1:F:169:MET:HE2  | 2.30                     | 0.66              |
| 1:G:1:MET:HG3    | 1:G:2:SER:O      | 1.95                     | 0.66              |
| 1:F:246:ARG:HH11 | 1:F:246:ARG:CG   | 2.08                     | 0.66              |
| 1:B:160:ARG:HD2  | 1:O:254:ARG:HH11 | 1.60                     | 0.65              |
| 1:Q:114:MET:HE3  | 1:R:69:PRO:HG2   | 1.76                     | 0.65              |
| 1:G:258:ARG:HG3  | 1:G:258:ARG:HH11 | 1.62                     | 0.65              |
| 1:Y:246:ARG:HH11 | 1:Y:246:ARG:CG   | 2.08                     | 0.65              |
| 1:b:246:ARG:HH11 | 1:b:246:ARG:CG   | 2.07                     | 0.65              |
| 1:c:246:ARG:HH11 | 1:c:246:ARG:CG   | 2.08                     | 0.65              |
| 1:X:246:ARG:HH11 | 1:X:246:ARG:CG   | 2.07                     | 0.65              |
| 1:N:246:ARG:HH11 | 1:N:246:ARG:CG   | 2.08                     | 0.65              |
| 1:R:254:ARG:HH11 | 1:W:160:ARG:HD2  | 1.62                     | 0.65              |
| 1:W:246:ARG:HH11 | 1:W:246:ARG:CG   | 2.07                     | 0.65              |
| 1:G:246:ARG:HH11 | 1:G:246:ARG:CG   | 2.08                     | 0.65              |
| 1:Q:196:GLU:OE2  | 1:Q:200:ARG:NH2  | 2.29                     | 0.65              |
| 1:V:258:ARG:HH11 | 1:V:258:ARG:CG   | 2.09                     | 0.65              |
| 1:X:15:ARG:NH2   | 1:X:33:GLU:OE2   | 2.30                     | 0.65              |
| 1:B:114:MET:HE3  | 1:C:69:PRO:HG2   | 1.79                     | 0.64              |
| 1:M:246:ARG:HH11 | 1:M:246:ARG:CG   | 2.08                     | 0.64              |
| 1:A:114:MET:HE3  | 1:B:69:PRO:HG2   | 1.78                     | 0.64              |
| 1:N:43:HIS:CE1   | 1:O:43:HIS:HD2   | 2.15                     | 0.64              |
| 1:M:156:HIS:CD2  | 1:O:169:MET:HE2  | 2.32                     | 0.64              |
| 1:S:156:HIS:CD2  | 1:U:169:MET:HE2  | 2.31                     | 0.64              |
| 1:N:169:MET:HE2  | 1:O:156:HIS:CD2  | 2.33                     | 0.64              |
| 1:S:15:ARG:NH2   | 1:S:33:GLU:OE2   | 2.31                     | 0.64              |
| 1:V:246:ARG:HH11 | 1:V:246:ARG:CG   | 2.08                     | 0.64              |
| 1:D:7:ARG:HH21   | 1:D:7:ARG:HG3    | 1.63                     | 0.64              |
| 1:U:246:ARG:HH11 | 1:U:246:ARG:CG   | 2.08                     | 0.64              |
| 1:N:114:MET:HE3  | 1:O:69:PRO:HG2   | 1.79                     | 0.64              |
| 1:Y:63:SER:HB3   | 1:a:60:GLN:HE21  | 1.63                     | 0.64              |
| 1:a:246:ARG:HH11 | 1:a:246:ARG:CG   | 2.07                     | 0.64              |
| 1:S:235:SER:HB3  | 4:S:1103:HOH:O   | 1.98                     | 0.63              |
| 1:b:9:ILE:HG12   | 1:d:7:ARG:HH12   | 1.62                     | 0.63              |
| 1:A:246:ARG:HH11 | 1:A:246:ARG:CG   | 2.07                     | 0.63              |
| 1:J:160:ARG:HD2  | 1:c:254:ARG:HH11 | 1.63                     | 0.63              |
| 1:K:246:ARG:HH11 | 1:K:246:ARG:CG   | 2.08                     | 0.63              |
| 1:W:15:ARG:NH2   | 1:W:33:GLU:OE2   | 2.31                     | 0.63              |
| 1:E:114:MET:HE3  | 1:F:69:PRO:HG2   | 1.81                     | 0.63              |
| 1:Y:9:ILE:HD11   | 1:a:7:ARG:NH1    | 2.14                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:246:ARG:HH11 | 1:Z:246:ARG:CG   | 2.08                     | 0.63              |
| 1:H:1:MET:HG3    | 1:H:2:SER:O      | 1.99                     | 0.63              |
| 1:Y:114:MET:HE3  | 1:Z:69:PRO:HG2   | 1.79                     | 0.63              |
| 1:A:15:ARG:NH2   | 1:A:33:GLU:OE2   | 2.31                     | 0.63              |
| 1:D:246:ARG:HH11 | 1:D:246:ARG:CG   | 2.08                     | 0.63              |
| 1:G:69:PRO:HG2   | 1:I:114:MET:HE3  | 1.81                     | 0.62              |
| 1:a:72:LYS:HG2   | 1:a:100:GLN:NE2  | 2.15                     | 0.62              |
| 1:C:246:ARG:HH11 | 1:C:246:ARG:CG   | 2.08                     | 0.62              |
| 1:J:246:ARG:HH11 | 1:J:246:ARG:CG   | 2.08                     | 0.62              |
| 1:S:246:ARG:HH11 | 1:S:246:ARG:CG   | 2.08                     | 0.61              |
| 1:Z:7:ARG:HH12   | 1:a:9:ILE:HG12   | 1.65                     | 0.61              |
| 1:L:246:ARG:HH11 | 1:L:246:ARG:CG   | 2.07                     | 0.61              |
| 1:P:246:ARG:HH11 | 1:P:246:ARG:CG   | 2.08                     | 0.61              |
| 1:S:235:SER:CB   | 4:S:1103:HOH:O   | 2.48                     | 0.61              |
| 1:P:114:MET:HE3  | 1:Q:69:PRO:HG2   | 1.80                     | 0.61              |
| 1:V:102:ARG:NH1  | 1:V:106:THR:CG2  | 2.63                     | 0.61              |
| 1:W:169:MET:HE2  | 1:X:156:HIS:CD2  | 2.36                     | 0.61              |
| 1:H:246:ARG:HH11 | 1:H:246:ARG:CG   | 2.08                     | 0.61              |
| 1:A:69:PRO:HG2   | 1:C:114:MET:HE3  | 1.81                     | 0.60              |
| 1:J:246:ARG:CD   | 4:J:1101:HOH:O   | 2.49                     | 0.60              |
| 1:E:246:ARG:HH11 | 1:E:246:ARG:CG   | 2.08                     | 0.60              |
| 1:P:15:ARG:NH2   | 1:P:33:GLU:OE2   | 2.34                     | 0.60              |
| 1:F:15:ARG:NH2   | 1:F:33:GLU:OE2   | 2.34                     | 0.59              |
| 1:F:225:VAL:HG11 | 1:F:253:THR:HG21 | 1.84                     | 0.59              |
| 1:J:169:MET:HE2  | 1:K:156:HIS:CD2  | 2.37                     | 0.59              |
| 1:Z:70:ASP:HB3   | 1:Z:72:LYS:HG2   | 1.84                     | 0.59              |
| 1:N:246:ARG:HG2  | 1:N:246:ARG:NH1  | 2.09                     | 0.59              |
| 1:T:15:ARG:NH2   | 1:T:33:GLU:OE2   | 2.34                     | 0.59              |
| 1:U:18:ALA:O     | 1:U:19:ASP:OD1   | 2.21                     | 0.59              |
| 1:D:7:ARG:HH21   | 1:D:7:ARG:HG2    | 1.64                     | 0.59              |
| 1:R:246:ARG:HH11 | 1:R:246:ARG:CG   | 2.08                     | 0.59              |
| 1:M:254:ARG:HH11 | 1:Z:160:ARG:HD2  | 1.66                     | 0.59              |
| 1:X:235:SER:HB3  | 4:X:1102:HOH:O   | 2.02                     | 0.59              |
| 1:V:63:SER:HB3   | 1:X:60:GLN:HE21  | 1.67                     | 0.59              |
| 1:D:60:GLN:HE21  | 1:E:63:SER:HB3   | 1.68                     | 0.58              |
| 1:T:246:ARG:HH11 | 1:T:246:ARG:CG   | 2.08                     | 0.58              |
| 1:d:68:THR:CG2   | 4:d:1110:HOH:O   | 2.50                     | 0.58              |
| 1:T:213:ARG:HB3  | 1:T:213:ARG:HH21 | 1.68                     | 0.58              |
| 1:D:225:VAL:HG11 | 1:D:253:THR:HG21 | 1.86                     | 0.58              |
| 1:E:225:VAL:HG11 | 1:E:253:THR:HG21 | 1.85                     | 0.58              |
| 1:V:258:ARG:CG   | 1:V:258:ARG:NH1  | 2.64                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:254:ARG:HH11 | 1:C:254:ARG:CB   | 2.16                     | 0.58              |
| 2:Y:1001:VFE:C3  | 2:Y:1001:VFE:C13 | 2.82                     | 0.58              |
| 1:c:79:ARG:NH2   | 1:c:104:GLU:OE2  | 2.37                     | 0.58              |
| 1:L:258:ARG:NH1  | 4:L:1101:HOH:O   | 2.29                     | 0.57              |
| 1:A:60:GLN:HE21  | 1:B:63:SER:HB3   | 1.69                     | 0.57              |
| 1:X:18:ALA:O     | 1:X:19:ASP:OD1   | 2.21                     | 0.57              |
| 1:a:72:LYS:HG2   | 1:a:100:GLN:HE21 | 1.67                     | 0.57              |
| 1:Q:246:ARG:HH11 | 1:Q:246:ARG:CG   | 2.08                     | 0.57              |
| 1:D:160:ARG:HD2  | 1:P:254:ARG:NH1  | 2.18                     | 0.57              |
| 1:T:60:GLN:HE21  | 1:U:63:SER:HB3   | 1.69                     | 0.57              |
| 1:T:225:VAL:HG11 | 1:T:253:THR:HG21 | 1.86                     | 0.57              |
| 2:C:1001:VFE:C3  | 2:C:1001:VFE:C13 | 2.83                     | 0.57              |
| 1:O:253:THR:HG23 | 1:O:253:THR:O    | 2.05                     | 0.57              |
| 1:P:7:ARG:CZ     | 1:Q:9:ILE:HD11   | 2.34                     | 0.57              |
| 1:V:104:GLU:HG2  | 1:V:106:THR:HG22 | 1.87                     | 0.57              |
| 1:b:253:THR:O    | 1:b:253:THR:HG23 | 2.04                     | 0.57              |
| 1:D:246:ARG:HG2  | 1:D:246:ARG:NH1  | 2.09                     | 0.57              |
| 1:N:254:ARG:NH1  | 1:Q:160:ARG:HD2  | 2.17                     | 0.57              |
| 1:B:104:GLU:HG2  | 1:B:106:THR:HG22 | 1.86                     | 0.57              |
| 1:A:169:MET:HE2  | 1:B:156:HIS:CD2  | 2.40                     | 0.56              |
| 1:H:104:GLU:HG2  | 1:H:106:THR:HG22 | 1.87                     | 0.56              |
| 1:R:104:GLU:HG2  | 1:R:106:THR:HG22 | 1.87                     | 0.56              |
| 1:J:253:THR:HG23 | 1:J:253:THR:O    | 2.06                     | 0.56              |
| 1:S:104:GLU:HG2  | 1:S:106:THR:HG22 | 1.87                     | 0.56              |
| 1:A:104:GLU:HG2  | 1:A:106:THR:HG22 | 1.87                     | 0.56              |
| 1:G:225:VAL:HG11 | 1:G:253:THR:HG21 | 1.87                     | 0.56              |
| 1:M:104:GLU:HG2  | 1:M:106:THR:HG22 | 1.87                     | 0.56              |
| 1:N:104:GLU:HG2  | 1:N:106:THR:HG22 | 1.87                     | 0.56              |
| 1:S:63:SER:HB3   | 1:U:60:GLN:HE21  | 1.68                     | 0.56              |
| 1:V:246:ARG:CD   | 4:V:1101:HOH:O   | 2.54                     | 0.56              |
| 1:Q:225:VAL:HG11 | 1:Q:253:THR:HG21 | 1.88                     | 0.56              |
| 1:S:225:VAL:HG11 | 1:S:253:THR:HG21 | 1.88                     | 0.56              |
| 1:V:15:ARG:NH2   | 1:V:33:GLU:OE2   | 2.38                     | 0.56              |
| 1:C:225:VAL:HG11 | 1:C:253:THR:HG21 | 1.86                     | 0.56              |
| 1:G:7:ARG:CZ     | 1:H:9:ILE:HD11   | 2.36                     | 0.56              |
| 1:K:7:ARG:CZ     | 1:L:9:ILE:HD11   | 2.35                     | 0.56              |
| 1:M:63:SER:HB3   | 1:O:60:GLN:HE21  | 1.71                     | 0.56              |
| 1:D:246:ARG:NH1  | 1:D:247:ASP:OD1  | 2.39                     | 0.56              |
| 1:L:104:GLU:HG2  | 1:L:106:THR:HG22 | 1.87                     | 0.56              |
| 1:A:246:ARG:NH1  | 1:A:247:ASP:OD1  | 2.39                     | 0.56              |
| 1:O:246:ARG:NH1  | 1:O:247:ASP:OD1  | 2.40                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:169:MET:HE2  | 1:Q:156:HIS:CD2  | 2.41                     | 0.55              |
| 1:T:246:ARG:NH1  | 1:T:247:ASP:OD1  | 2.39                     | 0.55              |
| 1:b:60:GLN:HE21  | 1:c:63:SER:HB3   | 1.70                     | 0.55              |
| 1:C:104:GLU:HG2  | 1:C:106:THR:HG22 | 1.88                     | 0.55              |
| 1:I:104:GLU:HG2  | 1:I:106:THR:HG22 | 1.88                     | 0.55              |
| 1:K:104:GLU:HG2  | 1:K:106:THR:HG22 | 1.87                     | 0.55              |
| 1:c:246:ARG:NH1  | 1:c:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:b:246:ARG:NH1  | 1:b:247:ASP:OD1  | 2.39                     | 0.55              |
| 1:G:104:GLU:HG2  | 1:G:106:THR:HG22 | 1.88                     | 0.55              |
| 1:Q:104:GLU:HG2  | 1:Q:106:THR:HG22 | 1.88                     | 0.55              |
| 1:d:246:ARG:NH1  | 1:d:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:J:104:GLU:HG2  | 1:J:106:THR:HG22 | 1.88                     | 0.55              |
| 1:V:246:ARG:NH1  | 1:V:247:ASP:OD1  | 2.39                     | 0.55              |
| 1:d:104:GLU:HG2  | 1:d:106:THR:HG22 | 1.87                     | 0.55              |
| 1:C:246:ARG:NH1  | 1:C:247:ASP:OD1  | 2.39                     | 0.55              |
| 1:G:246:ARG:NH1  | 1:G:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:M:246:ARG:NH1  | 1:M:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:O:104:GLU:HG2  | 1:O:106:THR:HG22 | 1.87                     | 0.55              |
| 1:Q:246:ARG:NH1  | 1:Q:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:W:104:GLU:HG2  | 1:W:106:THR:HG22 | 1.88                     | 0.55              |
| 1:X:246:ARG:NH1  | 1:X:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:a:246:ARG:NH1  | 1:a:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:B:60:GLN:HE21  | 1:C:63:SER:HB3   | 1.71                     | 0.55              |
| 1:H:246:ARG:NH1  | 1:H:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:P:246:ARG:NH1  | 1:P:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:E:60:GLN:HE21  | 1:F:63:SER:HB3   | 1.71                     | 0.55              |
| 1:E:246:ARG:NH1  | 1:E:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:K:246:ARG:NH1  | 1:K:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:N:246:ARG:NH1  | 1:N:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:P:104:GLU:HG2  | 1:P:106:THR:HG22 | 1.87                     | 0.55              |
| 1:R:246:ARG:NH1  | 1:R:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:T:169:MET:HE2  | 1:U:156:HIS:CD2  | 2.42                     | 0.55              |
| 1:A:225:VAL:HG11 | 1:A:253:THR:HG21 | 1.88                     | 0.55              |
| 1:Z:246:ARG:NH1  | 1:Z:247:ASP:OD1  | 2.40                     | 0.55              |
| 1:H:253:THR:HG23 | 1:H:253:THR:O    | 2.07                     | 0.54              |
| 1:T:104:GLU:HG2  | 1:T:106:THR:HG22 | 1.88                     | 0.54              |
| 1:A:63:SER:HB3   | 1:C:60:GLN:HE21  | 1.72                     | 0.54              |
| 1:F:104:GLU:HG2  | 1:F:106:THR:HG22 | 1.88                     | 0.54              |
| 1:F:231:GLU:OE2  | 1:K:212:ARG:NH2  | 2.39                     | 0.54              |
| 1:L:246:ARG:NH1  | 1:L:247:ASP:OD1  | 2.40                     | 0.54              |
| 1:C:246:ARG:HG2  | 1:C:246:ARG:NH1  | 2.10                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:246:ARG:NH1   | 1:J:247:ASP:OD1   | 2.40                     | 0.54              |
| 1:U:246:ARG:NH1   | 1:U:247:ASP:OD1   | 2.40                     | 0.54              |
| 1:D:5:ASP:OD1     | 1:D:7:ARG:HG3     | 2.07                     | 0.54              |
| 1:D:5:ASP:OD1     | 1:D:7:ARG:NH2     | 2.40                     | 0.54              |
| 1:F:246:ARG:NH1   | 1:F:247:ASP:OD1   | 2.40                     | 0.54              |
| 1:W:246:ARG:NH1   | 1:W:247:ASP:OD1   | 2.40                     | 0.54              |
| 1:Y:246:ARG:NH1   | 1:Y:247:ASP:OD1   | 2.40                     | 0.54              |
| 1:G:258:ARG:HG3   | 1:G:258:ARG:NH1   | 2.23                     | 0.54              |
| 1:C:235:SER:HB3   | 4:C:1103:HOH:O    | 2.08                     | 0.54              |
| 1:M:246:ARG:HG2   | 1:M:246:ARG:NH1   | 2.09                     | 0.54              |
| 1:T:7:ARG:CZ      | 1:U:9:ILE:HD11    | 2.38                     | 0.54              |
| 1:b:63:SER:HB3    | 1:d:60:GLN:HE21   | 1.72                     | 0.54              |
| 1:S:246:ARG:NH1   | 1:S:247:ASP:OD1   | 2.40                     | 0.53              |
| 1:Q:57[B]:ARG:NH2 | 1:Q:57[B]:ARG:HG2 | 2.24                     | 0.53              |
| 1:U:253:THR:HG23  | 1:U:253:THR:O     | 2.08                     | 0.53              |
| 1:c:246:ARG:HG2   | 1:c:246:ARG:NH1   | 2.10                     | 0.53              |
| 1:L:225:VAL:HG11  | 1:L:253:THR:HG21  | 1.90                     | 0.53              |
| 1:V:60:GLN:HE21   | 1:W:63:SER:HB3    | 1.73                     | 0.53              |
| 1:a:225:VAL:HG11  | 1:a:253:THR:HG21  | 1.90                     | 0.53              |
| 1:E:164:HIS:HE1   | 1:E:201:ARG:HG3   | 1.73                     | 0.53              |
| 1:I:1:MET:HG2     | 1:I:2:SER:O       | 2.08                     | 0.53              |
| 1:d:57[B]:ARG:NH2 | 1:d:57[B]:ARG:CG  | 2.71                     | 0.53              |
| 1:G:258:ARG:HH11  | 1:G:258:ARG:CG    | 2.21                     | 0.53              |
| 1:c:104:GLU:OE1   | 1:c:106:THR:CG2   | 2.57                     | 0.53              |
| 1:D:5:ASP:OD1     | 1:D:7:ARG:CG      | 2.57                     | 0.53              |
| 1:G:114:MET:HE3   | 1:H:69:PRO:HG2    | 1.91                     | 0.52              |
| 1:Y:253:THR:HG23  | 1:Y:253:THR:O     | 2.09                     | 0.52              |
| 1:B:7:ARG:HH12    | 1:C:9:ILE:HG12    | 1.73                     | 0.52              |
| 1:P:9:ILE:HG23    | 1:P:27:ILE:HG12   | 1.91                     | 0.52              |
| 1:P:253:THR:HA    | 4:P:1105:HOH:O    | 2.09                     | 0.52              |
| 1:C:160:ARG:HD2   | 1:K:254:ARG:HH11  | 1.74                     | 0.52              |
| 1:E:164:HIS:CE1   | 1:E:201:ARG:HG3   | 2.45                     | 0.52              |
| 1:B:254:ARG:O     | 1:O:175:LYS:HG2   | 2.10                     | 0.52              |
| 1:H:258:ARG:NH1   | 4:H:1101:HOH:O    | 2.30                     | 0.52              |
| 1:J:246:ARG:HD2   | 4:J:1101:HOH:O    | 2.07                     | 0.52              |
| 1:E:1:MET:HG2     | 1:E:2:SER:O       | 2.10                     | 0.51              |
| 1:c:60:GLN:HE21   | 1:d:63:SER:HB3    | 1.75                     | 0.51              |
| 1:d:246:ARG:HG2   | 1:d:246:ARG:NH1   | 2.11                     | 0.51              |
| 1:G:169:MET:HE2   | 1:H:156:HIS:CD2   | 2.45                     | 0.51              |
| 1:L:72:LYS:HD2    | 1:L:100:GLN:HG2   | 1.93                     | 0.51              |
| 1:B:254:ARG:HH11  | 1:O:160:ARG:HD3   | 1.75                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:246:ARG:HG2   | 1:A:246:ARG:NH1    | 2.08                     | 0.51              |
| 1:V:114:MET:HE3   | 1:W:69:PRO:HG2     | 1.91                     | 0.51              |
| 1:W:253:THR:HG22  | 1:W:253:THR:O      | 2.11                     | 0.51              |
| 1:X:1:MET:HE3     | 1:X:2:SER:O        | 2.11                     | 0.51              |
| 1:I:253:THR:HG23  | 1:I:253:THR:O      | 2.11                     | 0.51              |
| 1:J:63:SER:HB3    | 1:L:60:GLN:HE21    | 1.76                     | 0.51              |
| 1:K:72:LYS:HD2    | 1:K:100:GLN:CG     | 2.41                     | 0.51              |
| 1:M:60:GLN:HE21   | 1:N:63:SER:HB3     | 1.77                     | 0.50              |
| 1:R:72:LYS:HD2    | 1:R:100:GLN:CG     | 2.41                     | 0.50              |
| 1:G:9:ILE:HD11    | 1:I:7:ARG:CZ       | 2.42                     | 0.50              |
| 1:M:235:SER:HB3   | 4:M:1102:HOH:O     | 2.10                     | 0.50              |
| 1:K:72:LYS:HD2    | 1:K:100:GLN:HG2    | 1.94                     | 0.50              |
| 1:L:246:ARG:HG2   | 1:L:246:ARG:NH1    | 2.09                     | 0.50              |
| 1:C:164:HIS:HE1   | 1:C:201:ARG:HG3    | 1.76                     | 0.50              |
| 1:Y:60:GLN:HE21   | 1:Z:63:SER:HB3     | 1.76                     | 0.50              |
| 1:R:253:THR:HG23  | 1:R:253:THR:O      | 2.10                     | 0.50              |
| 1:Q:57[B]:ARG:HG2 | 1:Q:57[B]:ARG:HH21 | 1.77                     | 0.50              |
| 1:R:72:LYS:HD2    | 1:R:100:GLN:HG2    | 1.93                     | 0.50              |
| 1:d:201:ARG:NE    | 4:d:1101:HOH:O     | 2.40                     | 0.50              |
| 1:P:63:SER:HB3    | 1:R:60:GLN:HE21    | 1.77                     | 0.49              |
| 1:X:253:THR:HG22  | 1:X:253:THR:O      | 2.11                     | 0.49              |
| 1:Z:70:ASP:CG     | 1:Z:72:LYS:HG2     | 2.37                     | 0.49              |
| 1:D:7:ARG:CG      | 1:D:7:ARG:NH2      | 2.64                     | 0.49              |
| 1:V:246:ARG:HG2   | 1:V:246:ARG:NH1    | 2.09                     | 0.49              |
| 1:X:57[A]:ARG:HD2 | 1:X:59:TYR:CE1     | 2.47                     | 0.49              |
| 1:Z:169:MET:HE2   | 1:a:156:HIS:NE2    | 2.27                     | 0.49              |
| 1:d:253:THR:O     | 1:d:253:THR:HG23   | 2.11                     | 0.49              |
| 1:F:160:ARG:HD2   | 1:L:254:ARG:NH1    | 2.18                     | 0.49              |
| 1:b:9:ILE:CG1     | 1:d:7:ARG:HH12     | 2.25                     | 0.49              |
| 1:N:60:GLN:HE21   | 1:O:63:SER:HB3     | 1.77                     | 0.49              |
| 1:P:246:ARG:HD2   | 4:P:1101:HOH:O     | 2.11                     | 0.49              |
| 1:C:164:HIS:CE1   | 1:C:201:ARG:HG3    | 2.46                     | 0.49              |
| 1:K:246:ARG:HG2   | 1:K:246:ARG:NH1    | 2.09                     | 0.49              |
| 1:V:253:THR:HG22  | 1:V:253:THR:O      | 2.12                     | 0.49              |
| 1:W:60:GLN:HE21   | 1:X:63:SER:HB3     | 1.78                     | 0.49              |
| 1:D:61:PHE:CZ     | 1:E:61:PHE:HA      | 2.48                     | 0.49              |
| 1:P:60:GLN:HE21   | 1:Q:63:SER:HB3     | 1.77                     | 0.49              |
| 1:Z:235:SER:HB2   | 4:Z:1110:HOH:O     | 2.10                     | 0.49              |
| 1:J:69:PRO:HG2    | 1:L:114:MET:HE3    | 1.95                     | 0.49              |
| 1:F:102:ARG:NH2   | 1:L:102:ARG:HG3    | 2.28                     | 0.48              |
| 1:W:7:ARG:CZ      | 1:X:9:ILE:HD11     | 2.42                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:Z:-2:GLY:O      | 1:Z:7:ARG:NH2      | 2.46                     | 0.48              |
| 1:B:169:MET:HE2   | 1:C:156:HIS:CD2    | 2.48                     | 0.48              |
| 1:Q:246:ARG:HG2   | 1:Q:246:ARG:NH1    | 2.08                     | 0.48              |
| 1:Z:169:MET:CE    | 1:a:156:HIS:CD2    | 2.88                     | 0.48              |
| 1:G:63:SER:HB3    | 1:I:60:GLN:HE21    | 1.78                     | 0.48              |
| 1:R:102:ARG:O     | 1:R:102:ARG:HG3    | 2.12                     | 0.48              |
| 1:L:72:LYS:HD2    | 1:L:100:GLN:CG     | 2.44                     | 0.48              |
| 1:b:7:ARG:CZ      | 1:c:9:ILE:HD11     | 2.44                     | 0.48              |
| 1:C:254:ARG:O     | 1:K:175:LYS:HG2    | 2.13                     | 0.48              |
| 1:M:9:ILE:HD11    | 1:O:7:ARG:CZ       | 2.43                     | 0.48              |
| 1:d:57[B]:ARG:NH2 | 1:d:57[B]:ARG:HG3  | 2.28                     | 0.48              |
| 1:S:164:HIS:CE1   | 1:S:201:ARG:HG3    | 2.49                     | 0.48              |
| 1:P:246:ARG:CD    | 4:P:1101:HOH:O     | 2.61                     | 0.48              |
| 1:Y:9:ILE:CD1     | 1:a:7:ARG:CZ       | 2.89                     | 0.47              |
| 1:V:164:HIS:CE1   | 1:V:201:ARG:HG3    | 2.50                     | 0.47              |
| 1:M:235:SER:CB    | 4:M:1102:HOH:O     | 2.62                     | 0.47              |
| 1:O:235:SER:CB    | 4:O:1103:HOH:O     | 2.63                     | 0.47              |
| 1:D:25:TRP:CZ2    | 1:E:25:TRP:HA      | 2.50                     | 0.47              |
| 2:F:1001:VFE:C3   | 2:F:1001:VFE:C13   | 2.92                     | 0.47              |
| 1:H:246:ARG:HG2   | 1:H:246:ARG:NH1    | 2.09                     | 0.47              |
| 1:S:169:MET:HE2   | 1:T:156:HIS:CD2    | 2.50                     | 0.47              |
| 1:c:253:THR:HG22  | 1:c:253:THR:O      | 2.13                     | 0.47              |
| 1:K:60:GLN:HE21   | 1:L:63:SER:HB3     | 1.79                     | 0.47              |
| 1:M:7:ARG:NH1     | 1:N:9:ILE:HD11     | 2.29                     | 0.47              |
| 1:D:164:HIS:CE1   | 1:D:201:ARG:HG3    | 2.50                     | 0.47              |
| 1:G:60:GLN:HE21   | 1:H:63:SER:HB3     | 1.80                     | 0.47              |
| 1:L:15:ARG:NH1    | 1:L:33:GLU:HB2     | 2.30                     | 0.47              |
| 1:P:253:THR:HG22  | 1:P:253:THR:O      | 2.15                     | 0.47              |
| 1:S:60:GLN:HE21   | 1:T:63:SER:HB3     | 1.80                     | 0.47              |
| 1:D:7:ARG:CZ      | 1:E:9:ILE:HD11     | 2.45                     | 0.47              |
| 1:E:231:GLU:OE2   | 1:U:212:ARG:NH2    | 2.47                     | 0.47              |
| 1:U:164:HIS:CE1   | 1:U:201:ARG:HG3    | 2.51                     | 0.47              |
| 1:S:164:HIS:HE1   | 1:S:201:ARG:HG3    | 1.80                     | 0.46              |
| 1:R:164:HIS:CE1   | 1:R:201:ARG:HG3    | 2.50                     | 0.46              |
| 1:L:15:ARG:HH11   | 1:L:15:ARG:HB2     | 1.80                     | 0.46              |
| 1:M:7:ARG:CZ      | 1:N:9:ILE:HD11     | 2.45                     | 0.46              |
| 1:Q:60:GLN:HE21   | 1:R:63:SER:HB3     | 1.79                     | 0.46              |
| 1:R:235:SER:HB3   | 4:R:1102:HOH:O     | 2.15                     | 0.46              |
| 1:Z:60:GLN:HE21   | 1:a:63:SER:HB3     | 1.81                     | 0.46              |
| 1:d:57[B]:ARG:CG  | 1:d:57[B]:ARG:HH21 | 2.28                     | 0.46              |
| 1:J:7:ARG:CZ      | 1:K:9:ILE:HD11     | 2.46                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:63:SER:HB3    | 1:F:60:GLN:HE21  | 1.80                     | 0.46              |
| 1:P:9:ILE:CG2     | 1:P:27:ILE:HG12  | 2.46                     | 0.46              |
| 1:R:164:HIS:HE1   | 1:R:201:ARG:HG3  | 1.80                     | 0.46              |
| 1:S:246:ARG:HG2   | 1:S:246:ARG:NH1  | 2.10                     | 0.46              |
| 1:c:104:GLU:OE1   | 1:c:106:THR:HG22 | 2.16                     | 0.46              |
| 1:C:235:SER:CB    | 4:C:1103:HOH:O   | 2.64                     | 0.46              |
| 1:T:246:ARG:HG2   | 1:T:246:ARG:NH1  | 2.10                     | 0.46              |
| 1:G:246:ARG:HG2   | 1:G:246:ARG:NH1  | 2.10                     | 0.46              |
| 1:H:164:HIS:CE1   | 1:H:201:ARG:HG3  | 2.51                     | 0.46              |
| 1:R:235:SER:CB    | 4:R:1102:HOH:O   | 2.63                     | 0.46              |
| 1:Z:253:THR:HG23  | 1:Z:253:THR:O    | 2.16                     | 0.46              |
| 1:C:72:LYS:HD2    | 1:C:100:GLN:HG2  | 1.98                     | 0.45              |
| 1:Y:25:TRP:HA     | 1:a:25:TRP:CZ2   | 2.52                     | 0.45              |
| 1:K:57[A]:ARG:HG2 | 1:K:59:TYR:CE1   | 2.51                     | 0.45              |
| 1:V:164:HIS:HE1   | 1:V:201:ARG:HG3  | 1.81                     | 0.45              |
| 1:W:164:HIS:HE1   | 1:W:201:ARG:HG3  | 1.81                     | 0.45              |
| 1:a:15:ARG:NH1    | 1:a:33:GLU:HB2   | 2.31                     | 0.45              |
| 1:B:253:THR:O     | 1:B:253:THR:HG23 | 2.15                     | 0.45              |
| 1:J:258:ARG:NH1   | 4:J:1102:HOH:O   | 2.49                     | 0.45              |
| 1:F:246:ARG:HG2   | 1:F:246:ARG:NH1  | 2.10                     | 0.45              |
| 1:Q:164:HIS:HE1   | 1:Q:201:ARG:HG2  | 1.81                     | 0.45              |
| 1:c:164:HIS:CE1   | 1:c:201:ARG:HG3  | 2.51                     | 0.45              |
| 1:F:102:ARG:HH21  | 1:L:102:ARG:HG3  | 1.82                     | 0.45              |
| 1:d:164:HIS:CE1   | 1:d:201:ARG:HG3  | 2.52                     | 0.45              |
| 1:X:246:ARG:HG2   | 1:X:246:ARG:NH1  | 2.09                     | 0.45              |
| 1:U:21:GLN:HE21   | 1:U:21:GLN:HB2   | 1.49                     | 0.45              |
| 1:Z:7:ARG:HH12    | 1:a:9:ILE:CG1    | 2.30                     | 0.45              |
| 1:c:164:HIS:HE1   | 1:c:201:ARG:HG3  | 1.82                     | 0.44              |
| 1:W:164:HIS:CE1   | 1:W:201:ARG:HG3  | 2.52                     | 0.44              |
| 1:D:164:HIS:HE1   | 1:D:201:ARG:HG3  | 1.82                     | 0.44              |
| 1:H:60:GLN:HE21   | 1:I:63:SER:HB3   | 1.82                     | 0.44              |
| 1:M:249:ILE:O     | 1:M:253:THR:OG1  | 2.35                     | 0.44              |
| 1:R:51:LYS:HE2    | 4:R:1108:HOH:O   | 2.17                     | 0.44              |
| 1:R:258:ARG:NH2   | 1:W:218:VAL:O    | 2.50                     | 0.44              |
| 1:b:246:ARG:HG2   | 1:b:246:ARG:NH1  | 2.10                     | 0.44              |
| 1:M:246:ARG:CG    | 1:M:246:ARG:NH1  | 2.75                     | 0.44              |
| 1:c:7:ARG:CZ      | 1:d:9:ILE:HD11   | 2.48                     | 0.44              |
| 1:a:72:LYS:HD2    | 1:a:100:GLN:HE21 | 1.82                     | 0.44              |
| 1:E:246:ARG:HG2   | 1:E:246:ARG:NH1  | 2.10                     | 0.44              |
| 1:A:196:GLU:OE1   | 1:A:199:ARG:NH1  | 2.51                     | 0.44              |
| 1:Q:169:MET:HE2   | 1:R:156:HIS:NE2  | 2.33                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:U:164:HIS:HE1    | 1:U:201:ARG:HG3   | 1.83                     | 0.44              |
| 1:H:164:HIS:HE1    | 1:H:201:ARG:HG3   | 1.82                     | 0.43              |
| 1:J:60:GLN:HE21    | 1:K:63:SER:HB3    | 1.83                     | 0.43              |
| 1:L:57[A]:ARG:HD2  | 1:L:59:TYR:CE1    | 2.54                     | 0.43              |
| 1:L:209:HIS:HB2    | 1:c:238:GLN:NE2   | 2.33                     | 0.43              |
| 1:Y:9:ILE:CD1      | 1:a:7:ARG:NH1     | 2.80                     | 0.43              |
| 1:O:246:ARG:HG2    | 1:O:246:ARG:NH1   | 2.10                     | 0.43              |
| 1:Q:164:HIS:CE1    | 1:Q:201:ARG:HG2   | 2.53                     | 0.43              |
| 1:Q:246:ARG:CG     | 1:Q:246:ARG:NH1   | 2.75                     | 0.43              |
| 1:Z:70:ASP:CB      | 1:Z:72:LYS:HG2    | 2.46                     | 0.43              |
| 1:c:114:MET:HE3    | 1:d:69:PRO:HG2    | 2.00                     | 0.43              |
| 1:a:246:ARG:CG     | 1:a:246:ARG:NH1   | 2.75                     | 0.43              |
| 1:b:156:HIS:NE2    | 1:d:169:MET:HE2   | 2.33                     | 0.43              |
| 1:D:7:ARG:HH11     | 1:E:9:ILE:HG12    | 1.83                     | 0.43              |
| 1:H:246:ARG:HD2    | 4:H:1102:HOH:O    | 2.17                     | 0.43              |
| 1:Z:7:ARG:CZ       | 1:a:9:ILE:HD11    | 2.48                     | 0.43              |
| 1:D:9:ILE:HG12     | 1:F:7:ARG:HH12    | 1.83                     | 0.43              |
| 1:K:72:LYS:CD      | 1:K:100:GLN:HG3   | 2.49                     | 0.43              |
| 1:Z:220:ARG:NH2    | 4:Z:1105:HOH:O    | 2.52                     | 0.43              |
| 4:D:1107:HOH:O     | 1:R:199:ARG:HD2   | 2.19                     | 0.43              |
| 1:L:212:ARG:NH2    | 1:c:231:GLU:CD    | 2.76                     | 0.43              |
| 1:d:164:HIS:HE1    | 1:d:201:ARG:HG3   | 1.82                     | 0.43              |
| 1:O:235:SER:HB2    | 4:O:1103:HOH:O    | 2.17                     | 0.43              |
| 1:A:160:ARG:HD2    | 1:H:254:ARG:HH11  | 1.84                     | 0.43              |
| 1:d:57[B]:ARG:HH21 | 1:d:57[B]:ARG:HG2 | 1.83                     | 0.43              |
| 1:F:164:HIS:CE1    | 1:F:201:ARG:HG3   | 2.54                     | 0.42              |
| 1:D:7:ARG:NH1      | 1:E:9:ILE:HG12    | 2.35                     | 0.42              |
| 1:H:114:MET:HE3    | 1:I:69:PRO:HG2    | 2.00                     | 0.42              |
| 1:M:133:ASN:HB2    | 2:M:1001:VFE:C27  | 2.48                     | 0.42              |
| 1:X:235:SER:CB     | 4:X:1102:HOH:O    | 2.64                     | 0.42              |
| 1:b:25:TRP:CZ2     | 1:c:25:TRP:HA     | 2.55                     | 0.42              |
| 1:P:246:ARG:HG2    | 1:P:246:ARG:NH1   | 2.09                     | 0.42              |
| 1:N:164:HIS:CE1    | 1:N:201:ARG:HG3   | 2.55                     | 0.42              |
| 1:E:61:PHE:CZ      | 1:F:61:PHE:HA     | 2.55                     | 0.42              |
| 1:Q:169:MET:CE     | 1:R:156:HIS:CD2   | 2.94                     | 0.42              |
| 1:c:246:ARG:CG     | 1:c:246:ARG:NH1   | 2.76                     | 0.42              |
| 1:A:164:HIS:CE1    | 1:A:201:ARG:HG3   | 2.55                     | 0.42              |
| 1:B:258:ARG:NH1    | 4:B:1102:HOH:O    | 2.53                     | 0.42              |
| 2:U:1001:VFE:C13   | 2:U:1001:VFE:C3   | 2.98                     | 0.42              |
| 2:X:1001:VFE:C13   | 2:X:1001:VFE:C3   | 2.97                     | 0.42              |
| 1:F:164:HIS:HE1    | 1:F:201:ARG:HG3   | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:9:ILE:HD11   | 1:I:7:ARG:NH1    | 2.35                     | 0.41              |
| 1:A:156:HIS:NE2  | 1:C:169:MET:HE2  | 2.33                     | 0.41              |
| 1:J:254:ARG:NH1  | 1:c:160:ARG:HD2  | 2.28                     | 0.41              |
| 1:Z:48:GLY:O     | 4:Z:1101:HOH:O   | 2.22                     | 0.41              |
| 1:b:61:PHE:CZ    | 1:c:61:PHE:HA    | 2.54                     | 0.41              |
| 1:Q:7:ARG:CZ     | 1:R:9:ILE:HD11   | 2.50                     | 0.41              |
| 1:R:254:ARG:NH1  | 1:W:160:ARG:HD2  | 2.30                     | 0.41              |
| 1:Z:246:ARG:HG2  | 1:Z:246:ARG:NH1  | 2.09                     | 0.41              |
| 1:M:175:LYS:HG2  | 1:Z:254:ARG:O    | 2.21                     | 0.41              |
| 1:N:246:ARG:CG   | 1:N:246:ARG:NH1  | 2.75                     | 0.41              |
| 1:A:74:LYS:HA    | 1:A:74:LYS:HD3   | 2.00                     | 0.41              |
| 1:A:164:HIS:HE1  | 1:A:201:ARG:HG3  | 1.85                     | 0.41              |
| 1:F:231:GLU:CD   | 1:K:212:ARG:NH2  | 2.78                     | 0.41              |
| 1:H:246:ARG:CG   | 1:H:246:ARG:NH1  | 2.75                     | 0.41              |
| 1:H:249:ILE:O    | 1:H:253:THR:HG22 | 2.21                     | 0.41              |
| 1:I:164:HIS:CE1  | 1:I:201:ARG:HG3  | 2.56                     | 0.41              |
| 1:J:246:ARG:CG   | 1:J:246:ARG:NH1  | 2.75                     | 0.41              |
| 1:L:72:LYS:CD    | 1:L:100:GLN:HG3  | 2.51                     | 0.41              |
| 1:M:114:MET:HE3  | 1:N:69:PRO:HG2   | 2.03                     | 0.41              |
| 1:d:132:VAL:HG11 | 2:d:1001:VFE:O20 | 2.20                     | 0.41              |
| 1:E:254:ARG:HH11 | 1:S:160:ARG:HD2  | 1.86                     | 0.41              |
| 1:G:246:ARG:CG   | 1:G:246:ARG:NH1  | 2.76                     | 0.41              |
| 1:F:72:LYS:O     | 1:F:74:LYS:HD2   | 2.21                     | 0.40              |
| 1:R:72:LYS:CD    | 1:R:100:GLN:HG3  | 2.50                     | 0.40              |
| 1:R:246:ARG:HG2  | 1:R:246:ARG:NH1  | 2.09                     | 0.40              |
| 1:M:89:ARG:HH11  | 1:M:89:ARG:HD3   | 1.77                     | 0.40              |
| 1:S:246:ARG:CG   | 1:S:246:ARG:NH1  | 2.76                     | 0.40              |
| 1:b:249:ILE:O    | 1:b:253:THR:HG22 | 2.20                     | 0.40              |
| 1:G:164:HIS:CE1  | 1:G:201:ARG:HG3  | 2.56                     | 0.40              |
| 1:T:196:GLU:OE2  | 1:T:199:ARG:NH1  | 2.55                     | 0.40              |
| 1:Y:89:ARG:HH11  | 1:Y:89:ARG:HD3   | 1.76                     | 0.40              |
| 1:c:169:MET:HE2  | 1:d:156:HIS:CD2  | 2.56                     | 0.40              |
| 1:D:231:GLU:OE2  | 1:R:212:ARG:NH2  | 2.50                     | 0.40              |
| 1:J:249:ILE:O    | 1:J:253:THR:HG22 | 2.21                     | 0.40              |
| 1:P:164:HIS:CE1  | 1:P:201:ARG:HG3  | 2.56                     | 0.40              |
| 1:U:89:ARG:HH11  | 1:U:89:ARG:HD3   | 1.77                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 257/261 (98%) | 246 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | B     | 257/261 (98%) | 247 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | C     | 256/261 (98%) | 246 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | D     | 256/261 (98%) | 246 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | E     | 257/261 (98%) | 246 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | F     | 256/261 (98%) | 246 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | G     | 257/261 (98%) | 247 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | H     | 257/261 (98%) | 246 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | I     | 257/261 (98%) | 245 (95%) | 12 (5%) | 0        | 100         | 100 |
| 1   | J     | 256/261 (98%) | 245 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | K     | 257/261 (98%) | 247 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | L     | 257/261 (98%) | 246 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | M     | 256/261 (98%) | 245 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | N     | 256/261 (98%) | 245 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | O     | 256/261 (98%) | 245 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | P     | 256/261 (98%) | 245 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | Q     | 256/261 (98%) | 246 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | R     | 257/261 (98%) | 246 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | S     | 257/261 (98%) | 247 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | T     | 257/261 (98%) | 247 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | U     | 258/261 (99%) | 245 (95%) | 13 (5%) | 0        | 100         | 100 |
| 1   | V     | 257/261 (98%) | 248 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 1   | W     | 257/261 (98%) | 247 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | X     | 259/261 (99%) | 246 (95%) | 13 (5%) | 0        | 100         | 100 |
| 1   | Y     | 257/261 (98%) | 247 (96%) | 10 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | Z     | 260/261 (100%)  | 251 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 1   | a     | 256/261 (98%)   | 246 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 1   | b     | 256/261 (98%)   | 244 (95%)  | 12 (5%)  | 0        | 100         | 100 |
| 1   | c     | 256/261 (98%)   | 245 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| 1   | d     | 260/261 (100%)  | 249 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| All | All   | 7707/7830 (98%) | 7387 (96%) | 320 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 207/208 (100%) | 191 (92%) | 16 (8%)  | 12          | 26 |
| 1   | B     | 207/208 (100%) | 188 (91%) | 19 (9%)  | 8           | 19 |
| 1   | C     | 206/208 (99%)  | 188 (91%) | 18 (9%)  | 9           | 21 |
| 1   | D     | 206/208 (99%)  | 185 (90%) | 21 (10%) | 7           | 15 |
| 1   | E     | 207/208 (100%) | 191 (92%) | 16 (8%)  | 12          | 26 |
| 1   | F     | 206/208 (99%)  | 191 (93%) | 15 (7%)  | 13          | 28 |
| 1   | G     | 207/208 (100%) | 187 (90%) | 20 (10%) | 8           | 17 |
| 1   | H     | 207/208 (100%) | 192 (93%) | 15 (7%)  | 13          | 28 |
| 1   | I     | 207/208 (100%) | 193 (93%) | 14 (7%)  | 14          | 31 |
| 1   | J     | 206/208 (99%)  | 189 (92%) | 17 (8%)  | 10          | 23 |
| 1   | K     | 207/208 (100%) | 187 (90%) | 20 (10%) | 8           | 17 |
| 1   | L     | 207/208 (100%) | 186 (90%) | 21 (10%) | 7           | 15 |
| 1   | M     | 206/208 (99%)  | 189 (92%) | 17 (8%)  | 10          | 23 |
| 1   | N     | 206/208 (99%)  | 189 (92%) | 17 (8%)  | 10          | 23 |
| 1   | O     | 206/208 (99%)  | 192 (93%) | 14 (7%)  | 14          | 31 |
| 1   | P     | 206/208 (99%)  | 186 (90%) | 20 (10%) | 8           | 17 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | Q     | 206/208 (99%)   | 189 (92%)  | 17 (8%)  | 10          | 23 |
| 1   | R     | 207/208 (100%)  | 184 (89%)  | 23 (11%) | 6           | 12 |
| 1   | S     | 207/208 (100%)  | 188 (91%)  | 19 (9%)  | 8           | 19 |
| 1   | T     | 207/208 (100%)  | 188 (91%)  | 19 (9%)  | 8           | 19 |
| 1   | U     | 208/208 (100%)  | 194 (93%)  | 14 (7%)  | 15          | 31 |
| 1   | V     | 207/208 (100%)  | 187 (90%)  | 20 (10%) | 8           | 17 |
| 1   | W     | 207/208 (100%)  | 190 (92%)  | 17 (8%)  | 10          | 23 |
| 1   | X     | 209/208 (100%)  | 190 (91%)  | 19 (9%)  | 9           | 20 |
| 1   | Y     | 207/208 (100%)  | 188 (91%)  | 19 (9%)  | 8           | 19 |
| 1   | Z     | 209/208 (100%)  | 191 (91%)  | 18 (9%)  | 10          | 21 |
| 1   | a     | 206/208 (99%)   | 189 (92%)  | 17 (8%)  | 10          | 23 |
| 1   | b     | 206/208 (99%)   | 185 (90%)  | 21 (10%) | 7           | 15 |
| 1   | c     | 206/208 (99%)   | 187 (91%)  | 19 (9%)  | 8           | 19 |
| 1   | d     | 209/208 (100%)  | 188 (90%)  | 21 (10%) | 7           | 16 |
| All | All   | 6205/6240 (99%) | 5662 (91%) | 543 (9%) | 10          | 21 |

All (543) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | SER  |
| 1   | A     | 15  | ARG  |
| 1   | A     | 51  | LYS  |
| 1   | A     | 63  | SER  |
| 1   | A     | 68  | THR  |
| 1   | A     | 71  | LEU  |
| 1   | A     | 72  | LYS  |
| 1   | A     | 90  | GLU  |
| 1   | A     | 102 | ARG  |
| 1   | A     | 106 | THR  |
| 1   | A     | 175 | LYS  |
| 1   | A     | 193 | MET  |
| 1   | A     | 196 | GLU  |
| 1   | A     | 199 | ARG  |
| 1   | A     | 212 | ARG  |
| 1   | A     | 246 | ARG  |
| 1   | B     | 1   | MET  |
| 1   | B     | 15  | ARG  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | B     | 51    | LYS  |
| 1   | B     | 57[A] | ARG  |
| 1   | B     | 57[B] | ARG  |
| 1   | B     | 63    | SER  |
| 1   | B     | 68    | THR  |
| 1   | B     | 74    | LYS  |
| 1   | B     | 90    | GLU  |
| 1   | B     | 100   | GLN  |
| 1   | B     | 106   | THR  |
| 1   | B     | 160   | ARG  |
| 1   | B     | 175   | LYS  |
| 1   | B     | 193   | MET  |
| 1   | B     | 196   | GLU  |
| 1   | B     | 199   | ARG  |
| 1   | B     | 212   | ARG  |
| 1   | B     | 226   | GLU  |
| 1   | B     | 258   | ARG  |
| 1   | C     | 2     | SER  |
| 1   | C     | 15    | ARG  |
| 1   | C     | 57[A] | ARG  |
| 1   | C     | 57[B] | ARG  |
| 1   | C     | 63    | SER  |
| 1   | C     | 68    | THR  |
| 1   | C     | 71    | LEU  |
| 1   | C     | 74    | LYS  |
| 1   | C     | 90    | GLU  |
| 1   | C     | 100   | GLN  |
| 1   | C     | 106   | THR  |
| 1   | C     | 175   | LYS  |
| 1   | C     | 193   | MET  |
| 1   | C     | 196   | GLU  |
| 1   | C     | 199   | ARG  |
| 1   | C     | 212   | ARG  |
| 1   | C     | 246   | ARG  |
| 1   | C     | 254   | ARG  |
| 1   | D     | 2     | SER  |
| 1   | D     | 3     | LEU  |
| 1   | D     | 4     | ILE  |
| 1   | D     | 7     | ARG  |
| 1   | D     | 15    | ARG  |
| 1   | D     | 57[A] | ARG  |
| 1   | D     | 57[B] | ARG  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | D     | 63    | SER  |
| 1   | D     | 68    | THR  |
| 1   | D     | 71    | LEU  |
| 1   | D     | 72    | LYS  |
| 1   | D     | 74    | LYS  |
| 1   | D     | 90    | GLU  |
| 1   | D     | 102   | ARG  |
| 1   | D     | 175   | LYS  |
| 1   | D     | 193   | MET  |
| 1   | D     | 196   | GLU  |
| 1   | D     | 199   | ARG  |
| 1   | D     | 212   | ARG  |
| 1   | D     | 246   | ARG  |
| 1   | D     | 258   | ARG  |
| 1   | E     | 2     | SER  |
| 1   | E     | 51    | LYS  |
| 1   | E     | 57[A] | ARG  |
| 1   | E     | 57[B] | ARG  |
| 1   | E     | 63    | SER  |
| 1   | E     | 71    | LEU  |
| 1   | E     | 74    | LYS  |
| 1   | E     | 90    | GLU  |
| 1   | E     | 100   | GLN  |
| 1   | E     | 175   | LYS  |
| 1   | E     | 193   | MET  |
| 1   | E     | 196   | GLU  |
| 1   | E     | 199   | ARG  |
| 1   | E     | 212   | ARG  |
| 1   | E     | 246   | ARG  |
| 1   | E     | 258   | ARG  |
| 1   | F     | 2     | SER  |
| 1   | F     | 51    | LYS  |
| 1   | F     | 63    | SER  |
| 1   | F     | 68    | THR  |
| 1   | F     | 74    | LYS  |
| 1   | F     | 90    | GLU  |
| 1   | F     | 100   | GLN  |
| 1   | F     | 106   | THR  |
| 1   | F     | 175   | LYS  |
| 1   | F     | 193   | MET  |
| 1   | F     | 196   | GLU  |
| 1   | F     | 199   | ARG  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | F     | 212   | ARG  |
| 1   | F     | 246   | ARG  |
| 1   | F     | 256   | ILE  |
| 1   | G     | 2     | SER  |
| 1   | G     | 15    | ARG  |
| 1   | G     | 51    | LYS  |
| 1   | G     | 57[A] | ARG  |
| 1   | G     | 57[B] | ARG  |
| 1   | G     | 63    | SER  |
| 1   | G     | 68    | THR  |
| 1   | G     | 71    | LEU  |
| 1   | G     | 72    | LYS  |
| 1   | G     | 74    | LYS  |
| 1   | G     | 90    | GLU  |
| 1   | G     | 102   | ARG  |
| 1   | G     | 106   | THR  |
| 1   | G     | 175   | LYS  |
| 1   | G     | 193   | MET  |
| 1   | G     | 196   | GLU  |
| 1   | G     | 199   | ARG  |
| 1   | G     | 212   | ARG  |
| 1   | G     | 246   | ARG  |
| 1   | G     | 258   | ARG  |
| 1   | H     | 2     | SER  |
| 1   | H     | 15    | ARG  |
| 1   | H     | 51    | LYS  |
| 1   | H     | 63    | SER  |
| 1   | H     | 68    | THR  |
| 1   | H     | 71    | LEU  |
| 1   | H     | 74    | LYS  |
| 1   | H     | 90    | GLU  |
| 1   | H     | 100   | GLN  |
| 1   | H     | 106   | THR  |
| 1   | H     | 175   | LYS  |
| 1   | H     | 193   | MET  |
| 1   | H     | 196   | GLU  |
| 1   | H     | 212   | ARG  |
| 1   | H     | 246   | ARG  |
| 1   | I     | 2     | SER  |
| 1   | I     | 51    | LYS  |
| 1   | I     | 63    | SER  |
| 1   | I     | 68    | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 71  | LEU  |
| 1   | I     | 72  | LYS  |
| 1   | I     | 74  | LYS  |
| 1   | I     | 90  | GLU  |
| 1   | I     | 106 | THR  |
| 1   | I     | 175 | LYS  |
| 1   | I     | 193 | MET  |
| 1   | I     | 196 | GLU  |
| 1   | I     | 199 | ARG  |
| 1   | I     | 212 | ARG  |
| 1   | J     | 15  | ARG  |
| 1   | J     | 63  | SER  |
| 1   | J     | 68  | THR  |
| 1   | J     | 71  | LEU  |
| 1   | J     | 72  | LYS  |
| 1   | J     | 74  | LYS  |
| 1   | J     | 90  | GLU  |
| 1   | J     | 102 | ARG  |
| 1   | J     | 106 | THR  |
| 1   | J     | 175 | LYS  |
| 1   | J     | 193 | MET  |
| 1   | J     | 196 | GLU  |
| 1   | J     | 199 | ARG  |
| 1   | J     | 212 | ARG  |
| 1   | J     | 220 | ARG  |
| 1   | J     | 226 | GLU  |
| 1   | J     | 246 | ARG  |
| 1   | K     | 1   | MET  |
| 1   | K     | 2   | SER  |
| 1   | K     | 51  | LYS  |
| 1   | K     | 63  | SER  |
| 1   | K     | 68  | THR  |
| 1   | K     | 71  | LEU  |
| 1   | K     | 72  | LYS  |
| 1   | K     | 74  | LYS  |
| 1   | K     | 90  | GLU  |
| 1   | K     | 100 | GLN  |
| 1   | K     | 106 | THR  |
| 1   | K     | 175 | LYS  |
| 1   | K     | 193 | MET  |
| 1   | K     | 196 | GLU  |
| 1   | K     | 199 | ARG  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | K     | 201   | ARG  |
| 1   | K     | 212   | ARG  |
| 1   | K     | 220   | ARG  |
| 1   | K     | 246   | ARG  |
| 1   | K     | 258   | ARG  |
| 1   | L     | 2     | SER  |
| 1   | L     | 51    | LYS  |
| 1   | L     | 57[A] | ARG  |
| 1   | L     | 57[B] | ARG  |
| 1   | L     | 63    | SER  |
| 1   | L     | 68    | THR  |
| 1   | L     | 71    | LEU  |
| 1   | L     | 72    | LYS  |
| 1   | L     | 74    | LYS  |
| 1   | L     | 90    | GLU  |
| 1   | L     | 100   | GLN  |
| 1   | L     | 106   | THR  |
| 1   | L     | 160   | ARG  |
| 1   | L     | 175   | LYS  |
| 1   | L     | 193   | MET  |
| 1   | L     | 196   | GLU  |
| 1   | L     | 199   | ARG  |
| 1   | L     | 201   | ARG  |
| 1   | L     | 212   | ARG  |
| 1   | L     | 246   | ARG  |
| 1   | L     | 258   | ARG  |
| 1   | M     | 15    | ARG  |
| 1   | M     | 51    | LYS  |
| 1   | M     | 57[A] | ARG  |
| 1   | M     | 57[B] | ARG  |
| 1   | M     | 63    | SER  |
| 1   | M     | 71    | LEU  |
| 1   | M     | 90    | GLU  |
| 1   | M     | 106   | THR  |
| 1   | M     | 160   | ARG  |
| 1   | M     | 193   | MET  |
| 1   | M     | 196   | GLU  |
| 1   | M     | 199   | ARG  |
| 1   | M     | 201   | ARG  |
| 1   | M     | 212   | ARG  |
| 1   | M     | 220   | ARG  |
| 1   | M     | 246   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 253 | THR  |
| 1   | N     | 2   | SER  |
| 1   | N     | 15  | ARG  |
| 1   | N     | 51  | LYS  |
| 1   | N     | 63  | SER  |
| 1   | N     | 68  | THR  |
| 1   | N     | 71  | LEU  |
| 1   | N     | 72  | LYS  |
| 1   | N     | 74  | LYS  |
| 1   | N     | 90  | GLU  |
| 1   | N     | 99  | VAL  |
| 1   | N     | 106 | THR  |
| 1   | N     | 175 | LYS  |
| 1   | N     | 193 | MET  |
| 1   | N     | 196 | GLU  |
| 1   | N     | 199 | ARG  |
| 1   | N     | 212 | ARG  |
| 1   | N     | 246 | ARG  |
| 1   | O     | 2   | SER  |
| 1   | O     | 15  | ARG  |
| 1   | O     | 51  | LYS  |
| 1   | O     | 63  | SER  |
| 1   | O     | 74  | LYS  |
| 1   | O     | 90  | GLU  |
| 1   | O     | 106 | THR  |
| 1   | O     | 175 | LYS  |
| 1   | O     | 193 | MET  |
| 1   | O     | 196 | GLU  |
| 1   | O     | 199 | ARG  |
| 1   | O     | 212 | ARG  |
| 1   | O     | 220 | ARG  |
| 1   | O     | 246 | ARG  |
| 1   | P     | 2   | SER  |
| 1   | P     | 9   | ILE  |
| 1   | P     | 15  | ARG  |
| 1   | P     | 51  | LYS  |
| 1   | P     | 63  | SER  |
| 1   | P     | 71  | LEU  |
| 1   | P     | 72  | LYS  |
| 1   | P     | 74  | LYS  |
| 1   | P     | 90  | GLU  |
| 1   | P     | 100 | GLN  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | P     | 102   | ARG  |
| 1   | P     | 106   | THR  |
| 1   | P     | 175   | LYS  |
| 1   | P     | 193   | MET  |
| 1   | P     | 196   | GLU  |
| 1   | P     | 199   | ARG  |
| 1   | P     | 212   | ARG  |
| 1   | P     | 220   | ARG  |
| 1   | P     | 226   | GLU  |
| 1   | P     | 246   | ARG  |
| 1   | Q     | 2     | SER  |
| 1   | Q     | 51    | LYS  |
| 1   | Q     | 63    | SER  |
| 1   | Q     | 68    | THR  |
| 1   | Q     | 71    | LEU  |
| 1   | Q     | 72    | LYS  |
| 1   | Q     | 74    | LYS  |
| 1   | Q     | 90    | GLU  |
| 1   | Q     | 106   | THR  |
| 1   | Q     | 175   | LYS  |
| 1   | Q     | 193   | MET  |
| 1   | Q     | 196   | GLU  |
| 1   | Q     | 199   | ARG  |
| 1   | Q     | 200   | ARG  |
| 1   | Q     | 201   | ARG  |
| 1   | Q     | 212   | ARG  |
| 1   | Q     | 246   | ARG  |
| 1   | R     | 2     | SER  |
| 1   | R     | 15    | ARG  |
| 1   | R     | 51    | LYS  |
| 1   | R     | 57[A] | ARG  |
| 1   | R     | 57[B] | ARG  |
| 1   | R     | 63    | SER  |
| 1   | R     | 68    | THR  |
| 1   | R     | 71    | LEU  |
| 1   | R     | 72    | LYS  |
| 1   | R     | 74    | LYS  |
| 1   | R     | 90    | GLU  |
| 1   | R     | 99    | VAL  |
| 1   | R     | 100   | GLN  |
| 1   | R     | 102   | ARG  |
| 1   | R     | 106   | THR  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | R     | 175   | LYS  |
| 1   | R     | 193   | MET  |
| 1   | R     | 196   | GLU  |
| 1   | R     | 199   | ARG  |
| 1   | R     | 200   | ARG  |
| 1   | R     | 212   | ARG  |
| 1   | R     | 246   | ARG  |
| 1   | R     | 258   | ARG  |
| 1   | S     | 1     | MET  |
| 1   | S     | 2     | SER  |
| 1   | S     | 15    | ARG  |
| 1   | S     | 51    | LYS  |
| 1   | S     | 63    | SER  |
| 1   | S     | 68    | THR  |
| 1   | S     | 71    | LEU  |
| 1   | S     | 72    | LYS  |
| 1   | S     | 74    | LYS  |
| 1   | S     | 90    | GLU  |
| 1   | S     | 100   | GLN  |
| 1   | S     | 106   | THR  |
| 1   | S     | 175   | LYS  |
| 1   | S     | 193   | MET  |
| 1   | S     | 196   | GLU  |
| 1   | S     | 199   | ARG  |
| 1   | S     | 212   | ARG  |
| 1   | S     | 246   | ARG  |
| 1   | S     | 258   | ARG  |
| 1   | T     | 15    | ARG  |
| 1   | T     | 51    | LYS  |
| 1   | T     | 57[A] | ARG  |
| 1   | T     | 57[B] | ARG  |
| 1   | T     | 63    | SER  |
| 1   | T     | 68    | THR  |
| 1   | T     | 71    | LEU  |
| 1   | T     | 74    | LYS  |
| 1   | T     | 90    | GLU  |
| 1   | T     | 106   | THR  |
| 1   | T     | 175   | LYS  |
| 1   | T     | 193   | MET  |
| 1   | T     | 196   | GLU  |
| 1   | T     | 199   | ARG  |
| 1   | T     | 212   | ARG  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | T     | 213   | ARG  |
| 1   | T     | 226   | GLU  |
| 1   | T     | 246   | ARG  |
| 1   | T     | 258   | ARG  |
| 1   | U     | 51    | LYS  |
| 1   | U     | 63    | SER  |
| 1   | U     | 68    | THR  |
| 1   | U     | 71    | LEU  |
| 1   | U     | 74    | LYS  |
| 1   | U     | 90    | GLU  |
| 1   | U     | 100   | GLN  |
| 1   | U     | 102   | ARG  |
| 1   | U     | 175   | LYS  |
| 1   | U     | 193   | MET  |
| 1   | U     | 196   | GLU  |
| 1   | U     | 199   | ARG  |
| 1   | U     | 212   | ARG  |
| 1   | U     | 246   | ARG  |
| 1   | V     | 1     | MET  |
| 1   | V     | 2     | SER  |
| 1   | V     | 15    | ARG  |
| 1   | V     | 57[A] | ARG  |
| 1   | V     | 57[B] | ARG  |
| 1   | V     | 63    | SER  |
| 1   | V     | 68    | THR  |
| 1   | V     | 71    | LEU  |
| 1   | V     | 72    | LYS  |
| 1   | V     | 74    | LYS  |
| 1   | V     | 90    | GLU  |
| 1   | V     | 102   | ARG  |
| 1   | V     | 106   | THR  |
| 1   | V     | 175   | LYS  |
| 1   | V     | 193   | MET  |
| 1   | V     | 196   | GLU  |
| 1   | V     | 199   | ARG  |
| 1   | V     | 212   | ARG  |
| 1   | V     | 246   | ARG  |
| 1   | V     | 258   | ARG  |
| 1   | W     | 51    | LYS  |
| 1   | W     | 57[A] | ARG  |
| 1   | W     | 57[B] | ARG  |
| 1   | W     | 63    | SER  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | W     | 68     | THR  |
| 1   | W     | 72     | LYS  |
| 1   | W     | 74     | LYS  |
| 1   | W     | 90     | GLU  |
| 1   | W     | 100    | GLN  |
| 1   | W     | 106    | THR  |
| 1   | W     | 175    | LYS  |
| 1   | W     | 193    | MET  |
| 1   | W     | 196    | GLU  |
| 1   | W     | 199    | ARG  |
| 1   | W     | 212    | ARG  |
| 1   | W     | 246    | ARG  |
| 1   | W     | 258    | ARG  |
| 1   | X     | 4      | ILE  |
| 1   | X     | 57[A]  | ARG  |
| 1   | X     | 57[B]  | ARG  |
| 1   | X     | 63     | SER  |
| 1   | X     | 68     | THR  |
| 1   | X     | 71     | LEU  |
| 1   | X     | 72     | LYS  |
| 1   | X     | 74     | LYS  |
| 1   | X     | 90     | GLU  |
| 1   | X     | 102[A] | ARG  |
| 1   | X     | 102[B] | ARG  |
| 1   | X     | 175    | LYS  |
| 1   | X     | 193    | MET  |
| 1   | X     | 196    | GLU  |
| 1   | X     | 199    | ARG  |
| 1   | X     | 201    | ARG  |
| 1   | X     | 212    | ARG  |
| 1   | X     | 226    | GLU  |
| 1   | X     | 246    | ARG  |
| 1   | Y     | 1      | MET  |
| 1   | Y     | 2      | SER  |
| 1   | Y     | 15     | ARG  |
| 1   | Y     | 51     | LYS  |
| 1   | Y     | 63     | SER  |
| 1   | Y     | 68     | THR  |
| 1   | Y     | 71     | LEU  |
| 1   | Y     | 72     | LYS  |
| 1   | Y     | 74     | LYS  |
| 1   | Y     | 90     | GLU  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | Y     | 102   | ARG  |
| 1   | Y     | 175   | LYS  |
| 1   | Y     | 193   | MET  |
| 1   | Y     | 196   | GLU  |
| 1   | Y     | 199   | ARG  |
| 1   | Y     | 201   | ARG  |
| 1   | Y     | 212   | ARG  |
| 1   | Y     | 246   | ARG  |
| 1   | Y     | 257   | THR  |
| 1   | Z     | 4     | ILE  |
| 1   | Z     | 15    | ARG  |
| 1   | Z     | 51    | LYS  |
| 1   | Z     | 57[A] | ARG  |
| 1   | Z     | 57[B] | ARG  |
| 1   | Z     | 63    | SER  |
| 1   | Z     | 71    | LEU  |
| 1   | Z     | 74    | LYS  |
| 1   | Z     | 90    | GLU  |
| 1   | Z     | 100   | GLN  |
| 1   | Z     | 175   | LYS  |
| 1   | Z     | 193   | MET  |
| 1   | Z     | 196   | GLU  |
| 1   | Z     | 199   | ARG  |
| 1   | Z     | 212   | ARG  |
| 1   | Z     | 220   | ARG  |
| 1   | Z     | 246   | ARG  |
| 1   | Z     | 258   | ARG  |
| 1   | a     | 2     | SER  |
| 1   | a     | 31    | GLU  |
| 1   | a     | 51    | LYS  |
| 1   | a     | 57[A] | ARG  |
| 1   | a     | 57[B] | ARG  |
| 1   | a     | 63    | SER  |
| 1   | a     | 71    | LEU  |
| 1   | a     | 74    | LYS  |
| 1   | a     | 90    | GLU  |
| 1   | a     | 99    | VAL  |
| 1   | a     | 102   | ARG  |
| 1   | a     | 175   | LYS  |
| 1   | a     | 193   | MET  |
| 1   | a     | 196   | GLU  |
| 1   | a     | 199   | ARG  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | a     | 212   | ARG  |
| 1   | a     | 246   | ARG  |
| 1   | b     | 2     | SER  |
| 1   | b     | 15    | ARG  |
| 1   | b     | 51    | LYS  |
| 1   | b     | 57[A] | ARG  |
| 1   | b     | 57[B] | ARG  |
| 1   | b     | 63    | SER  |
| 1   | b     | 68    | THR  |
| 1   | b     | 71    | LEU  |
| 1   | b     | 72    | LYS  |
| 1   | b     | 74    | LYS  |
| 1   | b     | 90    | GLU  |
| 1   | b     | 102   | ARG  |
| 1   | b     | 149   | LEU  |
| 1   | b     | 160   | ARG  |
| 1   | b     | 175   | LYS  |
| 1   | b     | 193   | MET  |
| 1   | b     | 196   | GLU  |
| 1   | b     | 199   | ARG  |
| 1   | b     | 201   | ARG  |
| 1   | b     | 212   | ARG  |
| 1   | b     | 246   | ARG  |
| 1   | c     | 2     | SER  |
| 1   | c     | 15    | ARG  |
| 1   | c     | 51    | LYS  |
| 1   | c     | 57[A] | ARG  |
| 1   | c     | 57[B] | ARG  |
| 1   | c     | 63    | SER  |
| 1   | c     | 68    | THR  |
| 1   | c     | 71    | LEU  |
| 1   | c     | 74    | LYS  |
| 1   | c     | 90    | GLU  |
| 1   | c     | 100   | GLN  |
| 1   | c     | 102   | ARG  |
| 1   | c     | 106   | THR  |
| 1   | c     | 175   | LYS  |
| 1   | c     | 193   | MET  |
| 1   | c     | 196   | GLU  |
| 1   | c     | 199   | ARG  |
| 1   | c     | 212   | ARG  |
| 1   | c     | 246   | ARG  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | d     | -1    | SER  |
| 1   | d     | 4     | ILE  |
| 1   | d     | 15    | ARG  |
| 1   | d     | 51    | LYS  |
| 1   | d     | 57[A] | ARG  |
| 1   | d     | 57[B] | ARG  |
| 1   | d     | 63    | SER  |
| 1   | d     | 68    | THR  |
| 1   | d     | 71    | LEU  |
| 1   | d     | 74    | LYS  |
| 1   | d     | 90    | GLU  |
| 1   | d     | 100   | GLN  |
| 1   | d     | 106   | THR  |
| 1   | d     | 160   | ARG  |
| 1   | d     | 175   | LYS  |
| 1   | d     | 193   | MET  |
| 1   | d     | 196   | GLU  |
| 1   | d     | 199   | ARG  |
| 1   | d     | 212   | ARG  |
| 1   | d     | 246   | ARG  |
| 1   | d     | 258   | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 128 | HIS  |
| 1   | A     | 134 | ASN  |
| 1   | A     | 164 | HIS  |
| 1   | B     | 100 | GLN  |
| 1   | B     | 128 | HIS  |
| 1   | B     | 134 | ASN  |
| 1   | B     | 164 | HIS  |
| 1   | C     | 100 | GLN  |
| 1   | C     | 128 | HIS  |
| 1   | C     | 134 | ASN  |
| 1   | C     | 156 | HIS  |
| 1   | C     | 164 | HIS  |
| 1   | D     | 128 | HIS  |
| 1   | D     | 134 | ASN  |
| 1   | D     | 156 | HIS  |
| 1   | D     | 164 | HIS  |
| 1   | E     | 100 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 134 | ASN  |
| 1   | E     | 156 | HIS  |
| 1   | E     | 164 | HIS  |
| 1   | F     | 100 | GLN  |
| 1   | F     | 128 | HIS  |
| 1   | F     | 134 | ASN  |
| 1   | F     | 164 | HIS  |
| 1   | G     | 128 | HIS  |
| 1   | G     | 134 | ASN  |
| 1   | G     | 156 | HIS  |
| 1   | G     | 164 | HIS  |
| 1   | H     | 100 | GLN  |
| 1   | H     | 128 | HIS  |
| 1   | H     | 134 | ASN  |
| 1   | H     | 156 | HIS  |
| 1   | H     | 164 | HIS  |
| 1   | H     | 221 | GLN  |
| 1   | I     | 134 | ASN  |
| 1   | I     | 156 | HIS  |
| 1   | I     | 164 | HIS  |
| 1   | I     | 209 | HIS  |
| 1   | J     | 128 | HIS  |
| 1   | J     | 134 | ASN  |
| 1   | J     | 156 | HIS  |
| 1   | J     | 250 | GLN  |
| 1   | K     | 100 | GLN  |
| 1   | K     | 128 | HIS  |
| 1   | K     | 134 | ASN  |
| 1   | K     | 156 | HIS  |
| 1   | L     | 100 | GLN  |
| 1   | L     | 128 | HIS  |
| 1   | L     | 134 | ASN  |
| 1   | L     | 156 | HIS  |
| 1   | L     | 250 | GLN  |
| 1   | M     | 43  | HIS  |
| 1   | M     | 121 | HIS  |
| 1   | M     | 128 | HIS  |
| 1   | M     | 134 | ASN  |
| 1   | N     | 128 | HIS  |
| 1   | N     | 134 | ASN  |
| 1   | N     | 156 | HIS  |
| 1   | N     | 164 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 43  | HIS  |
| 1   | O     | 128 | HIS  |
| 1   | O     | 134 | ASN  |
| 1   | P     | 100 | GLN  |
| 1   | P     | 128 | HIS  |
| 1   | P     | 134 | ASN  |
| 1   | P     | 156 | HIS  |
| 1   | P     | 164 | HIS  |
| 1   | P     | 250 | GLN  |
| 1   | Q     | 128 | HIS  |
| 1   | Q     | 134 | ASN  |
| 1   | Q     | 156 | HIS  |
| 1   | Q     | 164 | HIS  |
| 1   | R     | 100 | GLN  |
| 1   | R     | 128 | HIS  |
| 1   | R     | 134 | ASN  |
| 1   | R     | 164 | HIS  |
| 1   | R     | 250 | GLN  |
| 1   | S     | 100 | GLN  |
| 1   | S     | 128 | HIS  |
| 1   | S     | 134 | ASN  |
| 1   | S     | 157 | GLN  |
| 1   | S     | 164 | HIS  |
| 1   | T     | 134 | ASN  |
| 1   | U     | 21  | GLN  |
| 1   | U     | 100 | GLN  |
| 1   | U     | 128 | HIS  |
| 1   | U     | 134 | ASN  |
| 1   | U     | 156 | HIS  |
| 1   | U     | 164 | HIS  |
| 1   | U     | 250 | GLN  |
| 1   | V     | 128 | HIS  |
| 1   | V     | 134 | ASN  |
| 1   | V     | 156 | HIS  |
| 1   | V     | 164 | HIS  |
| 1   | W     | 100 | GLN  |
| 1   | W     | 128 | HIS  |
| 1   | W     | 134 | ASN  |
| 1   | W     | 164 | HIS  |
| 1   | X     | 121 | HIS  |
| 1   | X     | 128 | HIS  |
| 1   | X     | 134 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 128 | HIS  |
| 1   | Y     | 134 | ASN  |
| 1   | Y     | 250 | GLN  |
| 1   | Z     | 100 | GLN  |
| 1   | Z     | 134 | ASN  |
| 1   | a     | 100 | GLN  |
| 1   | a     | 134 | ASN  |
| 1   | a     | 164 | HIS  |
| 1   | b     | 128 | HIS  |
| 1   | b     | 134 | ASN  |
| 1   | c     | 100 | GLN  |
| 1   | c     | 128 | HIS  |
| 1   | c     | 134 | ASN  |
| 1   | d     | 100 | GLN  |
| 1   | d     | 134 | ASN  |
| 1   | d     | 156 | HIS  |
| 1   | d     | 164 | HIS  |
| 1   | d     | 221 | GLN  |
| 1   | d     | 250 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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 | $\# Z  > 2$ |
| 2   | VFE  | A     | 1001 | -    | 31,31,31     | 1.73 | 6 (19%)     | 39,41,41    | 2.06 | 13 (33%)    |
| 2   | VFE  | E     | 1001 | -    | 31,31,31     | 1.58 | 4 (12%)     | 39,41,41    | 2.30 | 11 (28%)    |
| 2   | VFE  | c     | 1001 | -    | 31,31,31     | 1.16 | 3 (9%)      | 39,41,41    | 1.50 | 7 (17%)     |
| 2   | VFE  | F     | 1001 | -    | 31,31,31     | 1.30 | 3 (9%)      | 39,41,41    | 1.47 | 7 (17%)     |
| 2   | VFE  | C     | 1001 | -    | 31,31,31     | 1.65 | 4 (12%)     | 39,41,41    | 2.17 | 8 (20%)     |
| 2   | VFE  | Z     | 1001 | -    | 31,31,31     | 1.67 | 5 (16%)     | 39,41,41    | 2.04 | 10 (25%)    |
| 2   | VFE  | Y     | 1001 | -    | 31,31,31     | 1.36 | 5 (16%)     | 39,41,41    | 1.45 | 6 (15%)     |
| 2   | VFE  | U     | 1001 | -    | 31,31,31     | 1.96 | 6 (19%)     | 39,41,41    | 2.00 | 10 (25%)    |
| 2   | VFE  | G     | 1001 | -    | 31,31,31     | 1.23 | 2 (6%)      | 39,41,41    | 1.65 | 9 (23%)     |
| 2   | VFE  | d     | 1001 | -    | 31,31,31     | 1.33 | 4 (12%)     | 39,41,41    | 1.94 | 12 (30%)    |
| 2   | VFE  | S     | 1001 | -    | 31,31,31     | 1.32 | 5 (16%)     | 39,41,41    | 1.56 | 9 (23%)     |
| 2   | VFE  | V     | 1001 | -    | 31,31,31     | 1.49 | 4 (12%)     | 39,41,41    | 1.73 | 8 (20%)     |
| 2   | VFE  | W     | 1001 | -    | 31,31,31     | 1.35 | 5 (16%)     | 39,41,41    | 1.75 | 10 (25%)    |
| 2   | VFE  | D     | 1001 | -    | 31,31,31     | 1.98 | 5 (16%)     | 39,41,41    | 2.14 | 10 (25%)    |
| 2   | VFE  | J     | 1001 | -    | 31,31,31     | 1.35 | 2 (6%)      | 39,41,41    | 1.65 | 8 (20%)     |
| 2   | VFE  | P     | 1001 | -    | 31,31,31     | 1.56 | 6 (19%)     | 39,41,41    | 1.26 | 5 (12%)     |
| 2   | VFE  | O     | 1001 | -    | 31,31,31     | 1.49 | 6 (19%)     | 39,41,41    | 1.35 | 5 (12%)     |
| 2   | VFE  | Q     | 1001 | -    | 31,31,31     | 1.10 | 3 (9%)      | 39,41,41    | 1.85 | 7 (17%)     |
| 2   | VFE  | R     | 1001 | -    | 31,31,31     | 1.40 | 2 (6%)      | 39,41,41    | 1.96 | 15 (38%)    |
| 2   | VFE  | X     | 1001 | -    | 31,31,31     | 1.88 | 7 (22%)     | 39,41,41    | 1.57 | 8 (20%)     |
| 2   | VFE  | N     | 1001 | -    | 31,31,31     | 1.22 | 2 (6%)      | 39,41,41    | 1.39 | 6 (15%)     |
| 2   | VFE  | H     | 1001 | -    | 31,31,31     | 1.13 | 3 (9%)      | 39,41,41    | 1.80 | 8 (20%)     |
| 2   | VFE  | T     | 1001 | -    | 31,31,31     | 1.48 | 7 (22%)     | 39,41,41    | 2.05 | 13 (33%)    |
| 2   | VFE  | b     | 1001 | -    | 31,31,31     | 1.24 | 3 (9%)      | 39,41,41    | 1.18 | 4 (10%)     |
| 2   | VFE  | M     | 1001 | -    | 31,31,31     | 1.71 | 5 (16%)     | 39,41,41    | 2.39 | 13 (33%)    |
| 2   | VFE  | B     | 1001 | -    | 31,31,31     | 1.28 | 4 (12%)     | 39,41,41    | 1.31 | 4 (10%)     |
| 2   | VFE  | K     | 1001 | -    | 31,31,31     | 1.50 | 3 (9%)      | 39,41,41    | 1.60 | 8 (20%)     |
| 2   | VFE  | a     | 1001 | -    | 31,31,31     | 1.42 | 5 (16%)     | 39,41,41    | 1.88 | 13 (33%)    |
| 2   | VFE  | L     | 1001 | -    | 31,31,31     | 1.52 | 5 (16%)     | 39,41,41    | 2.12 | 15 (38%)    |
| 2   | VFE  | I     | 1001 | -    | 31,31,31     | 1.51 | 5 (16%)     | 39,41,41    | 2.06 | 14 (35%)    |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | VFE  | A     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | E     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | c     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | F     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | C     | 1001 | -    | -       | 4/23/23/23 | 0/3/3/3 |
| 2   | VFE  | Z     | 1001 | -    | -       | 4/23/23/23 | 0/3/3/3 |
| 2   | VFE  | Y     | 1001 | -    | -       | 3/23/23/23 | 0/3/3/3 |
| 2   | VFE  | U     | 1001 | -    | -       | 3/23/23/23 | 0/3/3/3 |
| 2   | VFE  | G     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | d     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | S     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | V     | 1001 | -    | -       | 4/23/23/23 | 0/3/3/3 |
| 2   | VFE  | W     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | D     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | J     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | P     | 1001 | -    | -       | 4/23/23/23 | 0/3/3/3 |
| 2   | VFE  | O     | 1001 | -    | -       | 4/23/23/23 | 0/3/3/3 |
| 2   | VFE  | Q     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | R     | 1001 | -    | -       | 3/23/23/23 | 0/3/3/3 |
| 2   | VFE  | X     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | N     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | H     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | T     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | b     | 1001 | -    | -       | 4/23/23/23 | 0/3/3/3 |
| 2   | VFE  | M     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | B     | 1001 | -    | -       | 4/23/23/23 | 0/3/3/3 |
| 2   | VFE  | K     | 1001 | -    | -       | 4/23/23/23 | 0/3/3/3 |
| 2   | VFE  | a     | 1001 | -    | -       | 2/23/23/23 | 0/3/3/3 |
| 2   | VFE  | L     | 1001 | -    | -       | 3/23/23/23 | 0/3/3/3 |
| 2   | VFE  | I     | 1001 | -    | -       | 5/23/23/23 | 0/3/3/3 |

All (129) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1001 | VFE  | C23-S22 | 6.03  | 1.86        | 1.77     |
| 2   | K     | 1001 | VFE  | C23-S22 | 5.83  | 1.86        | 1.77     |
| 2   | E     | 1001 | VFE  | C23-S22 | 5.79  | 1.86        | 1.77     |
| 2   | D     | 1001 | VFE  | C25-C24 | 5.79  | 1.48        | 1.38     |
| 2   | D     | 1001 | VFE  | C27-C28 | 5.73  | 1.50        | 1.38     |
| 2   | M     | 1001 | VFE  | C23-S22 | 5.50  | 1.85        | 1.77     |
| 2   | X     | 1001 | VFE  | C25-C24 | -5.41 | 1.29        | 1.38     |
| 2   | X     | 1001 | VFE  | C27-C28 | -5.23 | 1.28        | 1.38     |
| 2   | C     | 1001 | VFE  | C23-S22 | 5.22  | 1.85        | 1.77     |
| 2   | U     | 1001 | VFE  | C23-S22 | 5.03  | 1.84        | 1.77     |
| 2   | V     | 1001 | VFE  | C23-S22 | 4.79  | 1.84        | 1.77     |
| 2   | U     | 1001 | VFE  | C25-C24 | 4.69  | 1.46        | 1.38     |
| 2   | I     | 1001 | VFE  | C23-S22 | 4.59  | 1.84        | 1.77     |
| 2   | Z     | 1001 | VFE  | C23-S22 | 4.35  | 1.83        | 1.77     |
| 2   | J     | 1001 | VFE  | C23-S22 | 4.32  | 1.83        | 1.77     |
| 2   | U     | 1001 | VFE  | C26-C27 | -4.30 | 1.31        | 1.38     |
| 2   | L     | 1001 | VFE  | C19-N6  | 4.26  | 1.43        | 1.35     |
| 2   | P     | 1001 | VFE  | C23-S22 | 4.20  | 1.83        | 1.77     |
| 2   | D     | 1001 | VFE  | C23-S22 | 4.09  | 1.83        | 1.77     |
| 2   | G     | 1001 | VFE  | C23-S22 | 3.86  | 1.83        | 1.77     |
| 2   | a     | 1001 | VFE  | C23-S22 | 3.75  | 1.82        | 1.77     |
| 2   | U     | 1001 | VFE  | C27-C28 | 3.74  | 1.46        | 1.38     |
| 2   | R     | 1001 | VFE  | C23-S22 | 3.68  | 1.82        | 1.77     |
| 2   | M     | 1001 | VFE  | C19-N6  | 3.61  | 1.42        | 1.35     |
| 2   | V     | 1001 | VFE  | C26-C27 | -3.38 | 1.33        | 1.38     |
| 2   | P     | 1001 | VFE  | C25-C24 | 3.37  | 1.44        | 1.38     |
| 2   | L     | 1001 | VFE  | C23-S22 | 3.27  | 1.82        | 1.77     |
| 2   | U     | 1001 | VFE  | C21-S22 | 3.25  | 1.88        | 1.80     |
| 2   | M     | 1001 | VFE  | C26-C27 | -3.24 | 1.33        | 1.38     |
| 2   | O     | 1001 | VFE  | C21-S22 | 3.23  | 1.88        | 1.80     |
| 2   | F     | 1001 | VFE  | C21-C19 | -3.20 | 1.46        | 1.51     |
| 2   | G     | 1001 | VFE  | C11-N14 | -3.19 | 1.37        | 1.43     |
| 2   | T     | 1001 | VFE  | C23-S22 | 3.18  | 1.82        | 1.77     |
| 2   | O     | 1001 | VFE  | C23-S22 | 3.16  | 1.82        | 1.77     |
| 2   | W     | 1001 | VFE  | C24-C23 | -3.12 | 1.34        | 1.39     |
| 2   | Z     | 1001 | VFE  | C19-N6  | 3.10  | 1.41        | 1.35     |
| 2   | Z     | 1001 | VFE  | C7-C8   | -3.05 | 1.45        | 1.51     |
| 2   | C     | 1001 | VFE  | C24-C23 | -3.05 | 1.34        | 1.39     |
| 2   | W     | 1001 | VFE  | C26-C27 | -3.03 | 1.33        | 1.38     |
| 2   | d     | 1001 | VFE  | O4-C3   | 3.01  | 1.29        | 1.23     |
| 2   | T     | 1001 | VFE  | C7-C8   | -2.98 | 1.46        | 1.51     |
| 2   | H     | 1001 | VFE  | C23-S22 | 2.93  | 1.81        | 1.77     |
| 2   | A     | 1001 | VFE  | C19-N6  | 2.93  | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | X     | 1001 | VFE  | C5-C3   | 2.90  | 1.57        | 1.52     |
| 2   | B     | 1001 | VFE  | C11-N14 | -2.88 | 1.37        | 1.43     |
| 2   | J     | 1001 | VFE  | C25-C24 | -2.85 | 1.34        | 1.38     |
| 2   | T     | 1001 | VFE  | C7-N6   | -2.83 | 1.42        | 1.46     |
| 2   | a     | 1001 | VFE  | C11-N14 | -2.81 | 1.37        | 1.43     |
| 2   | T     | 1001 | VFE  | C10-C9  | -2.80 | 1.34        | 1.38     |
| 2   | c     | 1001 | VFE  | C15-N14 | 2.79  | 1.38        | 1.34     |
| 2   | C     | 1001 | VFE  | C26-C27 | -2.78 | 1.34        | 1.38     |
| 2   | M     | 1001 | VFE  | C21-S22 | 2.78  | 1.87        | 1.80     |
| 2   | O     | 1001 | VFE  | C19-N6  | 2.76  | 1.40        | 1.35     |
| 2   | c     | 1001 | VFE  | C21-C19 | -2.75 | 1.47        | 1.51     |
| 2   | I     | 1001 | VFE  | C11-N14 | -2.73 | 1.38        | 1.43     |
| 2   | N     | 1001 | VFE  | C5-C3   | 2.71  | 1.57        | 1.52     |
| 2   | I     | 1001 | VFE  | C26-C27 | -2.70 | 1.34        | 1.38     |
| 2   | A     | 1001 | VFE  | C11-N14 | -2.64 | 1.38        | 1.43     |
| 2   | Q     | 1001 | VFE  | C5-N6   | 2.63  | 1.49        | 1.45     |
| 2   | S     | 1001 | VFE  | C23-S22 | 2.62  | 1.81        | 1.77     |
| 2   | b     | 1001 | VFE  | C7-C8   | -2.62 | 1.46        | 1.51     |
| 2   | X     | 1001 | VFE  | C7-N6   | -2.60 | 1.42        | 1.46     |
| 2   | Y     | 1001 | VFE  | C5-C3   | 2.57  | 1.57        | 1.52     |
| 2   | a     | 1001 | VFE  | C28-CL  | -2.56 | 1.67        | 1.73     |
| 2   | V     | 1001 | VFE  | C7-C8   | -2.56 | 1.46        | 1.51     |
| 2   | E     | 1001 | VFE  | C5-C3   | 2.55  | 1.57        | 1.52     |
| 2   | B     | 1001 | VFE  | C21-C19 | -2.54 | 1.47        | 1.51     |
| 2   | P     | 1001 | VFE  | C11-N14 | -2.53 | 1.38        | 1.43     |
| 2   | D     | 1001 | VFE  | C21-S22 | 2.52  | 1.86        | 1.80     |
| 2   | H     | 1001 | VFE  | C21-C19 | -2.52 | 1.47        | 1.51     |
| 2   | K     | 1001 | VFE  | C19-N6  | 2.51  | 1.40        | 1.35     |
| 2   | W     | 1001 | VFE  | C28-CL  | -2.51 | 1.67        | 1.73     |
| 2   | S     | 1001 | VFE  | C7-C8   | -2.51 | 1.46        | 1.51     |
| 2   | b     | 1001 | VFE  | C11-N14 | -2.49 | 1.38        | 1.43     |
| 2   | W     | 1001 | VFE  | C19-N6  | 2.46  | 1.40        | 1.35     |
| 2   | a     | 1001 | VFE  | C26-C27 | -2.46 | 1.34        | 1.38     |
| 2   | L     | 1001 | VFE  | C15-N14 | 2.44  | 1.38        | 1.34     |
| 2   | Q     | 1001 | VFE  | C19-N6  | 2.42  | 1.39        | 1.35     |
| 2   | Q     | 1001 | VFE  | C23-S22 | 2.40  | 1.80        | 1.77     |
| 2   | L     | 1001 | VFE  | C7-C8   | -2.40 | 1.47        | 1.51     |
| 2   | T     | 1001 | VFE  | C19-N6  | 2.39  | 1.39        | 1.35     |
| 2   | X     | 1001 | VFE  | C11-N14 | -2.37 | 1.38        | 1.43     |
| 2   | Y     | 1001 | VFE  | C19-N6  | 2.37  | 1.39        | 1.35     |
| 2   | S     | 1001 | VFE  | C19-N6  | 2.37  | 1.39        | 1.35     |
| 2   | a     | 1001 | VFE  | C21-S22 | 2.32  | 1.86        | 1.80     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 1001 | VFE  | C26-C27 | -2.32 | 1.34        | 1.38     |
| 2   | c     | 1001 | VFE  | C23-S22 | 2.31  | 1.80        | 1.77     |
| 2   | E     | 1001 | VFE  | C28-CL  | -2.30 | 1.68        | 1.73     |
| 2   | d     | 1001 | VFE  | C11-N14 | -2.26 | 1.38        | 1.43     |
| 2   | I     | 1001 | VFE  | C7-N6   | -2.25 | 1.43        | 1.46     |
| 2   | P     | 1001 | VFE  | N14-N18 | -2.25 | 1.33        | 1.36     |
| 2   | Y     | 1001 | VFE  | C23-S22 | 2.24  | 1.80        | 1.77     |
| 2   | b     | 1001 | VFE  | C21-S22 | 2.20  | 1.85        | 1.80     |
| 2   | P     | 1001 | VFE  | C15-N14 | 2.20  | 1.37        | 1.34     |
| 2   | W     | 1001 | VFE  | C15-N14 | 2.20  | 1.37        | 1.34     |
| 2   | S     | 1001 | VFE  | C11-N14 | -2.19 | 1.39        | 1.43     |
| 2   | Z     | 1001 | VFE  | C11-N14 | -2.19 | 1.39        | 1.43     |
| 2   | S     | 1001 | VFE  | C7-N6   | -2.19 | 1.43        | 1.46     |
| 2   | U     | 1001 | VFE  | C19-N6  | 2.17  | 1.39        | 1.35     |
| 2   | T     | 1001 | VFE  | C26-C27 | -2.17 | 1.35        | 1.38     |
| 2   | H     | 1001 | VFE  | C11-N14 | -2.16 | 1.39        | 1.43     |
| 2   | Z     | 1001 | VFE  | C21-S22 | 2.16  | 1.85        | 1.80     |
| 2   | L     | 1001 | VFE  | C5-N6   | 2.16  | 1.48        | 1.45     |
| 2   | A     | 1001 | VFE  | C10-C11 | -2.15 | 1.35        | 1.39     |
| 2   | C     | 1001 | VFE  | C21-S22 | 2.15  | 1.85        | 1.80     |
| 2   | T     | 1001 | VFE  | C21-C19 | -2.14 | 1.48        | 1.51     |
| 2   | M     | 1001 | VFE  | C11-N14 | -2.14 | 1.39        | 1.43     |
| 2   | Y     | 1001 | VFE  | C11-N14 | -2.14 | 1.39        | 1.43     |
| 2   | d     | 1001 | VFE  | N14-N18 | -2.14 | 1.33        | 1.36     |
| 2   | d     | 1001 | VFE  | C1-N2   | 2.13  | 1.49        | 1.45     |
| 2   | E     | 1001 | VFE  | C19-N6  | 2.13  | 1.39        | 1.35     |
| 2   | Y     | 1001 | VFE  | C12-C13 | -2.13 | 1.35        | 1.38     |
| 2   | A     | 1001 | VFE  | C28-CL  | -2.13 | 1.68        | 1.73     |
| 2   | D     | 1001 | VFE  | C13-C8  | -2.13 | 1.34        | 1.38     |
| 2   | V     | 1001 | VFE  | C11-N14 | -2.11 | 1.39        | 1.43     |
| 2   | O     | 1001 | VFE  | C26-C27 | -2.11 | 1.35        | 1.38     |
| 2   | F     | 1001 | VFE  | C11-N14 | -2.10 | 1.39        | 1.43     |
| 2   | X     | 1001 | VFE  | C28-C23 | -2.09 | 1.34        | 1.39     |
| 2   | O     | 1001 | VFE  | C5-C3   | 2.09  | 1.56        | 1.52     |
| 2   | P     | 1001 | VFE  | C7-N6   | -2.09 | 1.43        | 1.46     |
| 2   | K     | 1001 | VFE  | C7-C8   | -2.07 | 1.47        | 1.51     |
| 2   | F     | 1001 | VFE  | C1-N2   | 2.06  | 1.49        | 1.45     |
| 2   | I     | 1001 | VFE  | C21-S22 | 2.06  | 1.85        | 1.80     |
| 2   | N     | 1001 | VFE  | C24-C23 | -2.06 | 1.36        | 1.39     |
| 2   | R     | 1001 | VFE  | C21-C19 | -2.05 | 1.48        | 1.51     |
| 2   | O     | 1001 | VFE  | C15-N14 | 2.05  | 1.37        | 1.34     |
| 2   | X     | 1001 | VFE  | C15-N14 | 2.04  | 1.37        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1001 | VFE  | C10-C9  | -2.02 | 1.35        | 1.38     |
| 2   | B     | 1001 | VFE  | C23-S22 | 2.00  | 1.80        | 1.77     |

All (276) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | M     | 1001 | VFE  | C21-S22-C23 | 8.32  | 116.51      | 102.27   |
| 2   | Z     | 1001 | VFE  | C3-C5-N6    | -6.82 | 95.77       | 113.22   |
| 2   | E     | 1001 | VFE  | C21-S22-C23 | 6.28  | 113.02      | 102.27   |
| 2   | D     | 1001 | VFE  | C24-C23-C28 | -6.22 | 109.43      | 117.55   |
| 2   | V     | 1001 | VFE  | C24-C23-C28 | -5.98 | 109.74      | 117.55   |
| 2   | C     | 1001 | VFE  | C23-C28-CL  | -5.92 | 109.45      | 119.72   |
| 2   | Q     | 1001 | VFE  | C21-S22-C23 | 5.69  | 112.02      | 102.27   |
| 2   | A     | 1001 | VFE  | C24-C23-C28 | -5.49 | 110.38      | 117.55   |
| 2   | L     | 1001 | VFE  | C23-C28-CL  | -5.44 | 110.28      | 119.72   |
| 2   | H     | 1001 | VFE  | C21-S22-C23 | 5.38  | 111.47      | 102.27   |
| 2   | T     | 1001 | VFE  | C3-C5-N6    | -5.36 | 99.50       | 113.22   |
| 2   | E     | 1001 | VFE  | C24-C23-C28 | -5.32 | 110.60      | 117.55   |
| 2   | M     | 1001 | VFE  | C23-C28-CL  | -5.19 | 110.72      | 119.72   |
| 2   | C     | 1001 | VFE  | C26-C27-C28 | -5.00 | 111.92      | 119.42   |
| 2   | U     | 1001 | VFE  | C26-C25-C24 | 4.99  | 126.39      | 120.24   |
| 2   | C     | 1001 | VFE  | C24-C23-S22 | 4.99  | 133.55      | 121.48   |
| 2   | U     | 1001 | VFE  | C25-C26-C27 | -4.97 | 114.11      | 120.24   |
| 2   | C     | 1001 | VFE  | C27-C28-C23 | 4.96  | 132.71      | 122.28   |
| 2   | S     | 1001 | VFE  | C23-C28-CL  | -4.89 | 111.24      | 119.72   |
| 2   | I     | 1001 | VFE  | C8-C7-N6    | 4.88  | 120.83      | 113.15   |
| 2   | X     | 1001 | VFE  | O4-C3-C5    | 4.88  | 129.56      | 121.02   |
| 2   | Q     | 1001 | VFE  | C23-C28-CL  | -4.77 | 111.44      | 119.72   |
| 2   | a     | 1001 | VFE  | C3-C5-N6    | -4.71 | 101.15      | 113.22   |
| 2   | L     | 1001 | VFE  | C7-N6-C5    | -4.68 | 108.91      | 116.65   |
| 2   | J     | 1001 | VFE  | C23-C28-CL  | -4.68 | 111.60      | 119.72   |
| 2   | d     | 1001 | VFE  | C3-C5-N6    | -4.60 | 101.44      | 113.22   |
| 2   | A     | 1001 | VFE  | C3-C5-N6    | -4.50 | 101.69      | 113.22   |
| 2   | C     | 1001 | VFE  | C26-C25-C24 | 4.45  | 125.73      | 120.24   |
| 2   | D     | 1001 | VFE  | C24-C23-S22 | 4.44  | 132.23      | 121.48   |
| 2   | D     | 1001 | VFE  | C3-C5-N6    | -4.43 | 101.87      | 113.22   |
| 2   | E     | 1001 | VFE  | C23-C28-CL  | -4.42 | 112.06      | 119.72   |
| 2   | C     | 1001 | VFE  | C24-C23-C28 | -4.42 | 111.78      | 117.55   |
| 2   | Z     | 1001 | VFE  | C23-C28-CL  | -4.37 | 112.14      | 119.72   |
| 2   | I     | 1001 | VFE  | C7-N6-C19   | -4.36 | 110.21      | 121.78   |
| 2   | c     | 1001 | VFE  | O20-C19-N6  | 4.30  | 129.78      | 122.12   |
| 2   | N     | 1001 | VFE  | O4-C3-C5    | 4.28  | 128.51      | 121.02   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | M     | 1001 | VFE  | O20-C19-N6  | 4.27  | 129.72      | 122.12   |
| 2   | R     | 1001 | VFE  | C26-C27-C28 | -4.18 | 113.14      | 119.42   |
| 2   | D     | 1001 | VFE  | C25-C26-C27 | -4.12 | 115.16      | 120.24   |
| 2   | T     | 1001 | VFE  | C13-C8-C9   | 4.10  | 124.32      | 118.23   |
| 2   | I     | 1001 | VFE  | C23-C28-CL  | -4.09 | 112.62      | 119.72   |
| 2   | Y     | 1001 | VFE  | C23-C28-CL  | -4.08 | 112.65      | 119.72   |
| 2   | O     | 1001 | VFE  | C21-S22-C23 | 4.04  | 109.19      | 102.27   |
| 2   | M     | 1001 | VFE  | C15-N14-N18 | 4.02  | 113.90      | 109.26   |
| 2   | d     | 1001 | VFE  | C7-C8-C13   | -3.99 | 113.40      | 120.75   |
| 2   | E     | 1001 | VFE  | C8-C7-N6    | 3.97  | 119.39      | 113.15   |
| 2   | W     | 1001 | VFE  | C26-C25-C24 | 3.95  | 125.12      | 120.24   |
| 2   | Q     | 1001 | VFE  | O4-C3-C5    | 3.94  | 127.91      | 121.02   |
| 2   | A     | 1001 | VFE  | C23-C28-CL  | -3.93 | 112.91      | 119.72   |
| 2   | K     | 1001 | VFE  | C3-C5-N6    | -3.88 | 103.29      | 113.22   |
| 2   | R     | 1001 | VFE  | C23-C28-CL  | -3.84 | 113.06      | 119.72   |
| 2   | G     | 1001 | VFE  | C23-C28-CL  | -3.78 | 113.17      | 119.72   |
| 2   | d     | 1001 | VFE  | C21-S22-C23 | -3.72 | 95.91       | 102.27   |
| 2   | N     | 1001 | VFE  | C23-C28-CL  | -3.71 | 113.28      | 119.72   |
| 2   | U     | 1001 | VFE  | O4-C3-C5    | 3.70  | 127.50      | 121.02   |
| 2   | F     | 1001 | VFE  | C5-C3-N2    | -3.70 | 110.14      | 116.27   |
| 2   | H     | 1001 | VFE  | C23-C28-CL  | -3.69 | 113.32      | 119.72   |
| 2   | A     | 1001 | VFE  | C21-S22-C23 | 3.63  | 108.49      | 102.27   |
| 2   | D     | 1001 | VFE  | C26-C25-C24 | 3.62  | 124.70      | 120.24   |
| 2   | R     | 1001 | VFE  | C12-C11-N14 | 3.61  | 124.00      | 119.58   |
| 2   | M     | 1001 | VFE  | C24-C23-S22 | 3.60  | 130.21      | 121.48   |
| 2   | E     | 1001 | VFE  | C7-N6-C19   | -3.60 | 112.21      | 121.78   |
| 2   | a     | 1001 | VFE  | C15-N14-N18 | 3.60  | 113.41      | 109.26   |
| 2   | G     | 1001 | VFE  | C24-C23-C28 | -3.60 | 112.85      | 117.55   |
| 2   | E     | 1001 | VFE  | O4-C3-C5    | 3.58  | 127.28      | 121.02   |
| 2   | D     | 1001 | VFE  | C27-C28-C23 | 3.57  | 129.79      | 122.28   |
| 2   | a     | 1001 | VFE  | C8-C7-N6    | -3.57 | 107.54      | 113.15   |
| 2   | Q     | 1001 | VFE  | C24-C23-S22 | 3.57  | 130.12      | 121.48   |
| 2   | M     | 1001 | VFE  | C7-N6-C5    | -3.56 | 110.76      | 116.65   |
| 2   | P     | 1001 | VFE  | C25-C26-C27 | -3.56 | 115.85      | 120.24   |
| 2   | I     | 1001 | VFE  | C10-C11-N14 | -3.54 | 115.25      | 119.58   |
| 2   | W     | 1001 | VFE  | C3-C5-N6    | -3.54 | 104.16      | 113.22   |
| 2   | A     | 1001 | VFE  | C27-C28-C23 | 3.50  | 129.64      | 122.28   |
| 2   | L     | 1001 | VFE  | C10-C11-N14 | 3.50  | 123.86      | 119.58   |
| 2   | H     | 1001 | VFE  | C24-C23-S22 | 3.49  | 129.92      | 121.48   |
| 2   | U     | 1001 | VFE  | C23-C28-CL  | -3.48 | 113.69      | 119.72   |
| 2   | T     | 1001 | VFE  | O20-C19-N6  | 3.46  | 128.29      | 122.12   |
| 2   | K     | 1001 | VFE  | C23-C28-CL  | -3.43 | 113.77      | 119.72   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | L     | 1001 | VFE  | C7-C8-C13   | -3.43 | 114.44      | 120.75   |
| 2   | F     | 1001 | VFE  | O4-C3-C5    | 3.43  | 127.01      | 121.02   |
| 2   | S     | 1001 | VFE  | C24-C23-S22 | 3.41  | 129.74      | 121.48   |
| 2   | A     | 1001 | VFE  | C5-C3-N2    | -3.41 | 110.62      | 116.27   |
| 2   | I     | 1001 | VFE  | C7-C8-C9    | -3.41 | 114.47      | 120.75   |
| 2   | R     | 1001 | VFE  | C24-C23-C28 | -3.40 | 113.11      | 117.55   |
| 2   | F     | 1001 | VFE  | C8-C7-N6    | 3.39  | 118.49      | 113.15   |
| 2   | R     | 1001 | VFE  | C27-C28-C23 | 3.39  | 129.41      | 122.28   |
| 2   | E     | 1001 | VFE  | C27-C28-C23 | 3.39  | 129.41      | 122.28   |
| 2   | E     | 1001 | VFE  | C24-C23-S22 | 3.38  | 129.65      | 121.48   |
| 2   | I     | 1001 | VFE  | C24-C23-S22 | 3.33  | 129.55      | 121.48   |
| 2   | K     | 1001 | VFE  | C24-C23-C28 | -3.33 | 113.20      | 117.55   |
| 2   | F     | 1001 | VFE  | C23-C28-CL  | -3.32 | 113.95      | 119.72   |
| 2   | a     | 1001 | VFE  | C24-C23-C28 | -3.31 | 113.23      | 117.55   |
| 2   | E     | 1001 | VFE  | C25-C26-C27 | -3.30 | 116.16      | 120.24   |
| 2   | D     | 1001 | VFE  | C23-C28-CL  | -3.30 | 113.99      | 119.72   |
| 2   | K     | 1001 | VFE  | C24-C23-S22 | 3.28  | 129.43      | 121.48   |
| 2   | T     | 1001 | VFE  | C10-C11-N14 | -3.28 | 115.58      | 119.58   |
| 2   | M     | 1001 | VFE  | C27-C28-CL  | 3.28  | 124.88      | 118.42   |
| 2   | Z     | 1001 | VFE  | C24-C23-C28 | -3.27 | 113.28      | 117.55   |
| 2   | W     | 1001 | VFE  | C23-C28-CL  | -3.27 | 114.05      | 119.72   |
| 2   | G     | 1001 | VFE  | C24-C23-S22 | 3.23  | 129.31      | 121.48   |
| 2   | H     | 1001 | VFE  | O20-C19-N6  | 3.22  | 127.86      | 122.12   |
| 2   | E     | 1001 | VFE  | C12-C11-N14 | 3.21  | 123.51      | 119.58   |
| 2   | J     | 1001 | VFE  | C26-C27-C28 | -3.20 | 114.62      | 119.42   |
| 2   | B     | 1001 | VFE  | O4-C3-C5    | 3.19  | 126.60      | 121.02   |
| 2   | J     | 1001 | VFE  | C3-C5-N6    | -3.15 | 105.15      | 113.22   |
| 2   | a     | 1001 | VFE  | C27-C28-C23 | 3.15  | 128.90      | 122.28   |
| 2   | U     | 1001 | VFE  | C7-N6-C19   | -3.14 | 113.44      | 121.78   |
| 2   | B     | 1001 | VFE  | C26-C25-C24 | 3.14  | 124.11      | 120.24   |
| 2   | B     | 1001 | VFE  | C21-S22-C23 | 3.13  | 107.63      | 102.27   |
| 2   | R     | 1001 | VFE  | C7-N6-C19   | -3.09 | 113.56      | 121.78   |
| 2   | R     | 1001 | VFE  | C24-C23-S22 | 3.09  | 128.95      | 121.48   |
| 2   | d     | 1001 | VFE  | C23-C28-CL  | -3.08 | 114.37      | 119.72   |
| 2   | H     | 1001 | VFE  | C25-C26-C27 | -3.08 | 116.44      | 120.24   |
| 2   | O     | 1001 | VFE  | O4-C3-C5    | 3.07  | 126.39      | 121.02   |
| 2   | d     | 1001 | VFE  | O4-C3-C5    | 3.06  | 126.38      | 121.02   |
| 2   | Y     | 1001 | VFE  | O20-C19-N6  | 3.05  | 127.55      | 122.12   |
| 2   | V     | 1001 | VFE  | C23-C28-CL  | -3.04 | 114.44      | 119.72   |
| 2   | L     | 1001 | VFE  | C24-C23-S22 | 3.03  | 128.83      | 121.48   |
| 2   | L     | 1001 | VFE  | C24-C23-C28 | -3.03 | 113.59      | 117.55   |
| 2   | U     | 1001 | VFE  | C3-C5-N6    | -3.03 | 105.47      | 113.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | c     | 1001 | VFE  | C23-C28-CL  | -3.02 | 114.48      | 119.72   |
| 2   | L     | 1001 | VFE  | O20-C19-N6  | 3.01  | 127.49      | 122.12   |
| 2   | Z     | 1001 | VFE  | C8-C7-N6    | -3.00 | 108.44      | 113.15   |
| 2   | c     | 1001 | VFE  | C3-C5-N6    | -2.99 | 105.58      | 113.22   |
| 2   | U     | 1001 | VFE  | C24-C23-S22 | 2.95  | 128.62      | 121.48   |
| 2   | U     | 1001 | VFE  | C24-C23-C28 | -2.95 | 113.70      | 117.55   |
| 2   | J     | 1001 | VFE  | C24-C23-S22 | 2.93  | 128.56      | 121.48   |
| 2   | T     | 1001 | VFE  | C5-N6-C19   | 2.93  | 129.38      | 120.81   |
| 2   | a     | 1001 | VFE  | O20-C19-C21 | 2.92  | 127.02      | 121.19   |
| 2   | T     | 1001 | VFE  | C21-S22-C23 | 2.91  | 107.25      | 102.27   |
| 2   | A     | 1001 | VFE  | C24-C23-S22 | 2.91  | 128.51      | 121.48   |
| 2   | P     | 1001 | VFE  | C5-N6-C19   | 2.90  | 129.31      | 120.81   |
| 2   | L     | 1001 | VFE  | O4-C3-C5    | -2.90 | 115.94      | 121.02   |
| 2   | d     | 1001 | VFE  | C7-N6-C5    | -2.90 | 111.85      | 116.65   |
| 2   | X     | 1001 | VFE  | C21-S22-C23 | 2.90  | 107.24      | 102.27   |
| 2   | Z     | 1001 | VFE  | C7-N6-C19   | -2.89 | 114.09      | 121.78   |
| 2   | C     | 1001 | VFE  | C7-N6-C19   | -2.89 | 114.12      | 121.78   |
| 2   | d     | 1001 | VFE  | C7-C8-C9    | 2.88  | 126.06      | 120.75   |
| 2   | W     | 1001 | VFE  | C8-C7-N6    | 2.88  | 117.68      | 113.15   |
| 2   | S     | 1001 | VFE  | C7-N6-C19   | -2.87 | 114.16      | 121.78   |
| 2   | T     | 1001 | VFE  | C13-C12-C11 | -2.87 | 116.67      | 120.30   |
| 2   | A     | 1001 | VFE  | C15-N14-N18 | 2.86  | 112.56      | 109.26   |
| 2   | T     | 1001 | VFE  | C7-N6-C5    | -2.86 | 111.93      | 116.65   |
| 2   | L     | 1001 | VFE  | C5-N6-C19   | 2.84  | 129.13      | 120.81   |
| 2   | I     | 1001 | VFE  | C5-N6-C19   | 2.79  | 128.99      | 120.81   |
| 2   | F     | 1001 | VFE  | C24-C23-S22 | 2.78  | 128.21      | 121.48   |
| 2   | I     | 1001 | VFE  | C13-C12-C11 | -2.77 | 116.79      | 120.30   |
| 2   | H     | 1001 | VFE  | C15-N14-N18 | 2.76  | 112.44      | 109.26   |
| 2   | S     | 1001 | VFE  | C3-C5-N6    | -2.76 | 106.17      | 113.22   |
| 2   | E     | 1001 | VFE  | C26-C25-C24 | 2.76  | 123.64      | 120.24   |
| 2   | B     | 1001 | VFE  | C23-C28-CL  | -2.75 | 114.94      | 119.72   |
| 2   | Q     | 1001 | VFE  | O20-C19-N6  | 2.75  | 127.01      | 122.12   |
| 2   | G     | 1001 | VFE  | C27-C28-C23 | 2.73  | 128.01      | 122.28   |
| 2   | L     | 1001 | VFE  | C27-C28-C23 | 2.72  | 128.00      | 122.28   |
| 2   | Z     | 1001 | VFE  | C7-N6-C5    | -2.72 | 112.15      | 116.65   |
| 2   | L     | 1001 | VFE  | C12-C11-N14 | -2.72 | 116.26      | 119.58   |
| 2   | L     | 1001 | VFE  | C8-C7-N6    | -2.71 | 108.89      | 113.15   |
| 2   | K     | 1001 | VFE  | C5-N6-C19   | 2.71  | 128.75      | 120.81   |
| 2   | a     | 1001 | VFE  | C26-C25-C24 | 2.70  | 123.58      | 120.24   |
| 2   | Y     | 1001 | VFE  | C7-N6-C5    | -2.69 | 112.20      | 116.65   |
| 2   | R     | 1001 | VFE  | C3-C5-N6    | -2.68 | 106.35      | 113.22   |
| 2   | M     | 1001 | VFE  | C13-C12-C11 | -2.68 | 116.91      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | U     | 1001 | VFE  | C15-N14-N18 | 2.65  | 112.31      | 109.26   |
| 2   | c     | 1001 | VFE  | C8-C7-N6    | -2.65 | 109.00      | 113.15   |
| 2   | V     | 1001 | VFE  | C27-C28-C23 | 2.64  | 127.82      | 122.28   |
| 2   | J     | 1001 | VFE  | C5-N6-C19   | 2.63  | 128.52      | 120.81   |
| 2   | X     | 1001 | VFE  | C8-C7-N6    | 2.60  | 117.24      | 113.15   |
| 2   | a     | 1001 | VFE  | C7-N6-C19   | -2.60 | 114.88      | 121.78   |
| 2   | Z     | 1001 | VFE  | C13-C8-C9   | 2.60  | 122.10      | 118.23   |
| 2   | Y     | 1001 | VFE  | C24-C23-S22 | 2.59  | 127.74      | 121.48   |
| 2   | X     | 1001 | VFE  | C3-C5-N6    | -2.59 | 106.60      | 113.22   |
| 2   | R     | 1001 | VFE  | C7-C8-C9    | -2.59 | 115.98      | 120.75   |
| 2   | K     | 1001 | VFE  | C12-C11-N14 | 2.58  | 122.74      | 119.58   |
| 2   | W     | 1001 | VFE  | C7-N6-C19   | -2.58 | 114.92      | 121.78   |
| 2   | G     | 1001 | VFE  | C7-N6-C19   | -2.57 | 114.95      | 121.78   |
| 2   | D     | 1001 | VFE  | C8-C7-N6    | 2.57  | 117.19      | 113.15   |
| 2   | W     | 1001 | VFE  | C27-C28-C23 | 2.55  | 127.65      | 122.28   |
| 2   | I     | 1001 | VFE  | C7-C8-C13   | 2.55  | 125.45      | 120.75   |
| 2   | S     | 1001 | VFE  | C27-C28-CL  | 2.55  | 123.45      | 118.42   |
| 2   | a     | 1001 | VFE  | C23-C28-CL  | -2.55 | 115.30      | 119.72   |
| 2   | d     | 1001 | VFE  | C8-C7-N6    | -2.54 | 109.17      | 113.15   |
| 2   | P     | 1001 | VFE  | C26-C27-C28 | 2.52  | 123.20      | 119.42   |
| 2   | V     | 1001 | VFE  | O4-C3-C5    | 2.52  | 125.42      | 121.02   |
| 2   | V     | 1001 | VFE  | C25-C24-C23 | 2.51  | 123.78      | 119.57   |
| 2   | D     | 1001 | VFE  | O4-C3-C5    | 2.51  | 125.41      | 121.02   |
| 2   | W     | 1001 | VFE  | C15-N14-N18 | 2.50  | 112.14      | 109.26   |
| 2   | Z     | 1001 | VFE  | C24-C23-S22 | 2.50  | 127.53      | 121.48   |
| 2   | T     | 1001 | VFE  | C26-C27-C28 | -2.50 | 115.67      | 119.42   |
| 2   | I     | 1001 | VFE  | C15-N14-N18 | 2.49  | 112.14      | 109.26   |
| 2   | G     | 1001 | VFE  | C21-S22-C23 | 2.49  | 106.53      | 102.27   |
| 2   | Z     | 1001 | VFE  | C5-N6-C19   | 2.48  | 128.07      | 120.81   |
| 2   | J     | 1001 | VFE  | C24-C23-C28 | -2.48 | 114.31      | 117.55   |
| 2   | G     | 1001 | VFE  | C15-N14-N18 | 2.48  | 112.12      | 109.26   |
| 2   | D     | 1001 | VFE  | C5-N6-C19   | 2.47  | 128.04      | 120.81   |
| 2   | d     | 1001 | VFE  | C5-N6-C19   | 2.46  | 128.03      | 120.81   |
| 2   | M     | 1001 | VFE  | C10-C11-N14 | -2.46 | 116.58      | 119.58   |
| 2   | L     | 1001 | VFE  | C10-C9-C8   | -2.45 | 117.78      | 121.00   |
| 2   | A     | 1001 | VFE  | C25-C24-C23 | 2.44  | 123.67      | 119.57   |
| 2   | d     | 1001 | VFE  | C15-N14-N18 | 2.44  | 112.07      | 109.26   |
| 2   | N     | 1001 | VFE  | C24-C23-S22 | 2.44  | 127.38      | 121.48   |
| 2   | R     | 1001 | VFE  | C5-C3-N2    | -2.44 | 112.24      | 116.27   |
| 2   | b     | 1001 | VFE  | O4-C3-C5    | 2.43  | 125.27      | 121.02   |
| 2   | G     | 1001 | VFE  | C5-N6-C19   | 2.43  | 127.91      | 120.81   |
| 2   | Y     | 1001 | VFE  | O4-C3-C5    | 2.42  | 125.26      | 121.02   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | R     | 1001 | VFE  | C19-C21-S22 | -2.42 | 104.19      | 112.07   |
| 2   | T     | 1001 | VFE  | C23-C28-CL  | -2.42 | 115.53      | 119.72   |
| 2   | M     | 1001 | VFE  | C5-N6-C19   | 2.41  | 127.88      | 120.81   |
| 2   | I     | 1001 | VFE  | C26-C25-C24 | 2.40  | 123.20      | 120.24   |
| 2   | a     | 1001 | VFE  | O20-C19-N6  | -2.39 | 117.87      | 122.12   |
| 2   | R     | 1001 | VFE  | C26-C25-C24 | 2.38  | 123.18      | 120.24   |
| 2   | I     | 1001 | VFE  | C12-C11-N14 | 2.37  | 122.49      | 119.58   |
| 2   | C     | 1001 | VFE  | C5-N6-C19   | 2.37  | 127.74      | 120.81   |
| 2   | T     | 1001 | VFE  | C12-C11-C10 | 2.36  | 123.68      | 119.18   |
| 2   | d     | 1001 | VFE  | O20-C19-N6  | 2.35  | 126.31      | 122.12   |
| 2   | X     | 1001 | VFE  | C24-C23-S22 | 2.35  | 127.17      | 121.48   |
| 2   | b     | 1001 | VFE  | C7-N6-C19   | -2.34 | 115.56      | 121.78   |
| 2   | V     | 1001 | VFE  | C24-C23-S22 | 2.34  | 127.15      | 121.48   |
| 2   | c     | 1001 | VFE  | C24-C23-S22 | 2.33  | 127.13      | 121.48   |
| 2   | K     | 1001 | VFE  | C25-C26-C27 | -2.33 | 117.37      | 120.24   |
| 2   | Z     | 1001 | VFE  | O20-C19-N6  | 2.32  | 126.25      | 122.12   |
| 2   | O     | 1001 | VFE  | C3-C5-N6    | -2.32 | 107.29      | 113.22   |
| 2   | V     | 1001 | VFE  | C12-C11-N14 | 2.32  | 122.42      | 119.58   |
| 2   | I     | 1001 | VFE  | C24-C23-C28 | -2.31 | 114.53      | 117.55   |
| 2   | P     | 1001 | VFE  | C12-C13-C8  | -2.31 | 117.97      | 121.00   |
| 2   | R     | 1001 | VFE  | C10-C11-N14 | -2.30 | 116.78      | 119.58   |
| 2   | J     | 1001 | VFE  | C7-C8-C13   | -2.29 | 116.52      | 120.75   |
| 2   | W     | 1001 | VFE  | C25-C26-C27 | -2.29 | 117.41      | 120.24   |
| 2   | Q     | 1001 | VFE  | C5-N6-C19   | 2.29  | 127.52      | 120.81   |
| 2   | a     | 1001 | VFE  | C5-N6-C19   | 2.29  | 127.51      | 120.81   |
| 2   | b     | 1001 | VFE  | C3-C5-N6    | -2.28 | 107.37      | 113.22   |
| 2   | A     | 1001 | VFE  | O4-C3-C5    | 2.28  | 125.01      | 121.02   |
| 2   | X     | 1001 | VFE  | C15-N14-N18 | 2.27  | 111.88      | 109.26   |
| 2   | R     | 1001 | VFE  | C21-S22-C23 | 2.27  | 106.16      | 102.27   |
| 2   | N     | 1001 | VFE  | C7-N6-C19   | -2.27 | 115.76      | 121.78   |
| 2   | T     | 1001 | VFE  | C10-C9-C8   | -2.26 | 118.03      | 121.00   |
| 2   | R     | 1001 | VFE  | O4-C3-C5    | 2.25  | 124.95      | 121.02   |
| 2   | a     | 1001 | VFE  | C26-C27-C28 | -2.23 | 116.07      | 119.42   |
| 2   | A     | 1001 | VFE  | C9-C10-C11  | -2.22 | 117.49      | 120.30   |
| 2   | d     | 1001 | VFE  | C26-C27-C28 | -2.22 | 116.09      | 119.42   |
| 2   | F     | 1001 | VFE  | O20-C19-N6  | 2.22  | 126.07      | 122.12   |
| 2   | T     | 1001 | VFE  | C5-C3-N2    | -2.21 | 112.61      | 116.27   |
| 2   | V     | 1001 | VFE  | C25-C26-C27 | -2.20 | 117.53      | 120.24   |
| 2   | L     | 1001 | VFE  | C13-C8-C9   | 2.19  | 121.50      | 118.23   |
| 2   | b     | 1001 | VFE  | C23-C28-CL  | -2.19 | 115.91      | 119.72   |
| 2   | S     | 1001 | VFE  | O4-C3-C5    | 2.19  | 124.85      | 121.02   |
| 2   | Q     | 1001 | VFE  | C27-C28-CL  | 2.18  | 122.71      | 118.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | O     | 1001 | VFE  | C5-N6-C19   | 2.18  | 127.18      | 120.81   |
| 2   | F     | 1001 | VFE  | C26-C25-C24 | 2.17  | 122.92      | 120.24   |
| 2   | U     | 1001 | VFE  | C21-S22-C23 | 2.16  | 105.98      | 102.27   |
| 2   | J     | 1001 | VFE  | C27-C28-C23 | 2.16  | 126.83      | 122.28   |
| 2   | S     | 1001 | VFE  | C21-S22-C23 | 2.16  | 105.97      | 102.27   |
| 2   | c     | 1001 | VFE  | C5-N6-C19   | 2.15  | 127.11      | 120.81   |
| 2   | S     | 1001 | VFE  | C26-C27-C28 | -2.15 | 116.19      | 119.42   |
| 2   | N     | 1001 | VFE  | C5-C3-N2    | -2.15 | 112.71      | 116.27   |
| 2   | M     | 1001 | VFE  | N14-C15-N16 | -2.14 | 105.91      | 110.38   |
| 2   | A     | 1001 | VFE  | C8-C7-N6    | 2.14  | 116.52      | 113.15   |
| 2   | W     | 1001 | VFE  | O20-C19-N6  | 2.14  | 125.93      | 122.12   |
| 2   | N     | 1001 | VFE  | C19-C21-S22 | 2.14  | 119.04      | 112.07   |
| 2   | X     | 1001 | VFE  | O20-C19-N6  | 2.13  | 125.92      | 122.12   |
| 2   | M     | 1001 | VFE  | C8-C7-N6    | 2.13  | 116.50      | 113.15   |
| 2   | L     | 1001 | VFE  | C26-C27-C28 | -2.12 | 116.23      | 119.42   |
| 2   | c     | 1001 | VFE  | C13-C12-C11 | 2.09  | 122.95      | 120.30   |
| 2   | H     | 1001 | VFE  | C27-C28-CL  | 2.09  | 122.54      | 118.42   |
| 2   | a     | 1001 | VFE  | C24-C23-S22 | 2.06  | 126.47      | 121.48   |
| 2   | Y     | 1001 | VFE  | C27-C28-CL  | 2.05  | 122.46      | 118.42   |
| 2   | W     | 1001 | VFE  | C26-C27-C28 | -2.04 | 116.36      | 119.42   |
| 2   | I     | 1001 | VFE  | C25-C26-C27 | -2.04 | 117.73      | 120.24   |
| 2   | M     | 1001 | VFE  | O20-C19-C21 | -2.02 | 117.17      | 121.19   |
| 2   | H     | 1001 | VFE  | C24-C23-C28 | -2.02 | 114.91      | 117.55   |
| 2   | X     | 1001 | VFE  | O20-C19-C21 | -2.02 | 117.17      | 121.19   |
| 2   | S     | 1001 | VFE  | C5-N6-C19   | 2.02  | 126.72      | 120.81   |
| 2   | G     | 1001 | VFE  | C25-C26-C27 | -2.01 | 117.76      | 120.24   |
| 2   | P     | 1001 | VFE  | C7-N6-C19   | -2.01 | 116.44      | 121.78   |
| 2   | A     | 1001 | VFE  | O20-C19-N6  | 2.01  | 125.70      | 122.12   |
| 2   | O     | 1001 | VFE  | C7-C8-C13   | -2.01 | 117.05      | 120.75   |
| 2   | K     | 1001 | VFE  | C7-N6-C19   | -2.00 | 116.46      | 121.78   |

There are no chirality outliers.

All (83) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 2   | I     | 1001 | VFE  | C5-C3-N2-C1  |
| 2   | I     | 1001 | VFE  | C3-C5-N6-C19 |
| 2   | K     | 1001 | VFE  | C5-C3-N2-C1  |
| 2   | L     | 1001 | VFE  | C5-C3-N2-C1  |
| 2   | O     | 1001 | VFE  | C5-C3-N2-C1  |
| 2   | Z     | 1001 | VFE  | C5-C3-N2-C1  |
| 2   | I     | 1001 | VFE  | O4-C3-N2-C1  |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 2   | K     | 1001 | VFE  | O4-C3-N2-C1 |
| 2   | G     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | L     | 1001 | VFE  | O4-C3-N2-C1 |
| 2   | A     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | Q     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | R     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | U     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | V     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | Y     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | Z     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | c     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | H     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | Z     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | A     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | D     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | G     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | K     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | R     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | U     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | V     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | Y     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | P     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | c     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | P     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | Q     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | B     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | C     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | D     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | K     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | N     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | b     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | B     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | H     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | b     | 1001 | VFE  | O4-C3-C5-N6 |
| 2   | O     | 1001 | VFE  | O4-C3-N2-C1 |
| 2   | P     | 1001 | VFE  | O4-C3-N2-C1 |
| 2   | Z     | 1001 | VFE  | O4-C3-N2-C1 |
| 2   | F     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | J     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | M     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | S     | 1001 | VFE  | N2-C3-C5-N6 |
| 2   | T     | 1001 | VFE  | N2-C3-C5-N6 |

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| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 2   | W     | 1001 | VFE  | N2-C3-C5-N6   |
| 2   | a     | 1001 | VFE  | N2-C3-C5-N6   |
| 2   | d     | 1001 | VFE  | N2-C3-C5-N6   |
| 2   | C     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | M     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | S     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | T     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | W     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | I     | 1001 | VFE  | N2-C3-C5-N6   |
| 2   | X     | 1001 | VFE  | N2-C3-C5-N6   |
| 2   | F     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | N     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | a     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | C     | 1001 | VFE  | C5-C3-N2-C1   |
| 2   | P     | 1001 | VFE  | C5-C3-N2-C1   |
| 2   | R     | 1001 | VFE  | C5-C3-N2-C1   |
| 2   | U     | 1001 | VFE  | C5-C3-N2-C1   |
| 2   | V     | 1001 | VFE  | C5-C3-N2-C1   |
| 2   | Y     | 1001 | VFE  | C5-C3-N2-C1   |
| 2   | b     | 1001 | VFE  | C5-C3-N2-C1   |
| 2   | b     | 1001 | VFE  | O4-C3-N2-C1   |
| 2   | I     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | J     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | E     | 1001 | VFE  | N2-C3-C5-N6   |
| 2   | d     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | L     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | O     | 1001 | VFE  | N2-C3-C5-N6   |
| 2   | E     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | C     | 1001 | VFE  | O4-C3-N2-C1   |
| 2   | X     | 1001 | VFE  | O4-C3-C5-N6   |
| 2   | B     | 1001 | VFE  | O20-C19-N6-C5 |
| 2   | B     | 1001 | VFE  | C21-C19-N6-C5 |
| 2   | V     | 1001 | VFE  | O4-C3-N2-C1   |
| 2   | O     | 1001 | VFE  | O4-C3-C5-N6   |

There are no ring outliers.

7 monomers are involved in 7 short contacts:

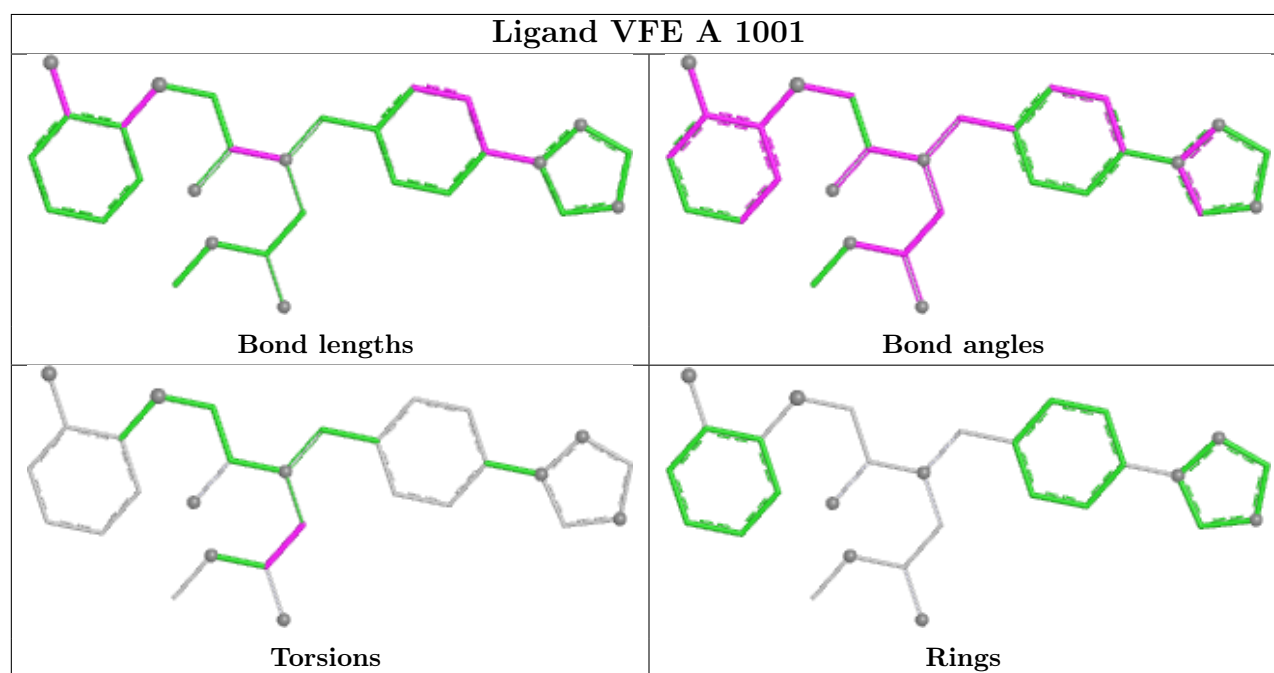
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | F     | 1001 | VFE  | 1       | 0            |
| 2   | C     | 1001 | VFE  | 1       | 0            |
| 2   | Y     | 1001 | VFE  | 1       | 0            |

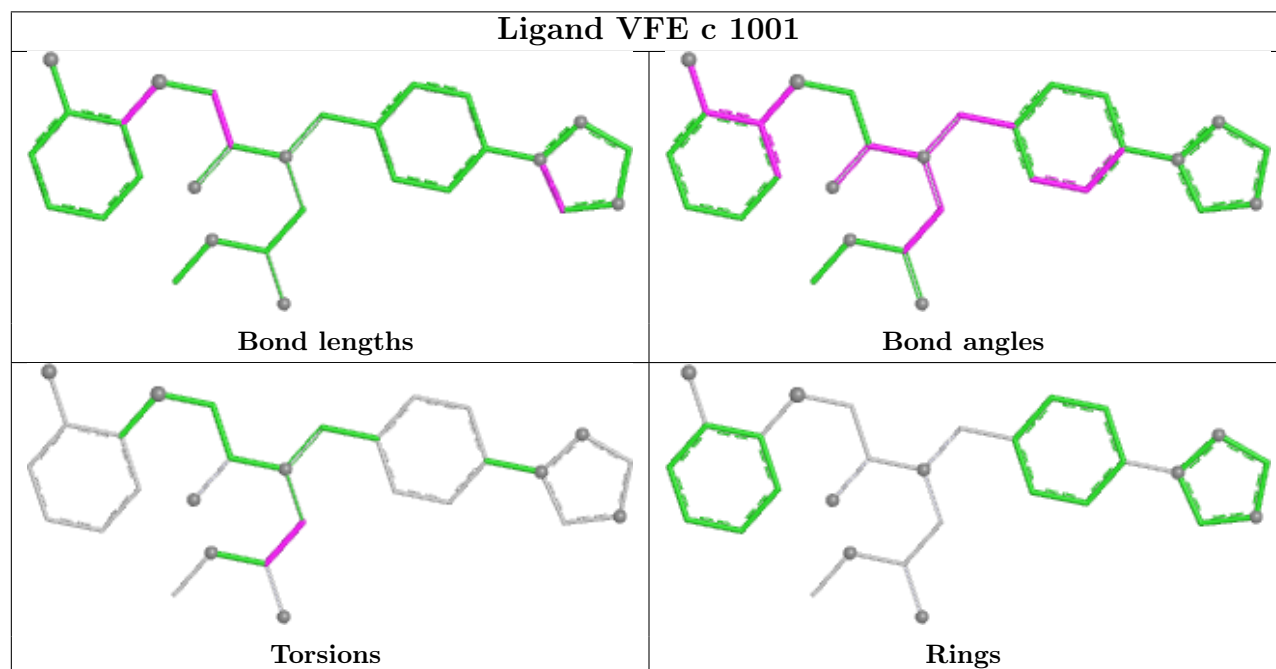
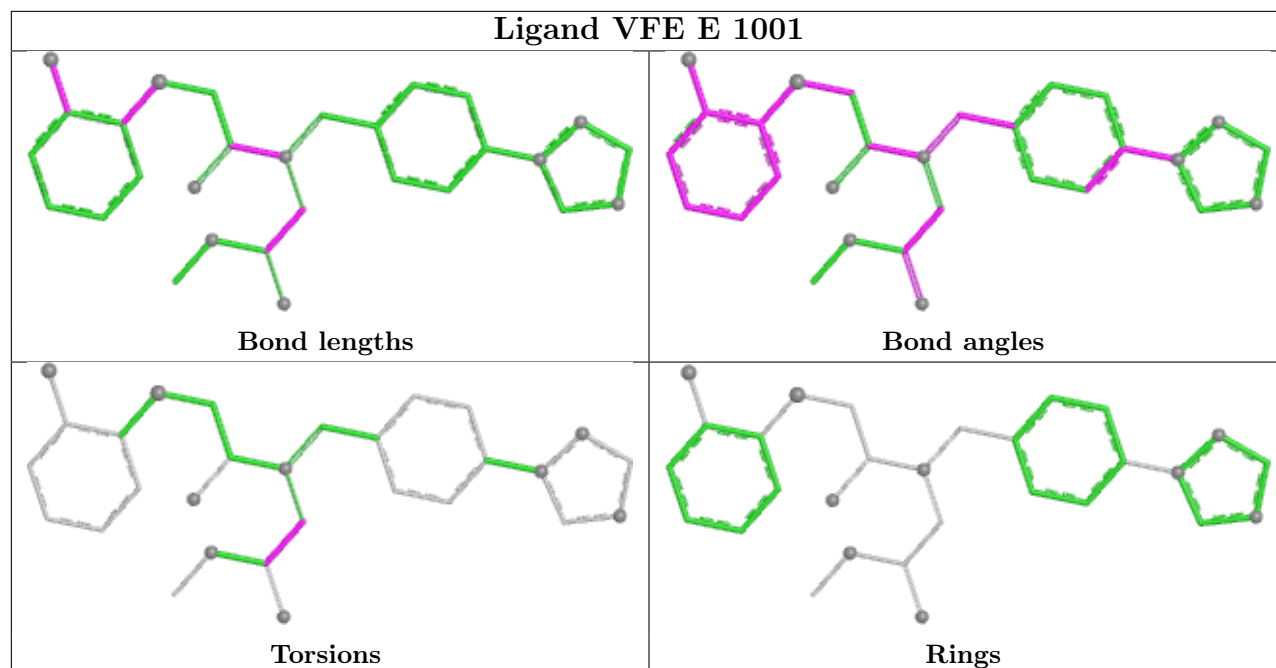
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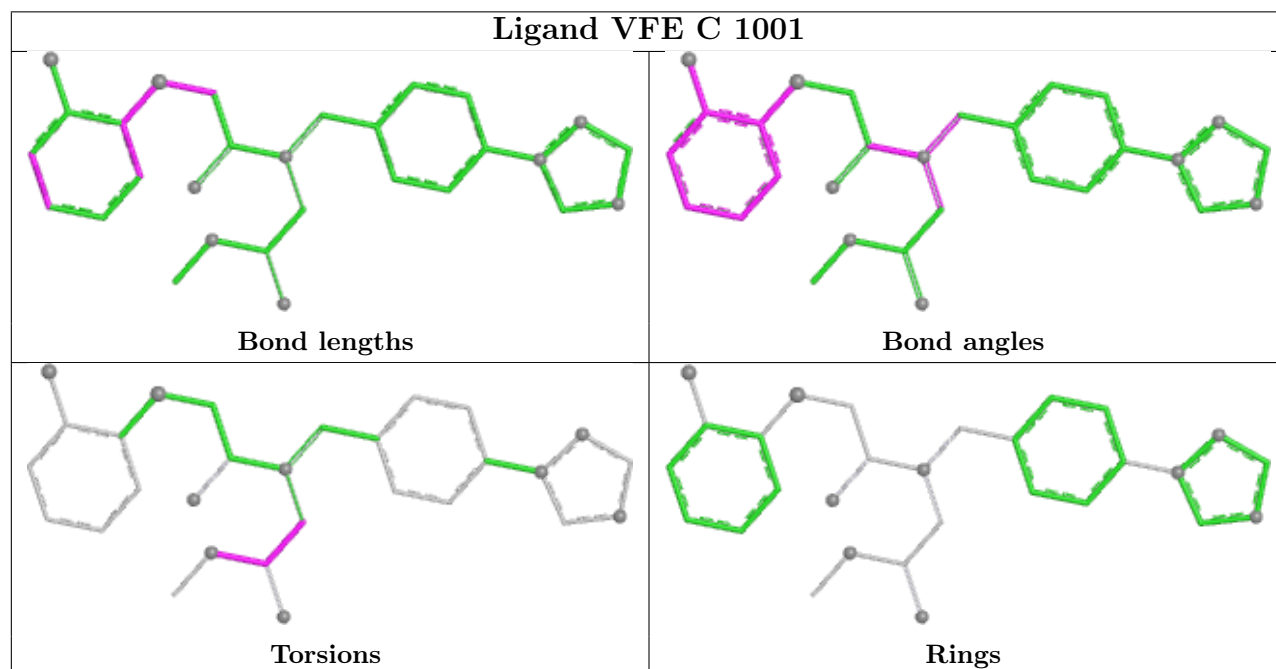
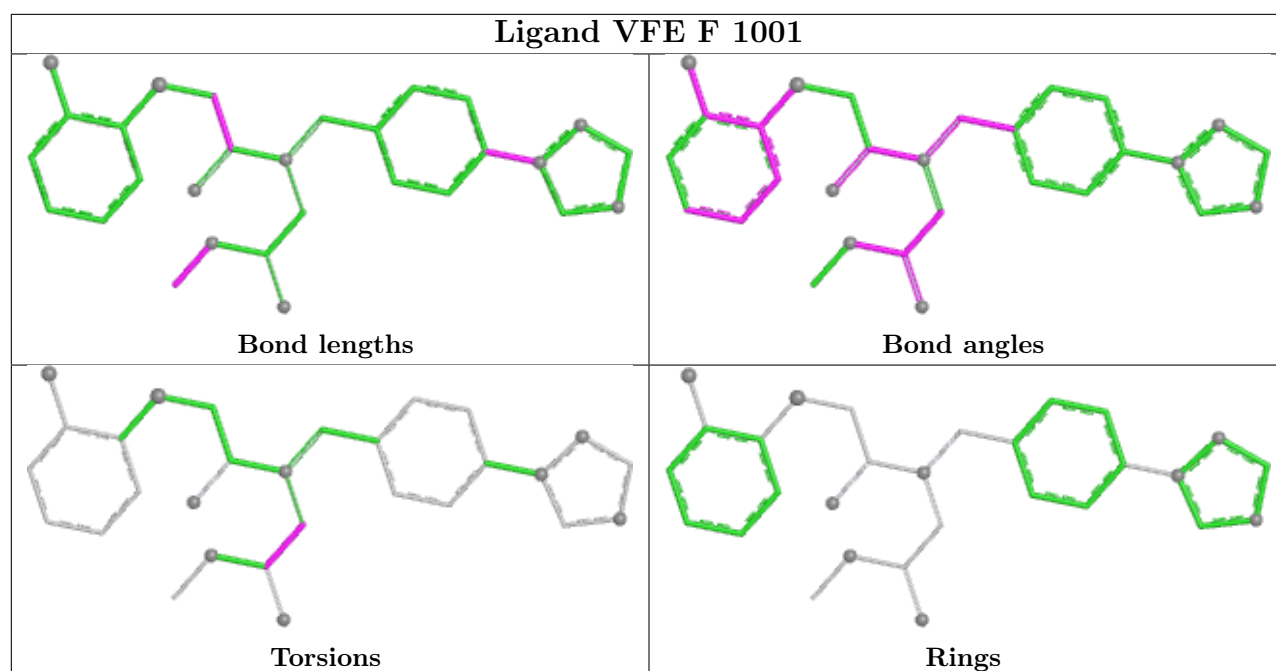
*Continued from previous page...*

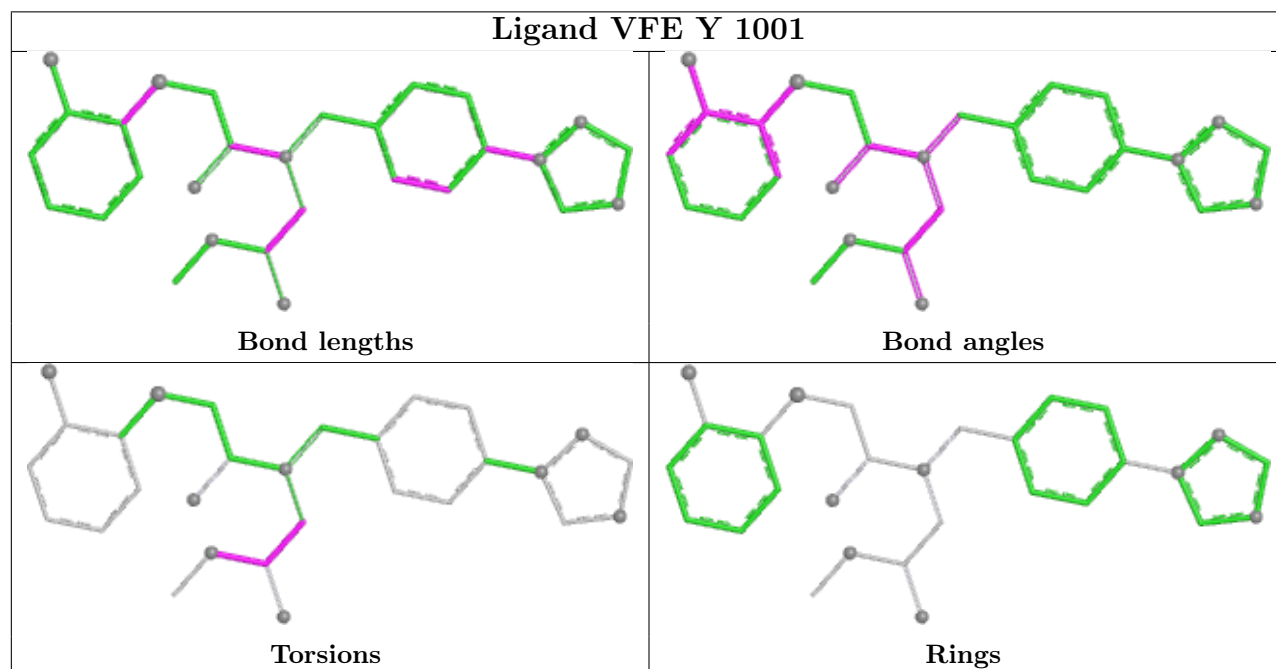
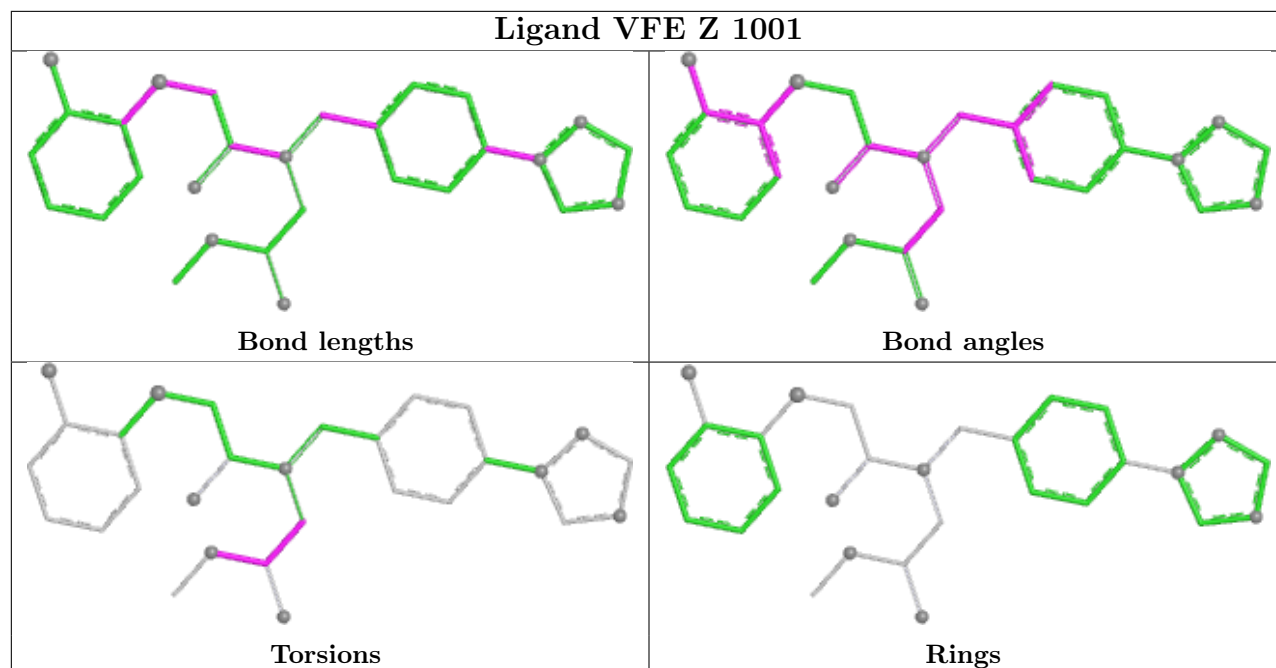
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | U     | 1001 | VFE  | 1       | 0            |
| 2   | d     | 1001 | VFE  | 1       | 0            |
| 2   | X     | 1001 | VFE  | 1       | 0            |
| 2   | M     | 1001 | VFE  | 1       | 0            |

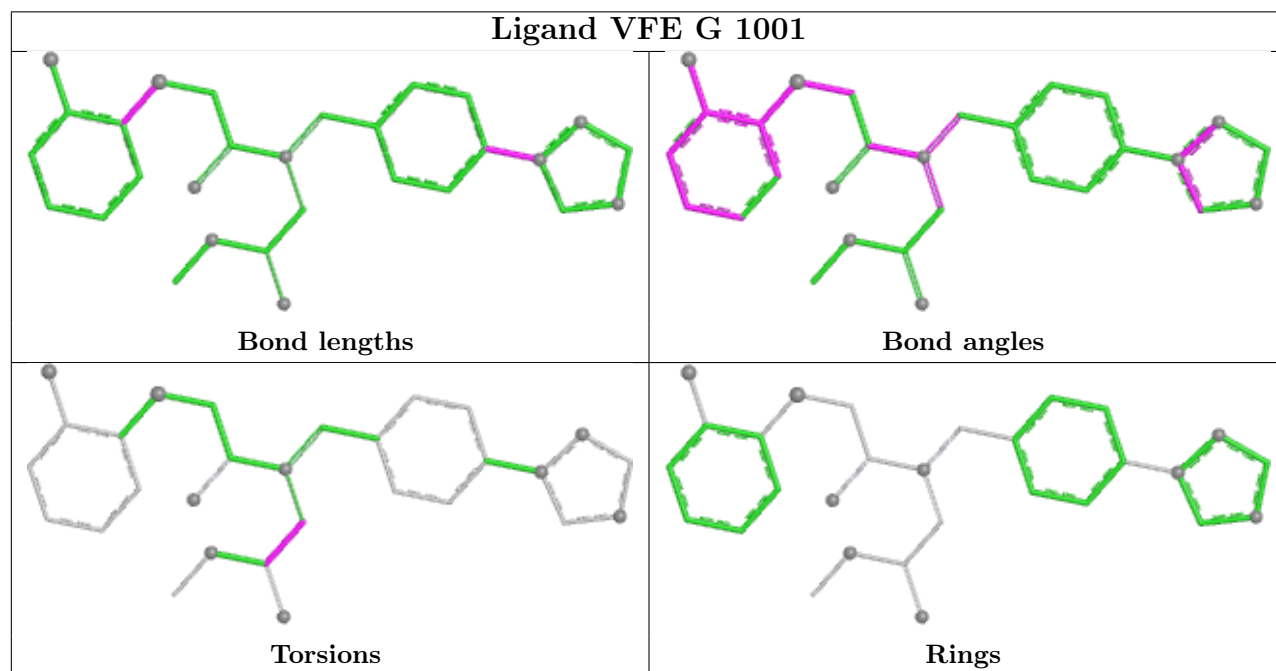
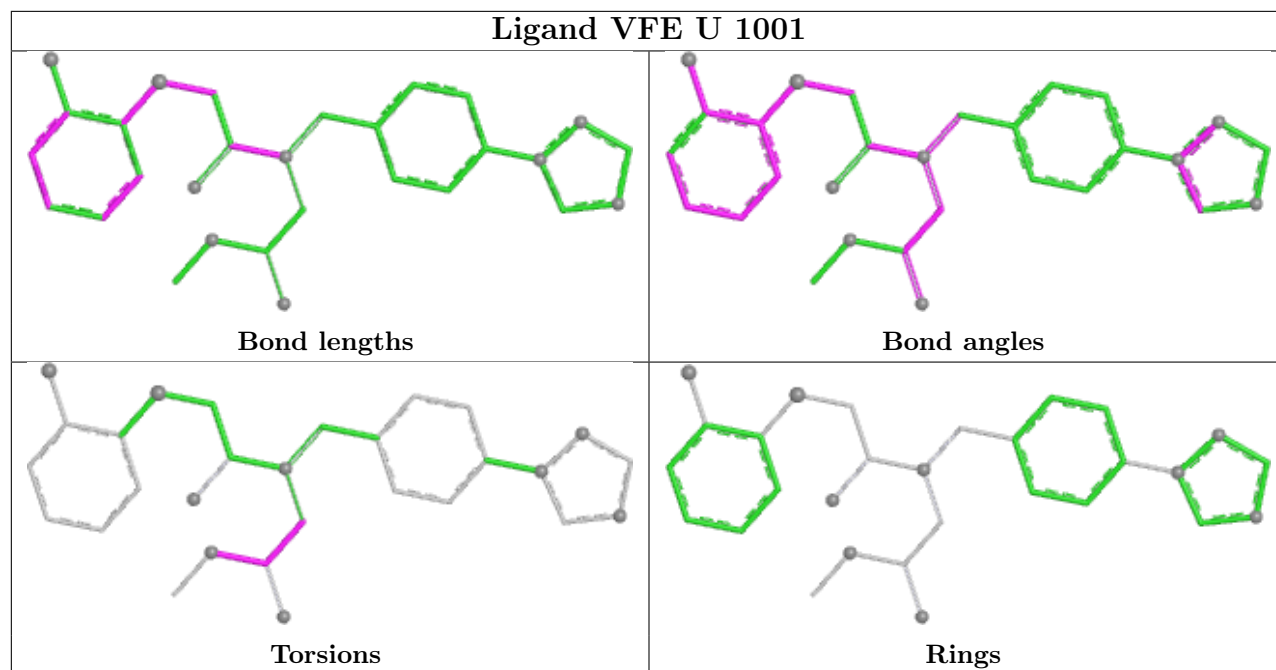
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



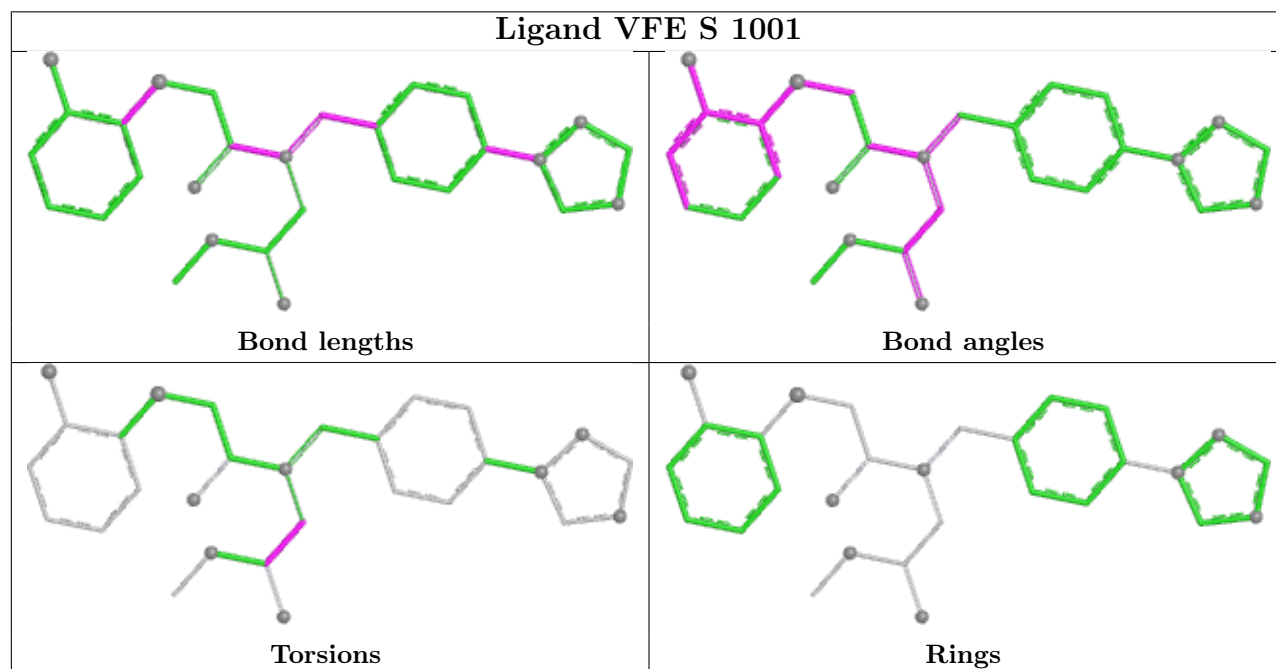
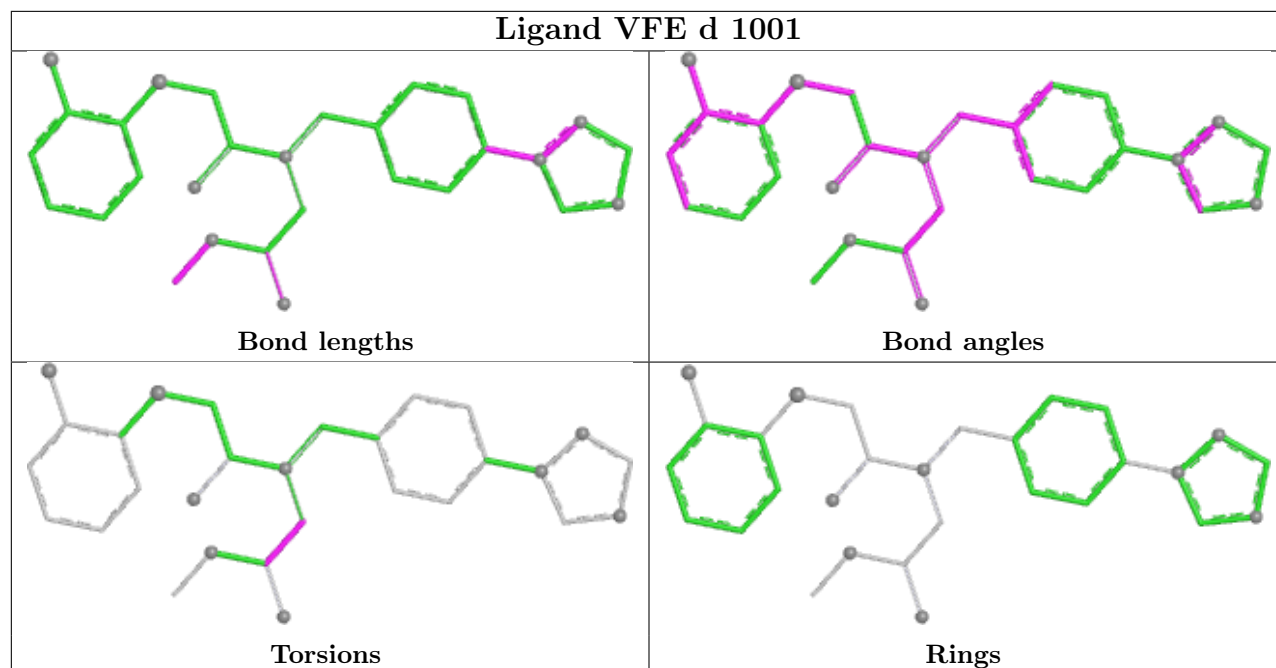


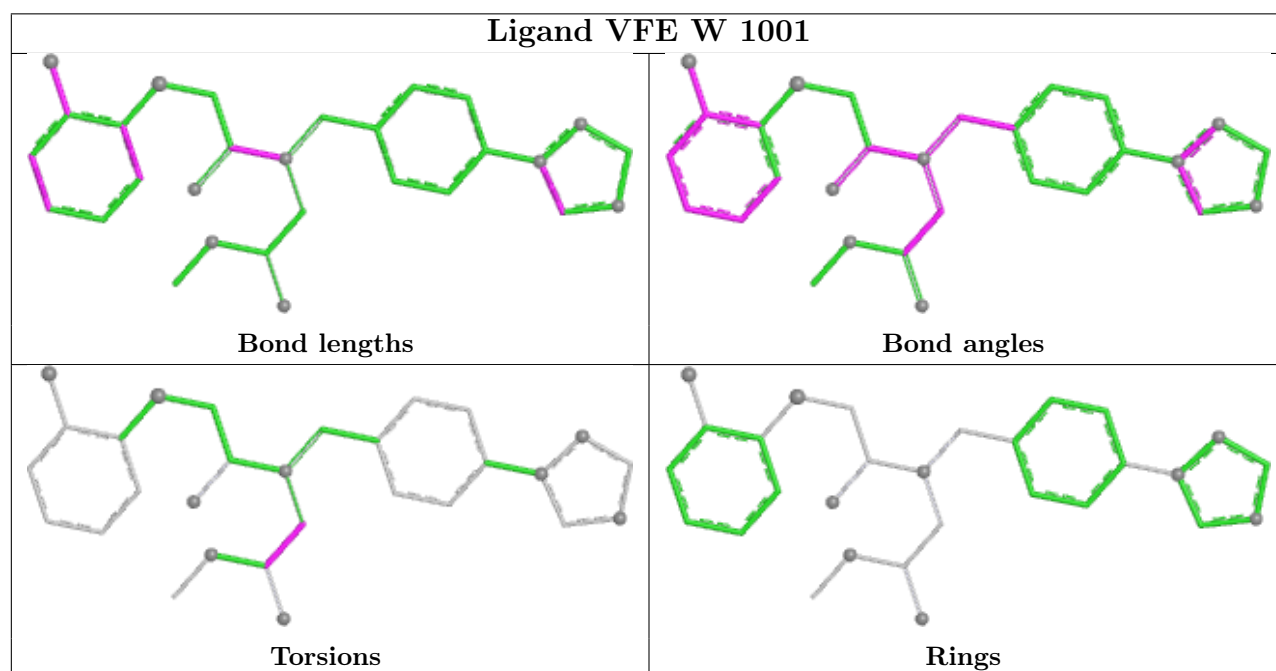
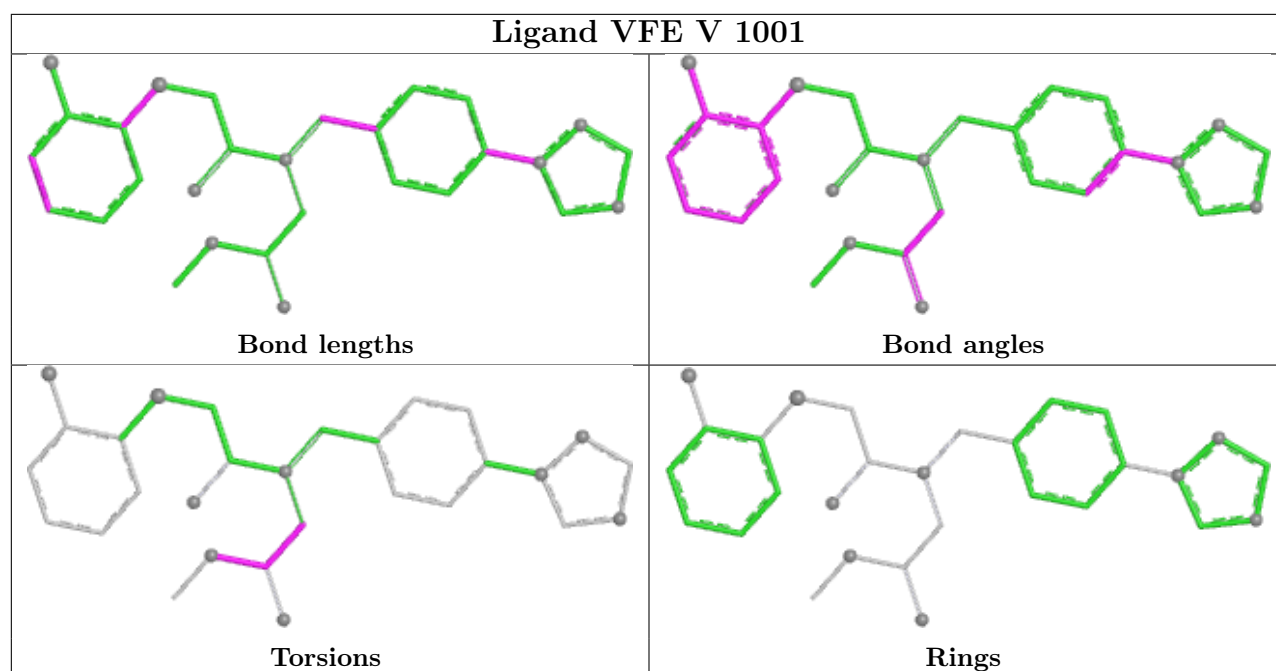




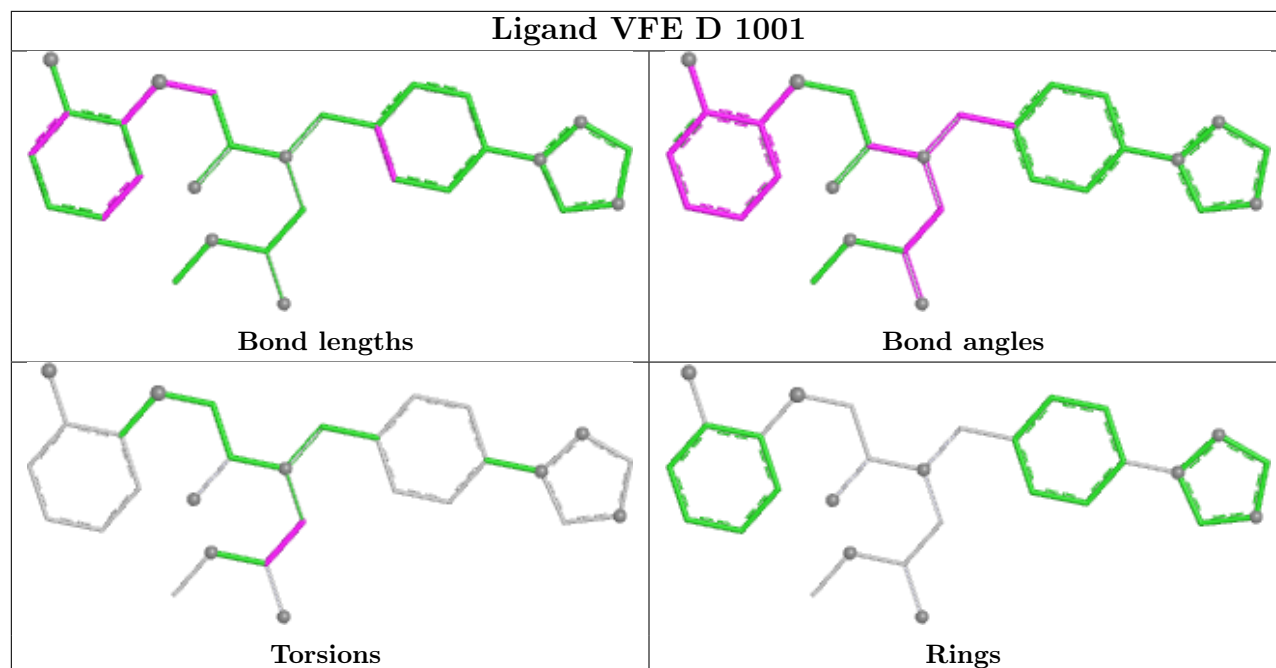




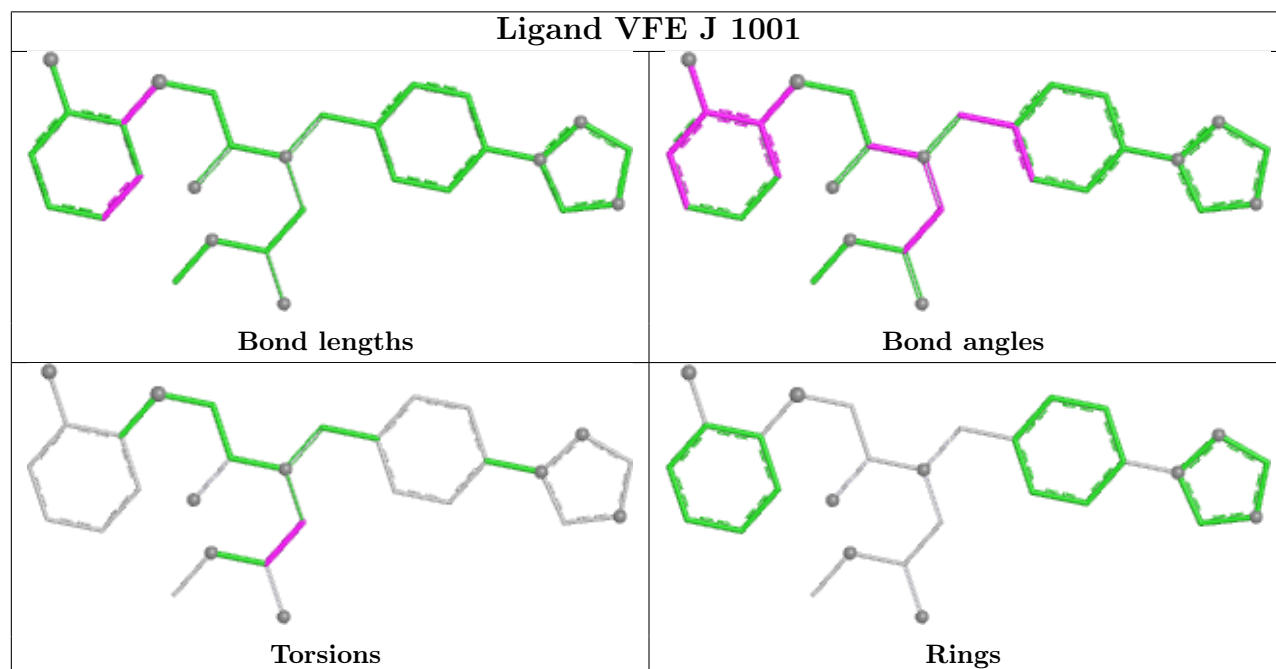


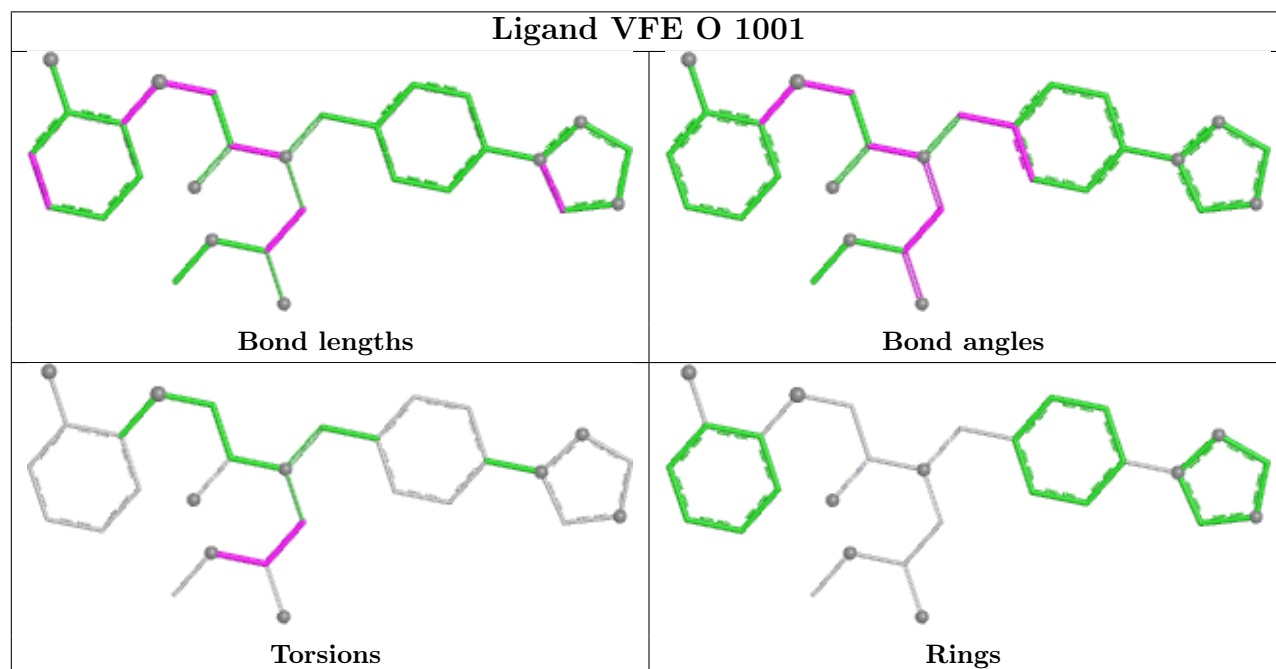
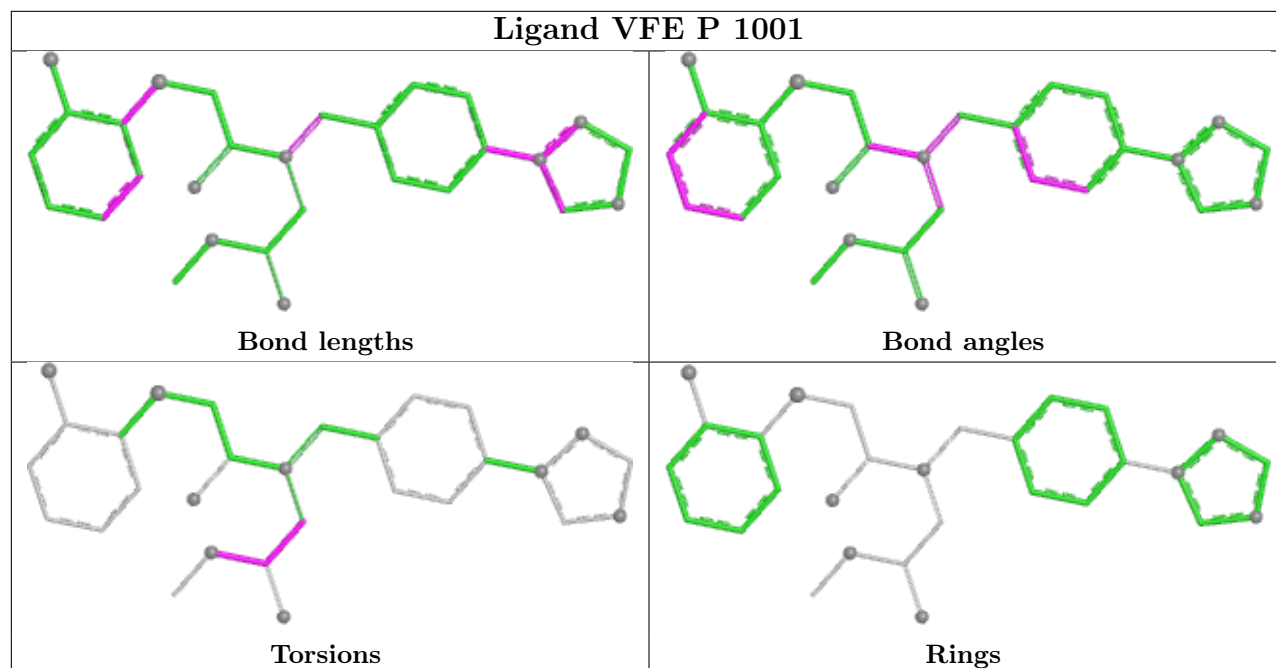


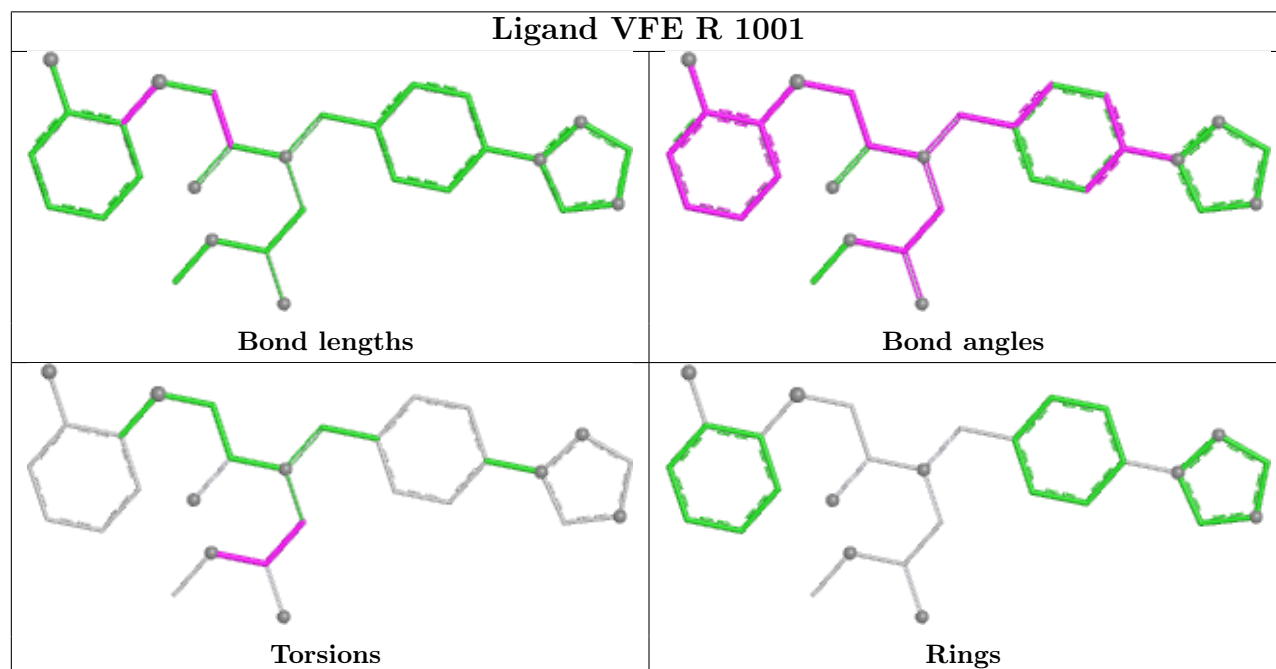
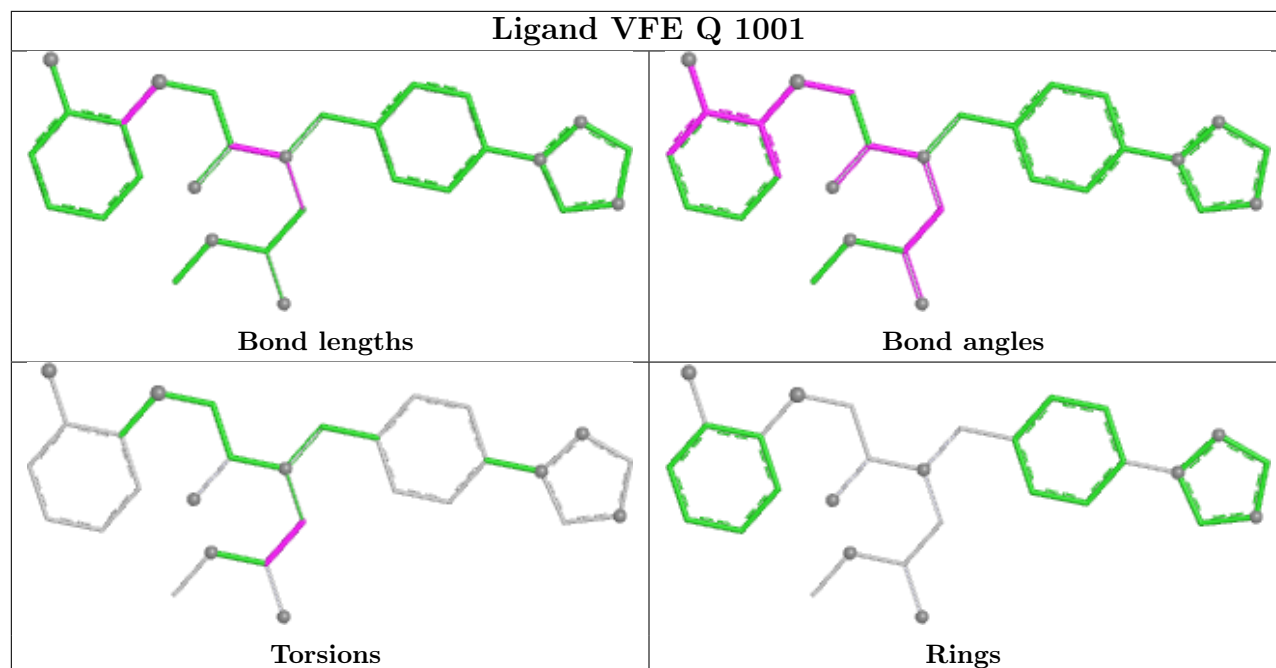
## Ligand VFE D 1001

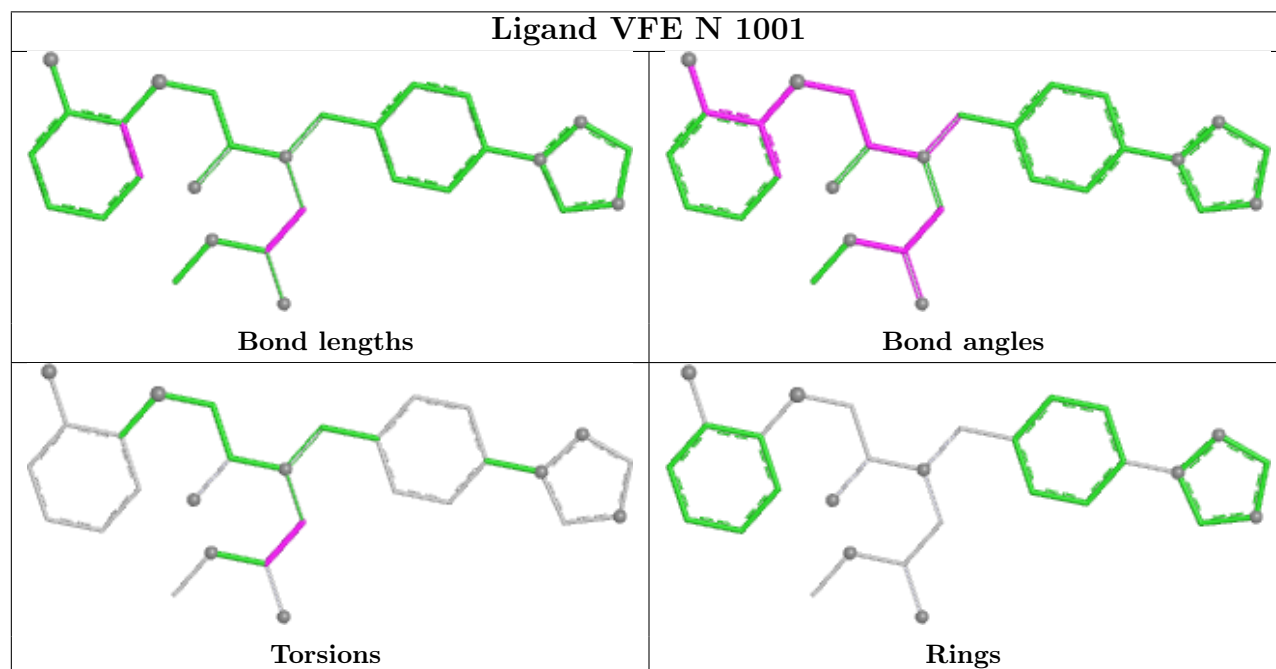
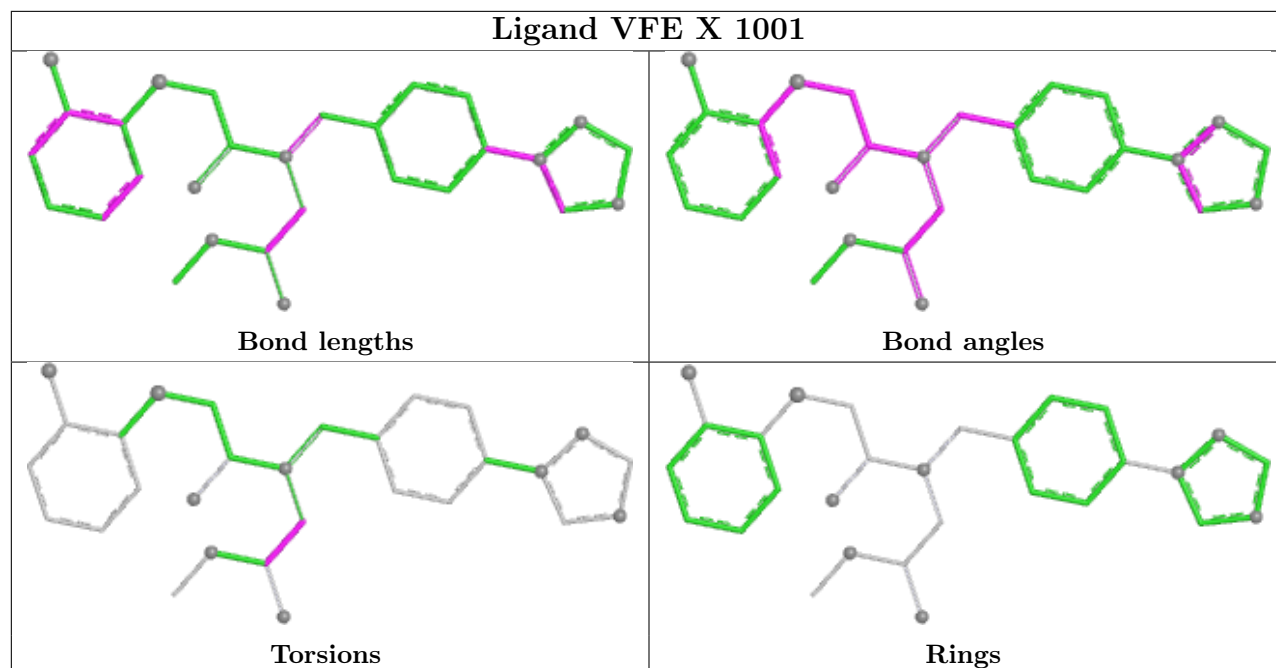


## Ligand VFE J 1001

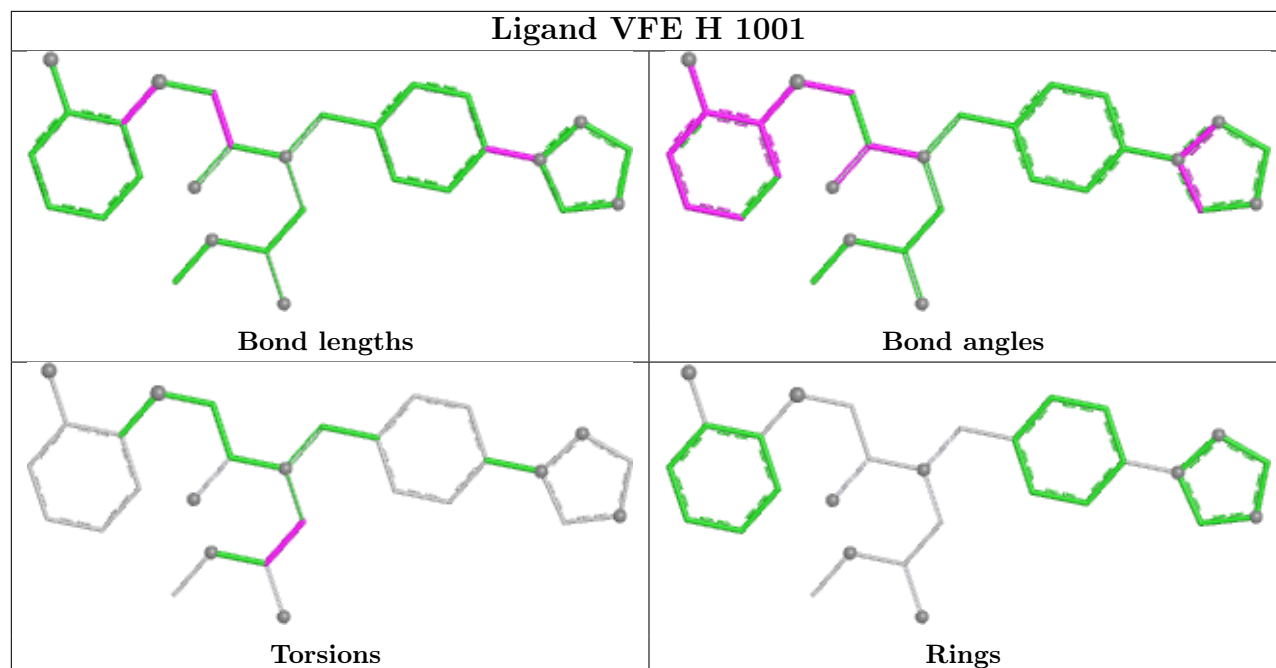




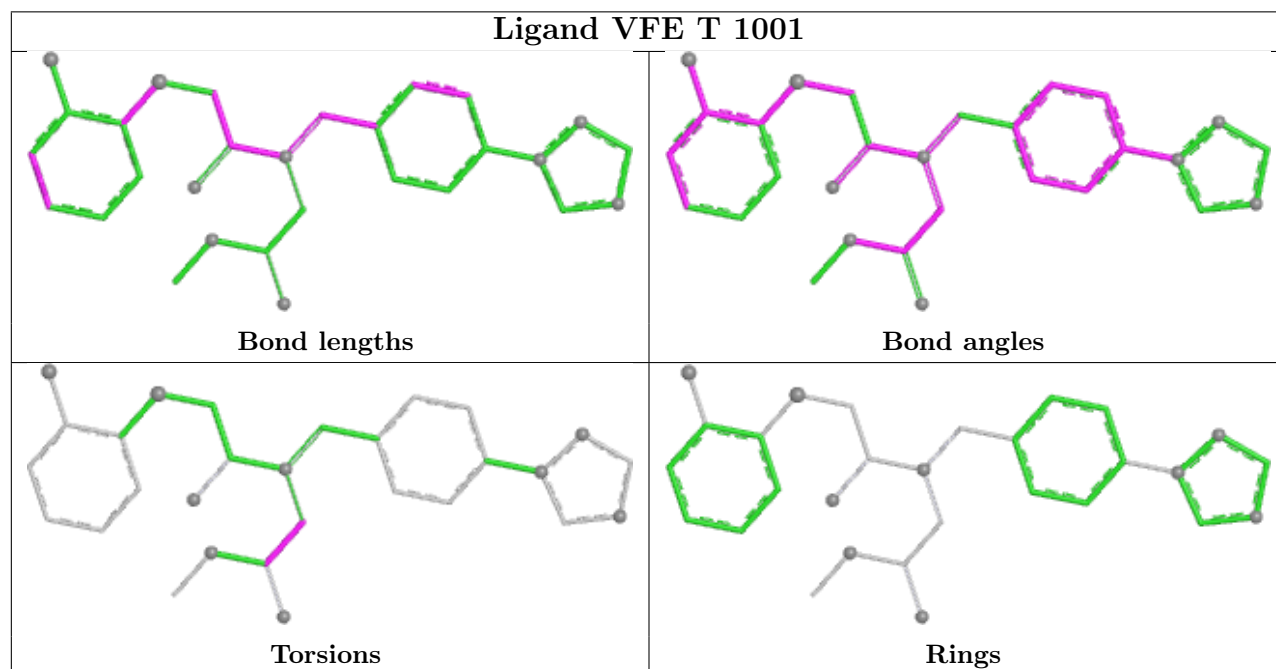


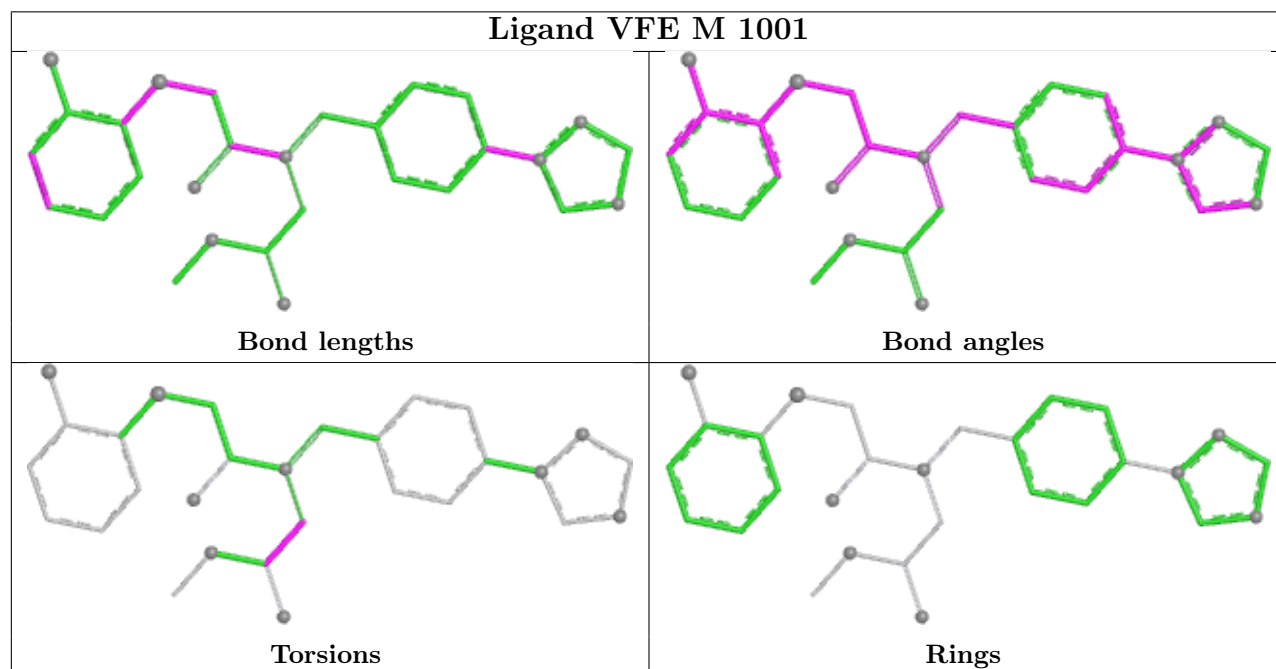
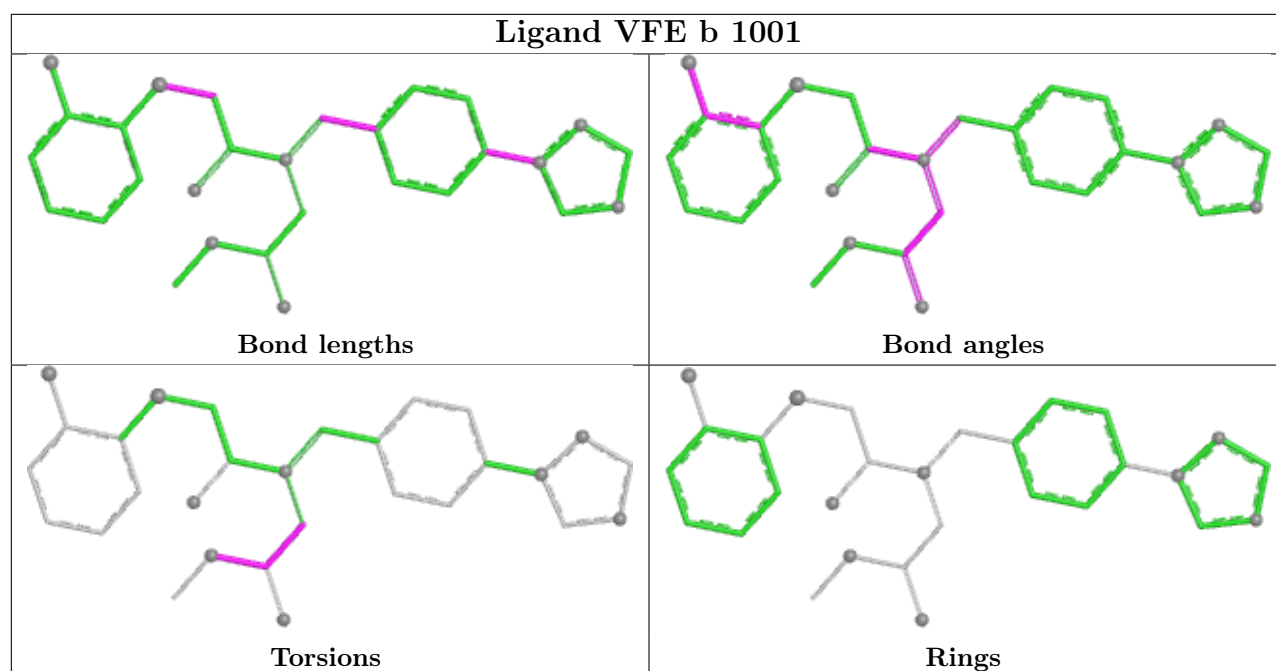


## Ligand VFE H 1001

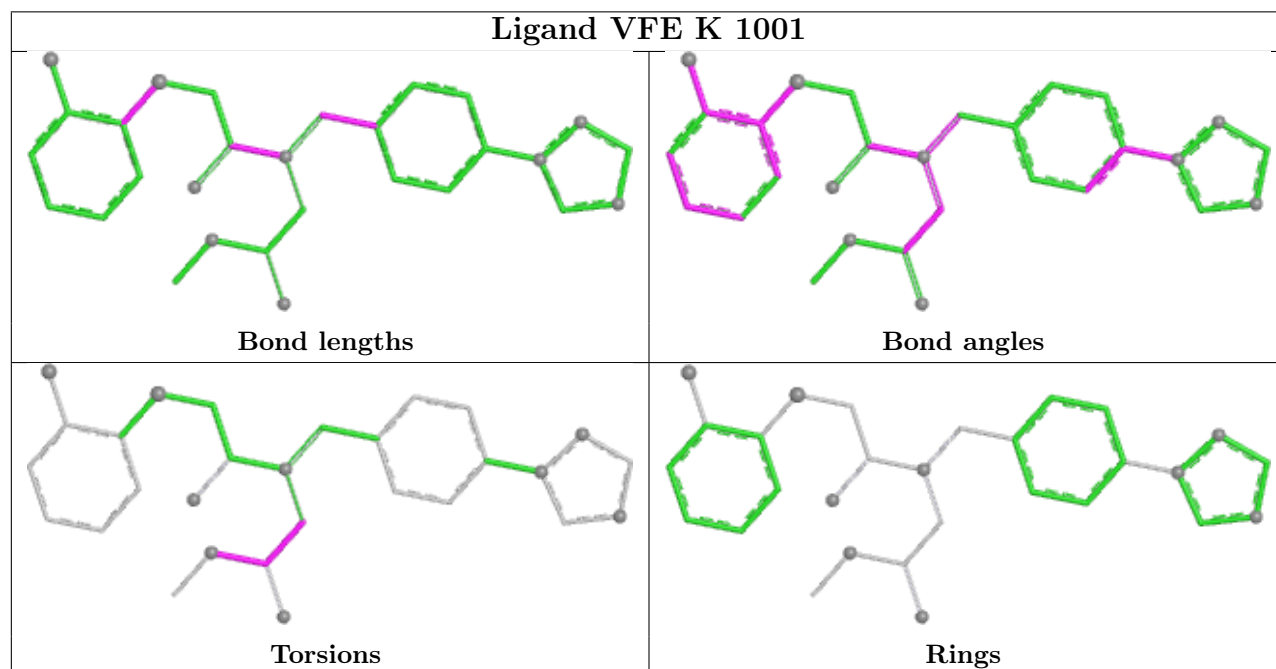
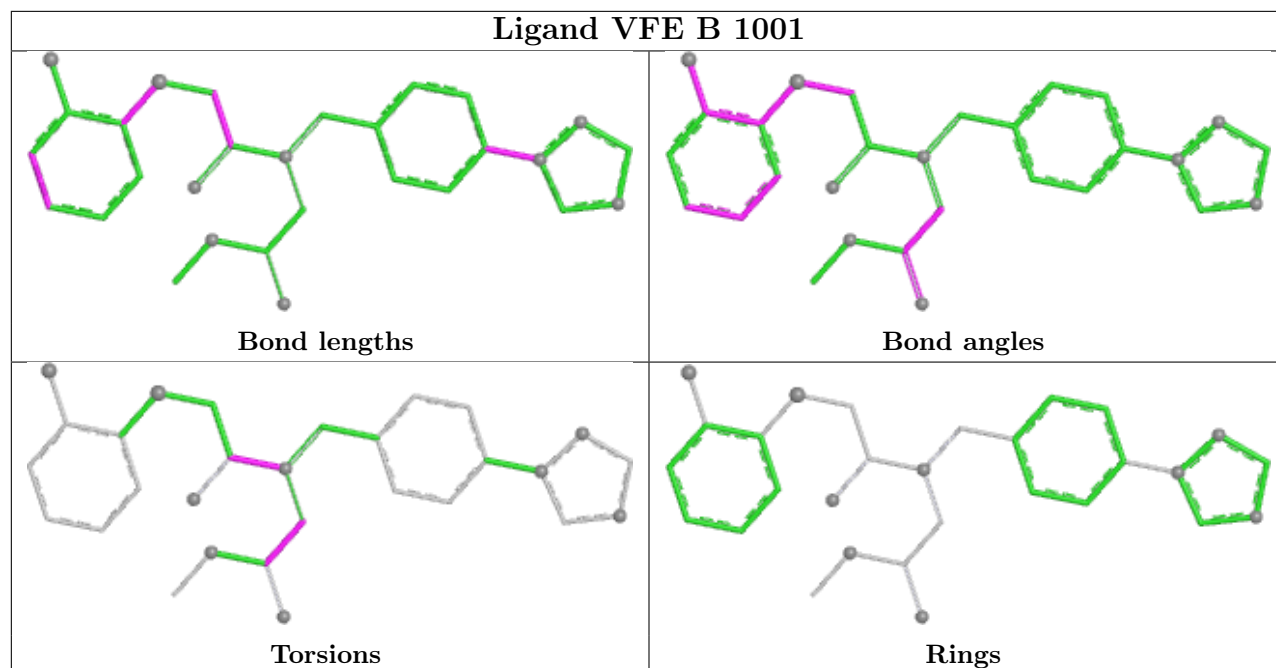


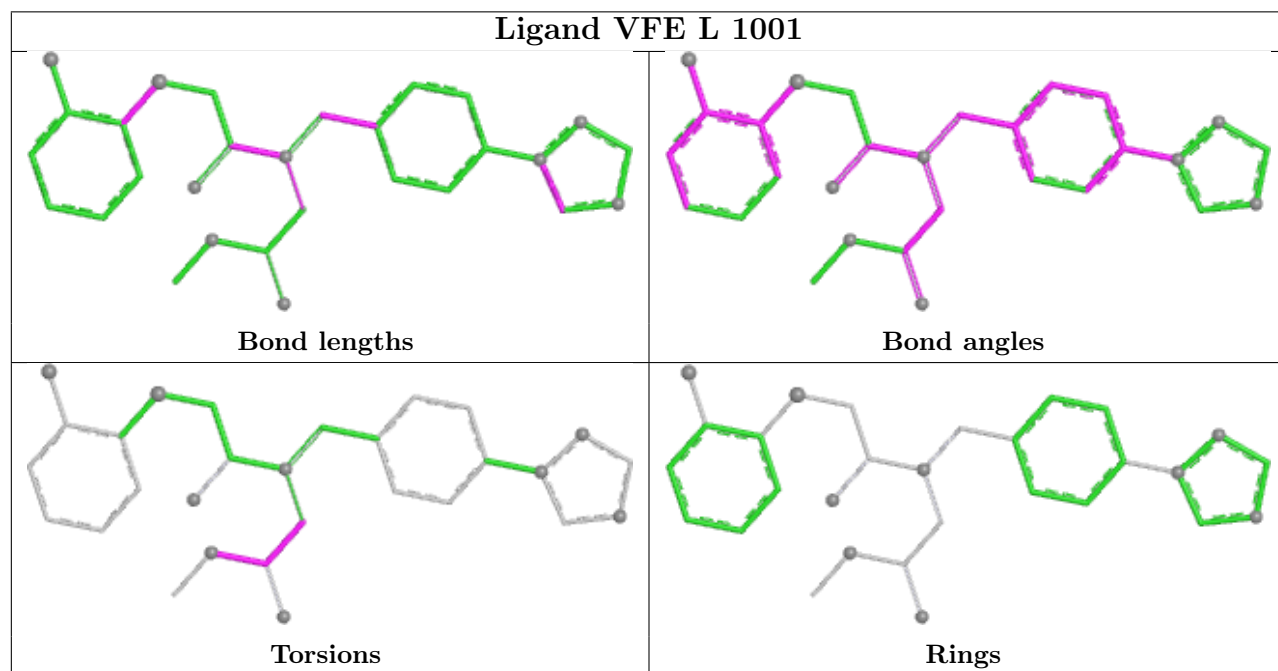
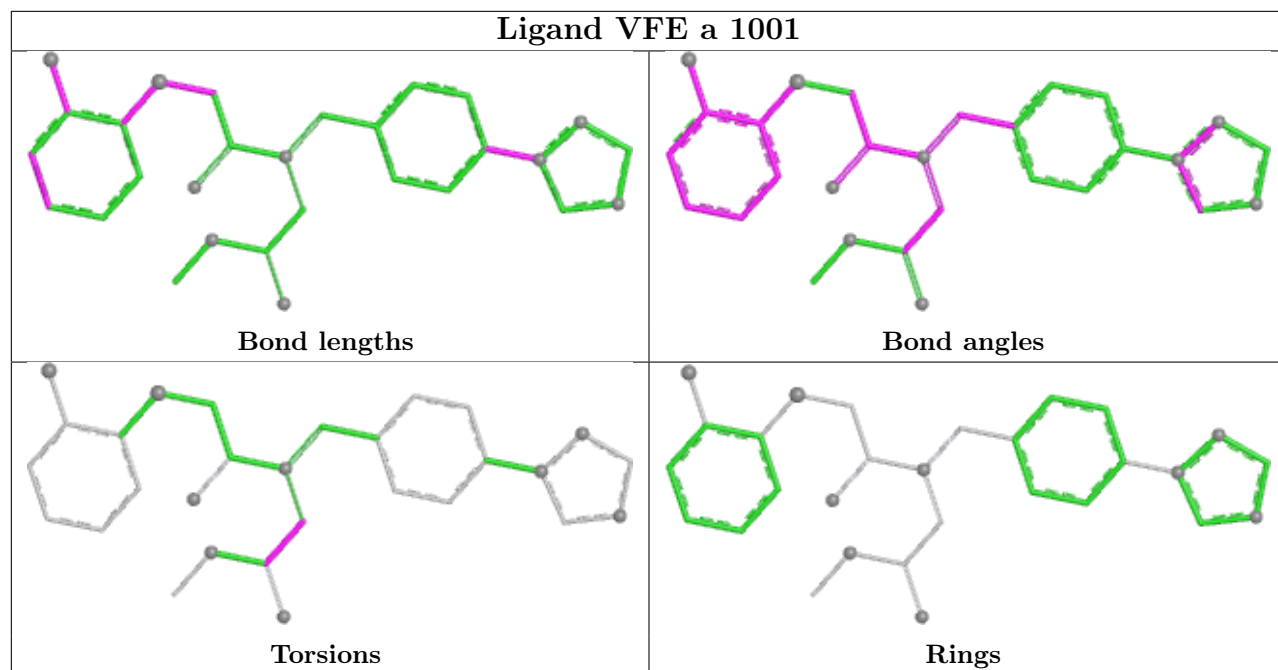
## Ligand VFE T 1001

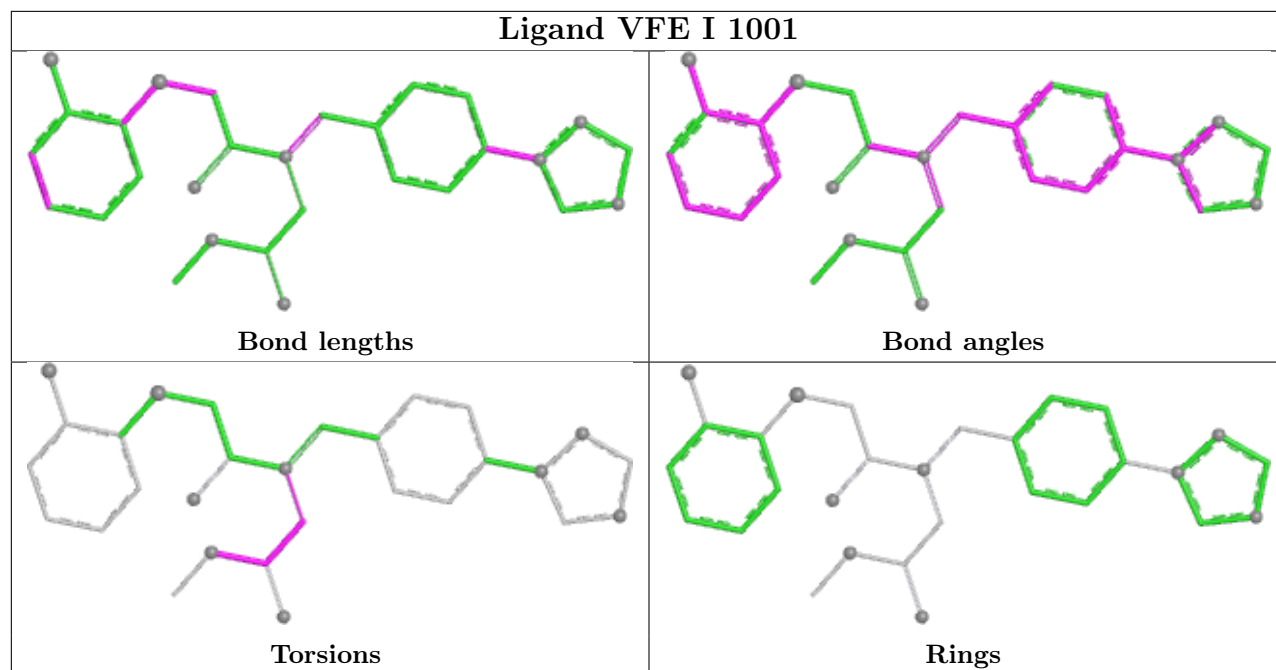












## 5.7 Other polymers [i](#)

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(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|---------|
| 1   | A     | 258/261 (98%) | 0.06   | 7 (2%) 56 47  | 23, 44, 73, 124       | 1 (0%)  |
| 1   | B     | 258/261 (98%) | 0.04   | 7 (2%) 56 47  | 24, 43, 71, 105       | 1 (0%)  |
| 1   | C     | 257/261 (98%) | -0.01  | 6 (2%) 61 52  | 21, 42, 69, 84        | 1 (0%)  |
| 1   | D     | 257/261 (98%) | 0.04   | 9 (3%) 47 37  | 22, 42, 69, 84        | 1 (0%)  |
| 1   | E     | 258/261 (98%) | -0.01  | 7 (2%) 56 47  | 23, 42, 69, 125       | 1 (0%)  |
| 1   | F     | 257/261 (98%) | -0.05  | 5 (1%) 66 59  | 23, 43, 70, 89        | 1 (0%)  |
| 1   | G     | 258/261 (98%) | 0.38   | 13 (5%) 34 27 | 37, 56, 93, 136       | 1 (0%)  |
| 1   | H     | 258/261 (98%) | 0.37   | 12 (4%) 36 29 | 35, 55, 93, 127       | 1 (0%)  |
| 1   | I     | 258/261 (98%) | 0.27   | 11 (4%) 40 31 | 35, 54, 89, 117       | 1 (0%)  |
| 1   | J     | 257/261 (98%) | 0.21   | 6 (2%) 61 52  | 34, 53, 87, 96        | 1 (0%)  |
| 1   | K     | 258/261 (98%) | 0.29   | 11 (4%) 40 31 | 34, 53, 88, 140       | 1 (0%)  |
| 1   | L     | 258/261 (98%) | 0.27   | 9 (3%) 47 37  | 37, 55, 90, 134       | 1 (0%)  |
| 1   | M     | 257/261 (98%) | 0.12   | 11 (4%) 40 31 | 32, 51, 82, 103       | 1 (0%)  |
| 1   | N     | 257/261 (98%) | 0.18   | 9 (3%) 47 37  | 33, 54, 88, 103       | 1 (0%)  |
| 1   | O     | 257/261 (98%) | 0.15   | 7 (2%) 56 47  | 32, 52, 86, 98        | 1 (0%)  |
| 1   | P     | 257/261 (98%) | 0.40   | 14 (5%) 31 24 | 34, 55, 91, 104       | 1 (0%)  |
| 1   | Q     | 257/261 (98%) | 0.29   | 12 (4%) 36 29 | 35, 55, 91, 102       | 1 (0%)  |
| 1   | R     | 258/261 (98%) | 0.24   | 9 (3%) 47 37  | 33, 52, 90, 122       | 1 (0%)  |
| 1   | S     | 258/261 (98%) | 0.00   | 5 (1%) 66 59  | 25, 45, 70, 123       | 1 (0%)  |
| 1   | T     | 258/261 (98%) | 0.08   | 6 (2%) 61 52  | 26, 46, 74, 110       | 1 (0%)  |
| 1   | U     | 259/261 (99%) | 0.07   | 11 (4%) 40 32 | 24, 43, 73, 117       | 1 (0%)  |
| 1   | V     | 258/261 (98%) | 0.07   | 7 (2%) 56 47  | 25, 46, 73, 121       | 1 (0%)  |
| 1   | W     | 258/261 (98%) | 0.08   | 8 (3%) 51 42  | 25, 45, 72, 107       | 1 (0%)  |
| 1   | X     | 259/261 (99%) | 0.08   | 11 (4%) 40 32 | 25, 43, 69, 121       | 2 (0%)  |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|----------------|-----------------------|---------|
| 1   | Y     | 258/261 (98%)   | 0.11   | 11 (4%) 40 31  | 24, 44, 76, 124       | 1 (0%)  |
| 1   | Z     | 261/261 (100%)  | -0.01  | 6 (2%) 61 52   | 23, 42, 69, 81        | 1 (0%)  |
| 1   | a     | 257/261 (98%)   | 0.03   | 7 (2%) 56 47   | 25, 44, 71, 91        | 1 (0%)  |
| 1   | b     | 257/261 (98%)   | 0.03   | 9 (3%) 47 37   | 22, 42, 69, 94        | 1 (0%)  |
| 1   | c     | 257/261 (98%)   | -0.02  | 6 (2%) 61 52   | 23, 43, 70, 87        | 1 (0%)  |
| 1   | d     | 261/261 (100%)  | 0.01   | 9 (3%) 48 38   | 21, 40, 67, 81        | 1 (0%)  |
| All | All   | 7736/7830 (98%) | 0.13   | 261 (3%) 48 38 | 21, 47, 81, 140       | 31 (0%) |

All (261) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | Y     | 1     | MET  | 6.6  |
| 1   | W     | 1     | MET  | 6.5  |
| 1   | U     | 1     | MET  | 5.9  |
| 1   | I     | 1     | MET  | 5.6  |
| 1   | E     | 1     | MET  | 5.5  |
| 1   | H     | 1     | MET  | 5.4  |
| 1   | K     | 1     | MET  | 5.4  |
| 1   | G     | 1     | MET  | 5.3  |
| 1   | M     | 2     | SER  | 5.3  |
| 1   | S     | 1     | MET  | 5.3  |
| 1   | L     | 1     | MET  | 5.2  |
| 1   | A     | 1     | MET  | 5.2  |
| 1   | U     | 0     | HIS  | 5.2  |
| 1   | R     | 1     | MET  | 5.0  |
| 1   | N     | 253   | THR  | 4.7  |
| 1   | X     | 1     | MET  | 4.7  |
| 1   | P     | 253   | THR  | 4.6  |
| 1   | V     | 1     | MET  | 4.6  |
| 1   | V     | 253   | THR  | 4.5  |
| 1   | X     | 0     | HIS  | 4.5  |
| 1   | G     | 57[A] | ARG  | 4.5  |
| 1   | T     | 1     | MET  | 4.5  |
| 1   | P     | 57[A] | ARG  | 4.4  |
| 1   | a     | 57[A] | ARG  | 4.4  |
| 1   | R     | 102   | ARG  | 4.4  |
| 1   | N     | 57[A] | ARG  | 4.3  |
| 1   | G     | 18    | ALA  | 4.1  |
| 1   | H     | 57[A] | ARG  | 4.1  |
| 1   | Q     | 2     | SER  | 4.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | b     | 2      | SER  | 4.1  |
| 1   | H     | 253    | THR  | 4.0  |
| 1   | Y     | 253    | THR  | 4.0  |
| 1   | P     | 71     | LEU  | 4.0  |
| 1   | J     | 253    | THR  | 4.0  |
| 1   | H     | 3      | LEU  | 3.9  |
| 1   | V     | 102    | ARG  | 3.9  |
| 1   | K     | 18     | ALA  | 3.9  |
| 1   | K     | 253    | THR  | 3.9  |
| 1   | X     | 102[A] | ARG  | 3.8  |
| 1   | P     | 18     | ALA  | 3.8  |
| 1   | c     | 102    | ARG  | 3.8  |
| 1   | F     | 2      | SER  | 3.8  |
| 1   | Q     | 57[A]  | ARG  | 3.8  |
| 1   | U     | 19     | ASP  | 3.7  |
| 1   | b     | 253    | THR  | 3.7  |
| 1   | C     | 2      | SER  | 3.7  |
| 1   | E     | 71     | LEU  | 3.7  |
| 1   | D     | 2      | SER  | 3.6  |
| 1   | I     | 57[A]  | ARG  | 3.6  |
| 1   | I     | 71     | LEU  | 3.6  |
| 1   | K     | 57[A]  | ARG  | 3.6  |
| 1   | X     | 57[A]  | ARG  | 3.6  |
| 1   | a     | 2      | SER  | 3.6  |
| 1   | V     | 258    | ARG  | 3.5  |
| 1   | J     | 226    | GLU  | 3.5  |
| 1   | R     | 253    | THR  | 3.5  |
| 1   | c     | 253    | THR  | 3.5  |
| 1   | J     | 57[A]  | ARG  | 3.5  |
| 1   | N     | 2      | SER  | 3.4  |
| 1   | O     | 57[A]  | ARG  | 3.4  |
| 1   | L     | 57[A]  | ARG  | 3.4  |
| 1   | P     | 2      | SER  | 3.4  |
| 1   | O     | 71     | LEU  | 3.3  |
| 1   | X     | 253    | THR  | 3.3  |
| 1   | U     | 71     | LEU  | 3.3  |
| 1   | M     | 57[A]  | ARG  | 3.3  |
| 1   | X     | 226    | GLU  | 3.3  |
| 1   | Y     | 102    | ARG  | 3.3  |
| 1   | K     | 68     | THR  | 3.3  |
| 1   | M     | 253    | THR  | 3.3  |
| 1   | d     | 253    | THR  | 3.3  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | B     | 1     | MET  | 3.2  |
| 1   | L     | 253   | THR  | 3.2  |
| 1   | A     | 102   | ARG  | 3.2  |
| 1   | Z     | 72    | LYS  | 3.2  |
| 1   | d     | 57[A] | ARG  | 3.2  |
| 1   | G     | 2     | SER  | 3.1  |
| 1   | Y     | 57[A] | ARG  | 3.1  |
| 1   | T     | 253   | THR  | 3.1  |
| 1   | R     | 57[A] | ARG  | 3.1  |
| 1   | P     | 12    | PRO  | 3.1  |
| 1   | Q     | 71    | LEU  | 3.1  |
| 1   | V     | 57[A] | ARG  | 3.0  |
| 1   | I     | 253   | THR  | 3.0  |
| 1   | S     | 57[A] | ARG  | 3.0  |
| 1   | W     | 57[A] | ARG  | 3.0  |
| 1   | b     | 57[A] | ARG  | 3.0  |
| 1   | c     | 57[A] | ARG  | 3.0  |
| 1   | c     | 72    | LYS  | 3.0  |
| 1   | a     | 253   | THR  | 3.0  |
| 1   | b     | 102   | ARG  | 3.0  |
| 1   | X     | 12    | PRO  | 3.0  |
| 1   | M     | 72    | LYS  | 3.0  |
| 1   | N     | 15    | ARG  | 3.0  |
| 1   | P     | 102   | ARG  | 3.0  |
| 1   | O     | 2     | SER  | 3.0  |
| 1   | L     | 71    | LEU  | 2.9  |
| 1   | M     | 77    | PRO  | 2.9  |
| 1   | W     | 77    | PRO  | 2.9  |
| 1   | D     | 72    | LYS  | 2.9  |
| 1   | Z     | 57[A] | ARG  | 2.9  |
| 1   | A     | 71    | LEU  | 2.9  |
| 1   | L     | 77    | PRO  | 2.9  |
| 1   | P     | 72    | LYS  | 2.9  |
| 1   | U     | 72    | LYS  | 2.9  |
| 1   | D     | 102   | ARG  | 2.9  |
| 1   | G     | 71    | LEU  | 2.9  |
| 1   | d     | 1     | MET  | 2.9  |
| 1   | S     | 226   | GLU  | 2.9  |
| 1   | B     | 253   | THR  | 2.9  |
| 1   | M     | 71    | LEU  | 2.9  |
| 1   | T     | 71    | LEU  | 2.9  |
| 1   | H     | 72    | LYS  | 2.8  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | H     | 71    | LEU  | 2.8  |
| 1   | N     | 18    | ALA  | 2.8  |
| 1   | G     | 6     | PRO  | 2.8  |
| 1   | C     | 57[A] | ARG  | 2.8  |
| 1   | Q     | 18    | ALA  | 2.8  |
| 1   | O     | 253   | THR  | 2.8  |
| 1   | I     | 77    | PRO  | 2.8  |
| 1   | U     | 12    | PRO  | 2.8  |
| 1   | c     | 71    | LEU  | 2.8  |
| 1   | B     | 2     | SER  | 2.8  |
| 1   | B     | 57[A] | ARG  | 2.7  |
| 1   | K     | 201   | ARG  | 2.7  |
| 1   | Q     | 253   | THR  | 2.7  |
| 1   | P     | 77    | PRO  | 2.7  |
| 1   | a     | 102   | ARG  | 2.7  |
| 1   | G     | 77    | PRO  | 2.7  |
| 1   | B     | 226   | GLU  | 2.7  |
| 1   | b     | 226   | GLU  | 2.7  |
| 1   | E     | 102   | ARG  | 2.7  |
| 1   | X     | 19    | ASP  | 2.7  |
| 1   | Q     | 102   | ARG  | 2.7  |
| 1   | A     | 77    | PRO  | 2.7  |
| 1   | D     | 71    | LEU  | 2.7  |
| 1   | H     | 2     | SER  | 2.7  |
| 1   | N     | 71    | LEU  | 2.7  |
| 1   | d     | 254   | ARG  | 2.6  |
| 1   | L     | 18    | ALA  | 2.6  |
| 1   | D     | 258   | ARG  | 2.6  |
| 1   | E     | 57[A] | ARG  | 2.6  |
| 1   | Y     | 258   | ARG  | 2.6  |
| 1   | Q     | 77    | PRO  | 2.6  |
| 1   | O     | 258   | ARG  | 2.6  |
| 1   | L     | 2     | SER  | 2.6  |
| 1   | M     | 18    | ALA  | 2.6  |
| 1   | Z     | 258   | ARG  | 2.5  |
| 1   | K     | 2     | SER  | 2.5  |
| 1   | A     | 57[A] | ARG  | 2.5  |
| 1   | M     | 258   | ARG  | 2.5  |
| 1   | I     | 74    | LYS  | 2.5  |
| 1   | B     | 71    | LEU  | 2.5  |
| 1   | Z     | 253   | THR  | 2.5  |
| 1   | T     | 57[A] | ARG  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Q     | 72  | LYS  | 2.5  |
| 1   | R     | 71  | LEU  | 2.5  |
| 1   | P     | 226 | GLU  | 2.5  |
| 1   | G     | 68  | THR  | 2.5  |
| 1   | L     | 68  | THR  | 2.5  |
| 1   | U     | 18  | ALA  | 2.5  |
| 1   | W     | 258 | ARG  | 2.5  |
| 1   | Q     | 74  | LYS  | 2.5  |
| 1   | H     | 226 | GLU  | 2.5  |
| 1   | G     | 17  | ALA  | 2.5  |
| 1   | N     | 106 | THR  | 2.4  |
| 1   | N     | 77  | PRO  | 2.4  |
| 1   | I     | 15  | ARG  | 2.4  |
| 1   | Q     | 15  | ARG  | 2.4  |
| 1   | M     | 226 | GLU  | 2.4  |
| 1   | V     | 71  | LEU  | 2.4  |
| 1   | I     | 12  | PRO  | 2.4  |
| 1   | U     | 258 | ARG  | 2.4  |
| 1   | J     | 2   | SER  | 2.4  |
| 1   | I     | 18  | ALA  | 2.4  |
| 1   | J     | 71  | LEU  | 2.4  |
| 1   | d     | 258 | ARG  | 2.4  |
| 1   | W     | 253 | THR  | 2.4  |
| 1   | W     | 71  | LEU  | 2.4  |
| 1   | G     | 258 | ARG  | 2.3  |
| 1   | H     | 15  | ARG  | 2.3  |
| 1   | K     | 254 | ARG  | 2.3  |
| 1   | U     | 226 | GLU  | 2.3  |
| 1   | Z     | 226 | GLU  | 2.3  |
| 1   | H     | 77  | PRO  | 2.3  |
| 1   | Q     | 7   | ARG  | 2.3  |
| 1   | T     | 258 | ARG  | 2.3  |
| 1   | Z     | 254 | ARG  | 2.3  |
| 1   | R     | 18  | ALA  | 2.3  |
| 1   | Y     | 226 | GLU  | 2.3  |
| 1   | Y     | 71  | LEU  | 2.3  |
| 1   | B     | 220 | ARG  | 2.3  |
| 1   | X     | 18  | ALA  | 2.3  |
| 1   | P     | 101 | ASP  | 2.3  |
| 1   | G     | 72  | LYS  | 2.3  |
| 1   | Y     | 256 | ILE  | 2.3  |
| 1   | D     | 253 | THR  | 2.3  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | R     | 15    | ARG  | 2.3  |
| 1   | U     | 102   | ARG  | 2.3  |
| 1   | b     | 258   | ARG  | 2.3  |
| 1   | K     | 77    | PRO  | 2.3  |
| 1   | A     | 253   | THR  | 2.3  |
| 1   | F     | 254   | ARG  | 2.3  |
| 1   | W     | 200   | ARG  | 2.3  |
| 1   | c     | 2     | SER  | 2.3  |
| 1   | a     | 226   | GLU  | 2.2  |
| 1   | X     | 72    | LYS  | 2.2  |
| 1   | b     | 72    | LYS  | 2.2  |
| 1   | d     | 72    | LYS  | 2.2  |
| 1   | E     | 253   | THR  | 2.2  |
| 1   | R     | 2     | SER  | 2.2  |
| 1   | F     | 71    | LEU  | 2.2  |
| 1   | L     | 226   | GLU  | 2.2  |
| 1   | N     | 72    | LYS  | 2.2  |
| 1   | a     | 72    | LYS  | 2.2  |
| 1   | D     | 57[A] | ARG  | 2.2  |
| 1   | U     | 57[A] | ARG  | 2.2  |
| 1   | P     | 6     | PRO  | 2.2  |
| 1   | b     | 77    | PRO  | 2.2  |
| 1   | I     | 2     | SER  | 2.2  |
| 1   | I     | 3     | LEU  | 2.2  |
| 1   | Q     | 226   | GLU  | 2.2  |
| 1   | C     | 253   | THR  | 2.2  |
| 1   | O     | 15    | ARG  | 2.2  |
| 1   | b     | 250   | GLN  | 2.2  |
| 1   | F     | 77    | PRO  | 2.2  |
| 1   | D     | 226   | GLU  | 2.2  |
| 1   | d     | 226   | GLU  | 2.2  |
| 1   | H     | 6     | PRO  | 2.1  |
| 1   | H     | 12    | PRO  | 2.1  |
| 1   | J     | 74    | LYS  | 2.1  |
| 1   | P     | 174   | GLY  | 2.1  |
| 1   | S     | 258   | ARG  | 2.1  |
| 1   | T     | 256   | ILE  | 2.1  |
| 1   | G     | 75    | GLY  | 2.1  |
| 1   | S     | 72    | LYS  | 2.1  |
| 1   | F     | 57[A] | ARG  | 2.1  |
| 1   | W     | 15    | ARG  | 2.1  |
| 1   | Y     | 15    | ARG  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Y     | 160 | ARG  | 2.1  |
| 1   | d     | 102 | ARG  | 2.1  |
| 1   | M     | 201 | ARG  | 2.1  |
| 1   | R     | 226 | GLU  | 2.1  |
| 1   | O     | 74  | LYS  | 2.0  |
| 1   | Y     | 72  | LYS  | 2.0  |
| 1   | K     | 3   | LEU  | 2.0  |
| 1   | X     | 3   | LEU  | 2.0  |
| 1   | A     | 254 | ARG  | 2.0  |
| 1   | C     | 254 | ARG  | 2.0  |
| 1   | C     | 258 | ARG  | 2.0  |
| 1   | E     | 258 | ARG  | 2.0  |
| 1   | P     | 258 | ARG  | 2.0  |
| 1   | V     | 254 | ARG  | 2.0  |
| 1   | G     | 253 | THR  | 2.0  |
| 1   | d     | 256 | ILE  | 2.0  |
| 1   | E     | 99  | VAL  | 2.0  |
| 1   | a     | 251 | SER  | 2.0  |
| 1   | M     | 3   | LEU  | 2.0  |
| 1   | K     | 258 | ARG  | 2.0  |
| 1   | C     | 68  | THR  | 2.0  |
| 1   | D     | 31  | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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<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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | VFE  | I     | 1001 | 29/29 | 0.91 | 0.16 | 58,63,70,80                 | 0     |

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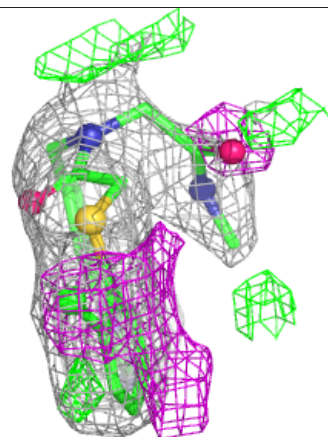
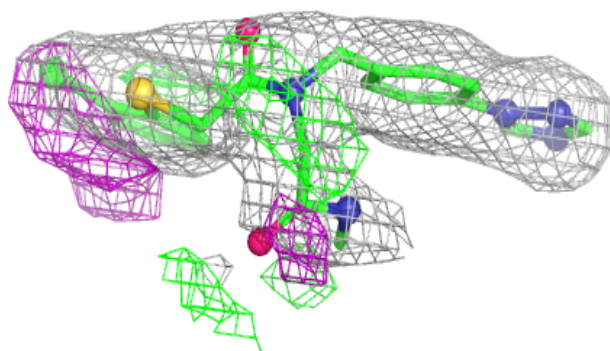
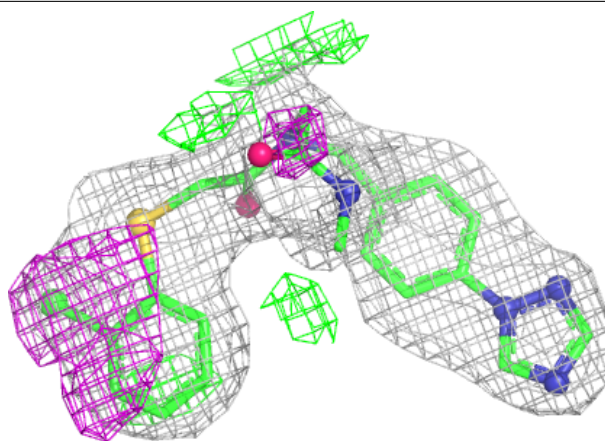
*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | VFE  | U     | 1001 | 29/29 | 0.91 | 0.16 | 53,58,66,71                 | 0     |
| 2   | VFE  | d     | 1001 | 29/29 | 0.91 | 0.16 | 44,57,66,70                 | 0     |
| 2   | VFE  | J     | 1001 | 29/29 | 0.92 | 0.14 | 55,59,69,71                 | 0     |
| 2   | VFE  | M     | 1001 | 29/29 | 0.92 | 0.15 | 53,62,70,82                 | 0     |
| 2   | VFE  | H     | 1001 | 29/29 | 0.92 | 0.15 | 61,69,73,82                 | 0     |
| 2   | VFE  | X     | 1001 | 29/29 | 0.92 | 0.14 | 51,57,67,72                 | 0     |
| 2   | VFE  | C     | 1001 | 29/29 | 0.92 | 0.14 | 49,56,62,81                 | 0     |
| 2   | VFE  | P     | 1001 | 29/29 | 0.93 | 0.13 | 56,60,66,77                 | 0     |
| 2   | VFE  | R     | 1001 | 29/29 | 0.93 | 0.14 | 52,58,80,80                 | 0     |
| 2   | VFE  | T     | 1001 | 29/29 | 0.93 | 0.14 | 47,57,69,72                 | 0     |
| 2   | VFE  | K     | 1001 | 29/29 | 0.93 | 0.13 | 61,67,77,82                 | 0     |
| 2   | VFE  | L     | 1001 | 29/29 | 0.93 | 0.14 | 59,63,73,81                 | 0     |
| 2   | VFE  | Z     | 1001 | 29/29 | 0.93 | 0.13 | 51,58,72,76                 | 0     |
| 2   | VFE  | a     | 1001 | 29/29 | 0.93 | 0.13 | 51,56,67,73                 | 0     |
| 2   | VFE  | c     | 1001 | 29/29 | 0.93 | 0.15 | 47,54,65,78                 | 0     |
| 2   | VFE  | D     | 1001 | 29/29 | 0.93 | 0.13 | 47,52,65,68                 | 0     |
| 2   | VFE  | B     | 1001 | 29/29 | 0.94 | 0.13 | 46,50,61,63                 | 0     |
| 2   | VFE  | V     | 1001 | 29/29 | 0.94 | 0.12 | 49,55,60,73                 | 0     |
| 2   | VFE  | O     | 1001 | 29/29 | 0.94 | 0.13 | 56,63,76,78                 | 0     |
| 2   | VFE  | Y     | 1001 | 29/29 | 0.94 | 0.13 | 50,58,71,73                 | 0     |
| 2   | VFE  | E     | 1001 | 29/29 | 0.94 | 0.12 | 49,55,64,72                 | 0     |
| 2   | VFE  | Q     | 1001 | 29/29 | 0.94 | 0.13 | 57,65,72,78                 | 0     |
| 2   | VFE  | b     | 1001 | 29/29 | 0.94 | 0.13 | 54,59,73,82                 | 0     |
| 2   | VFE  | G     | 1001 | 29/29 | 0.94 | 0.12 | 56,65,69,74                 | 0     |
| 2   | VFE  | A     | 1001 | 29/29 | 0.94 | 0.12 | 46,53,62,69                 | 0     |
| 2   | VFE  | W     | 1001 | 29/29 | 0.95 | 0.12 | 52,55,67,72                 | 0     |
| 2   | VFE  | F     | 1001 | 29/29 | 0.95 | 0.12 | 46,52,65,76                 | 0     |
| 2   | VFE  | N     | 1001 | 29/29 | 0.95 | 0.10 | 50,57,64,73                 | 0     |
| 2   | VFE  | S     | 1001 | 29/29 | 0.95 | 0.11 | 45,54,59,71                 | 0     |
| 3   | MG   | D     | 1002 | 1/1   | 0.95 | 0.10 | 58,58,58,58                 | 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.

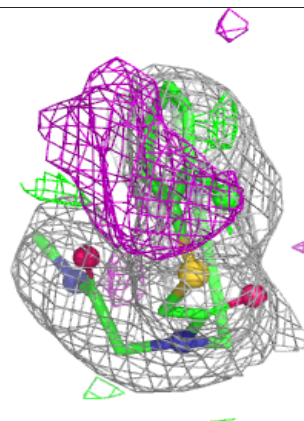
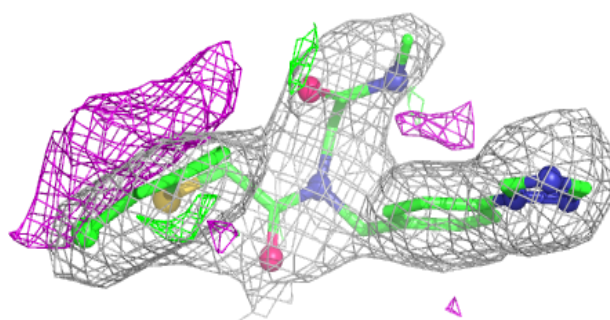
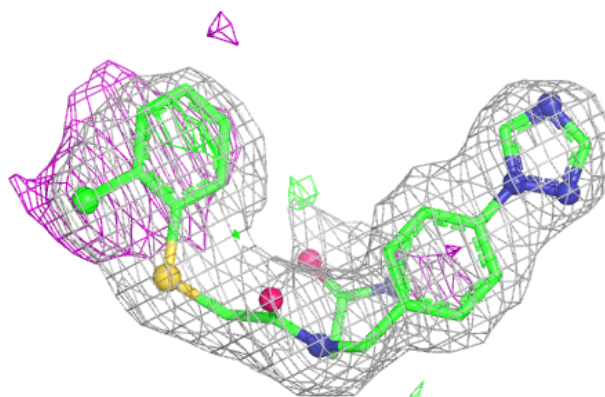
**Electron density around VFE I 1001:**

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



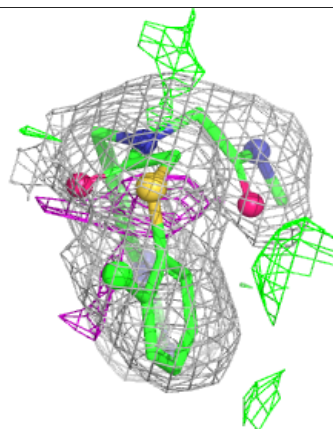
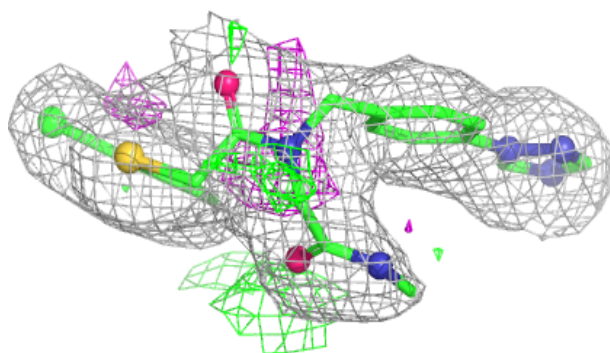
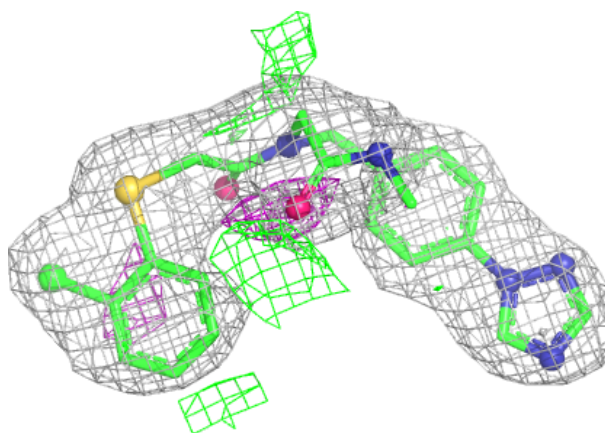
**Electron density around VFE U 1001:**

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

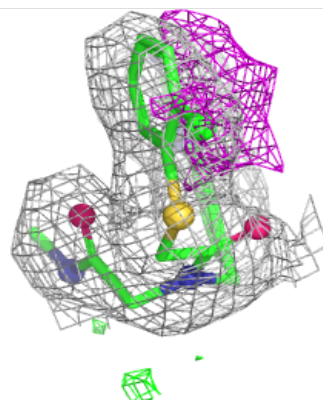
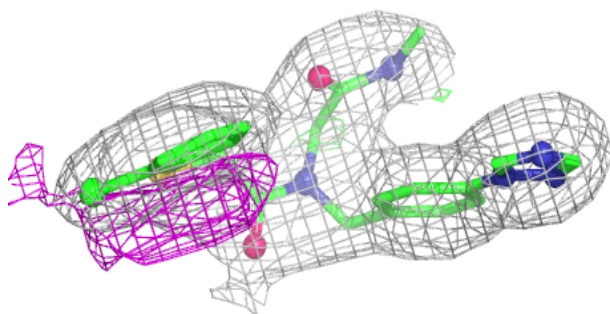
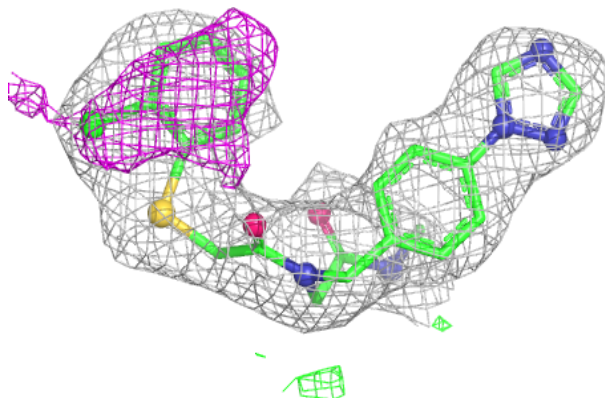


**Electron density around VFE d 1001:**

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

**Electron density around VFE J 1001:**

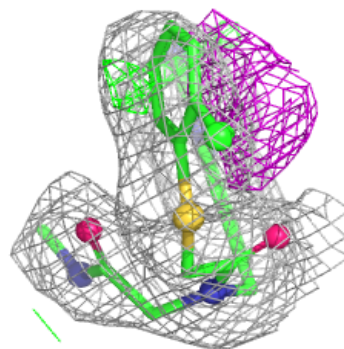
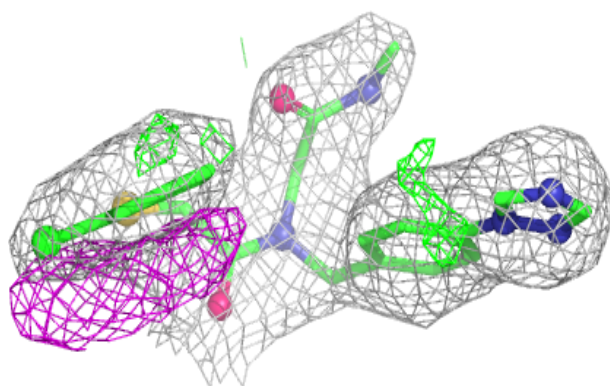
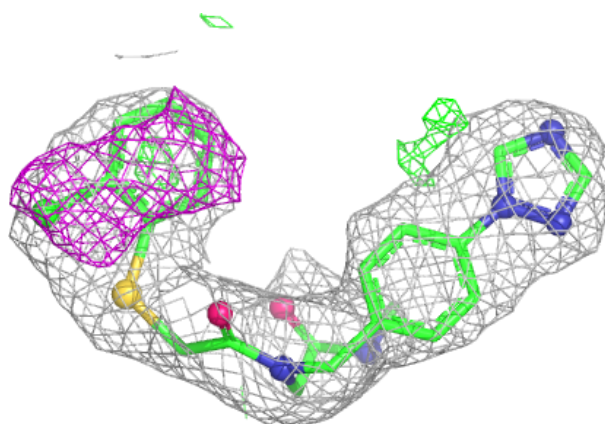
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around VFE M 1001:**

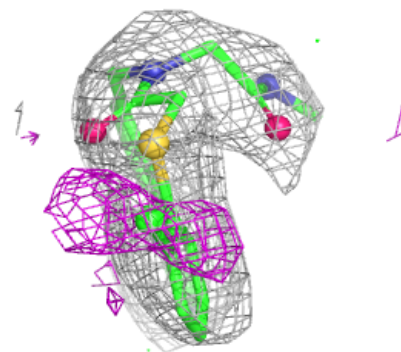
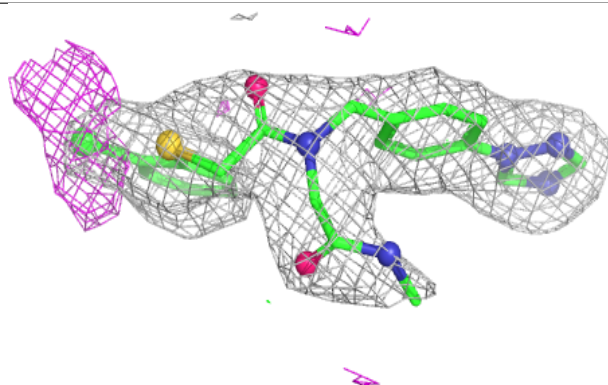
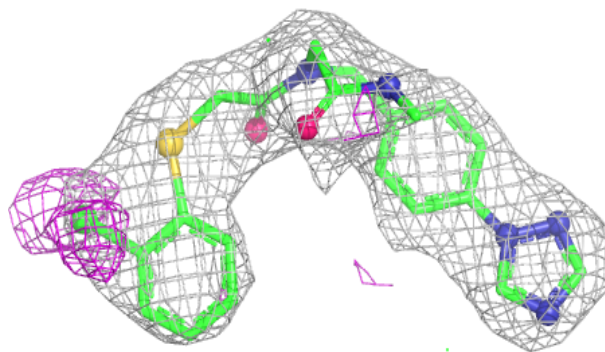
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



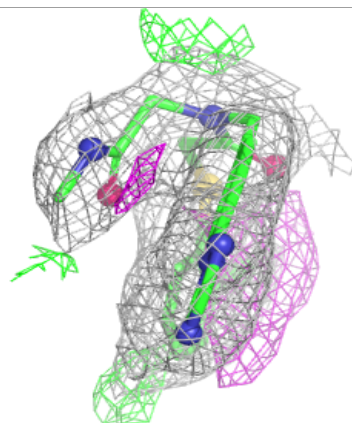
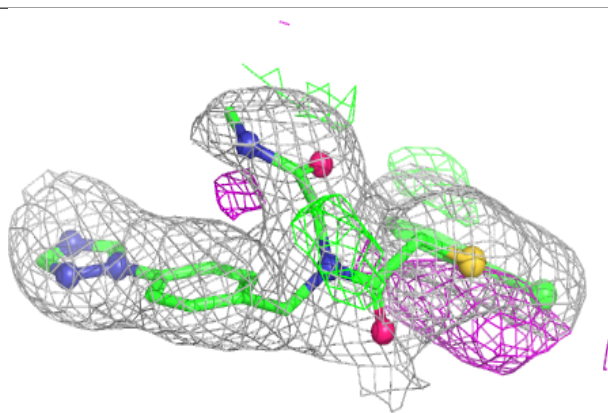
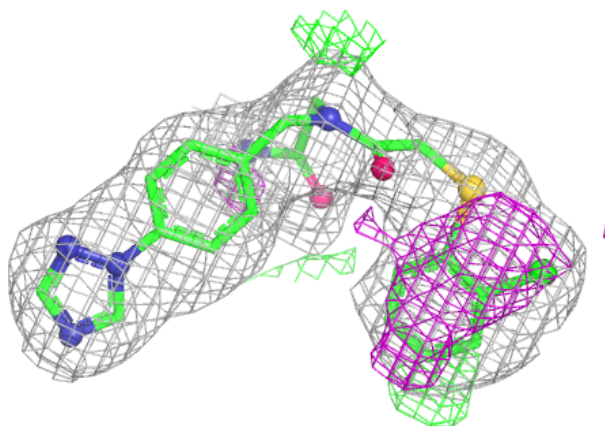


**Electron density around VFE H 1001:**

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

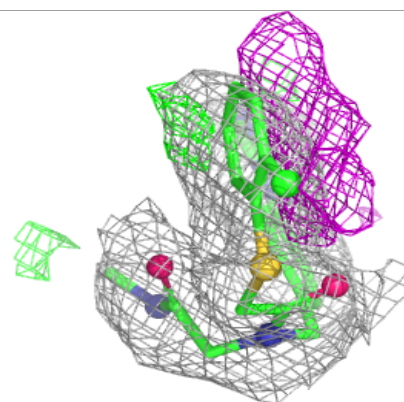
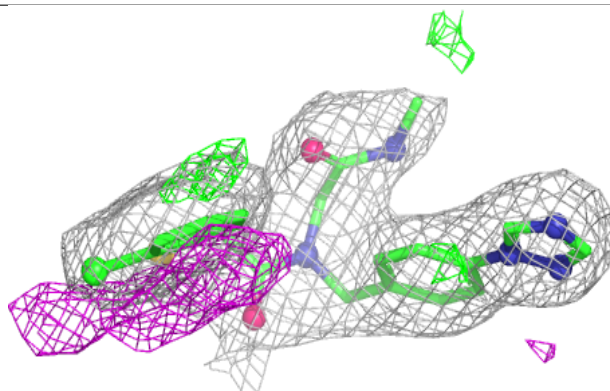
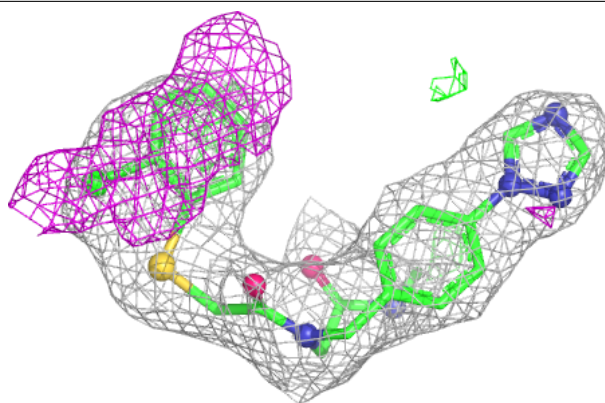
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and green (positive)

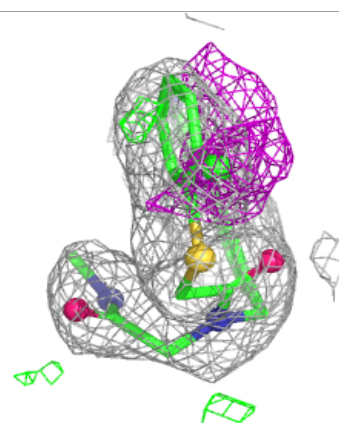
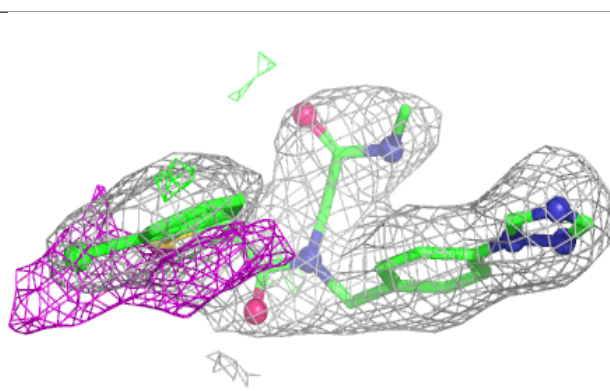
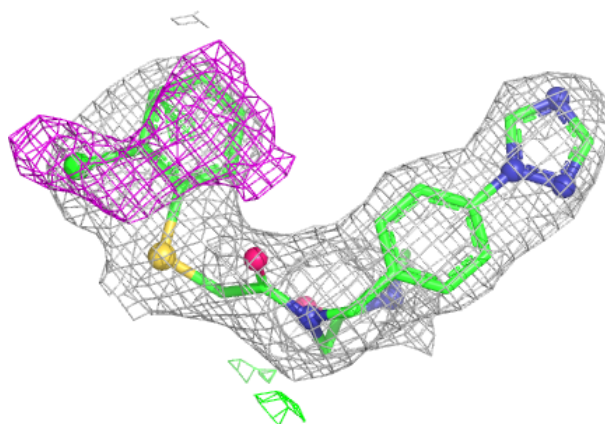


**Electron density around VFE C 1001:**

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

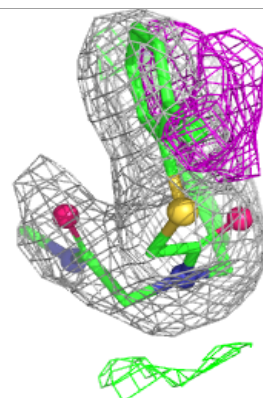
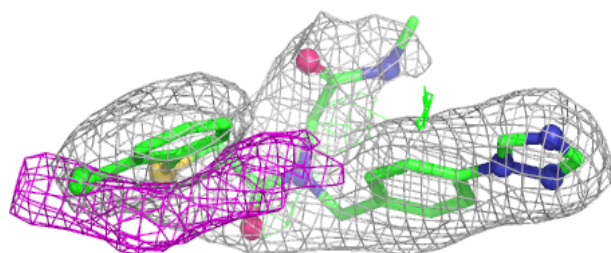
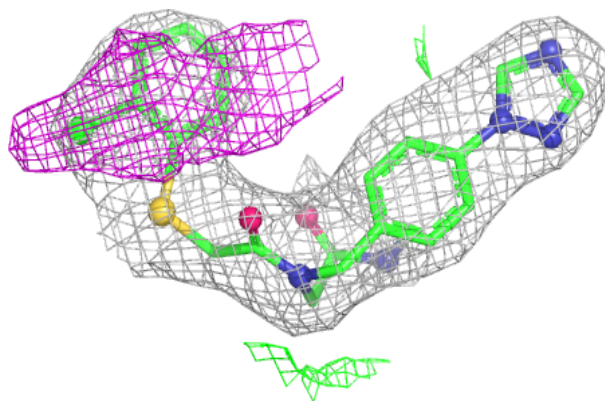
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and green (positive)

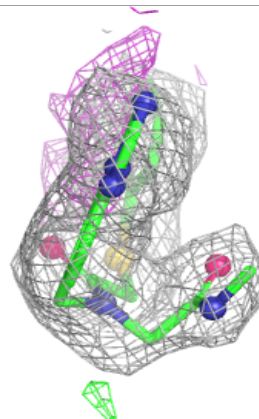
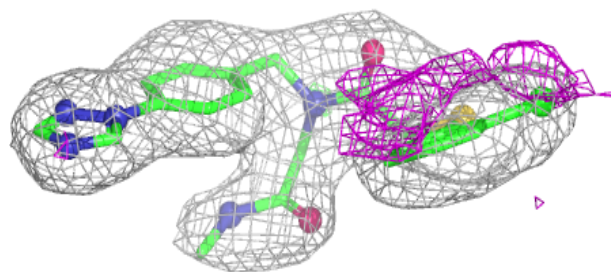
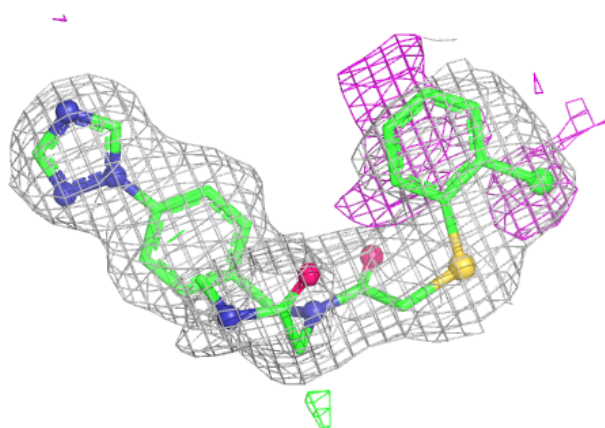


**Electron density around VFE R 1001:**

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and green (positive)

**Electron density around VFE T 1001:**

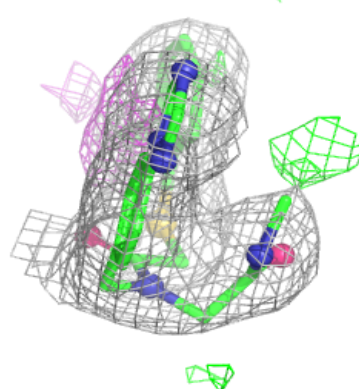
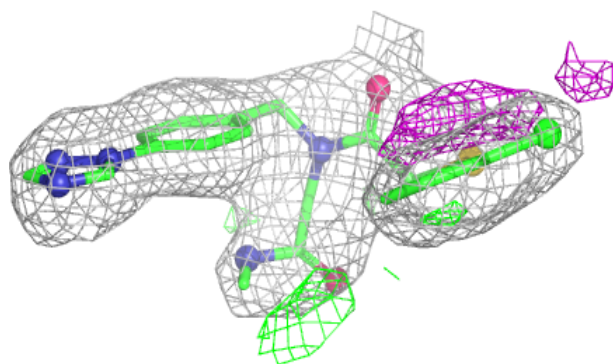
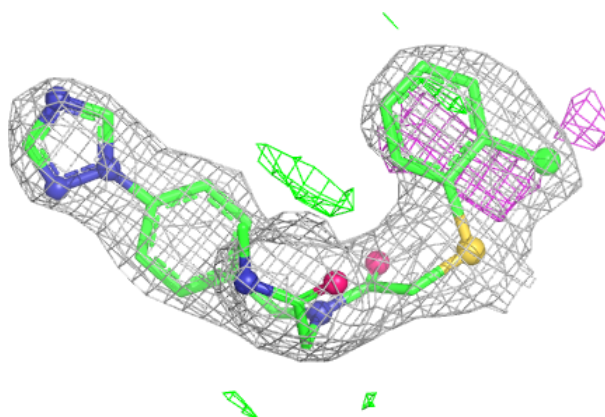
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



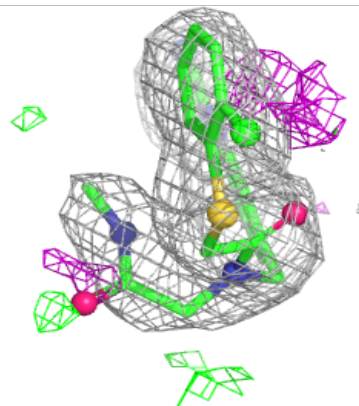
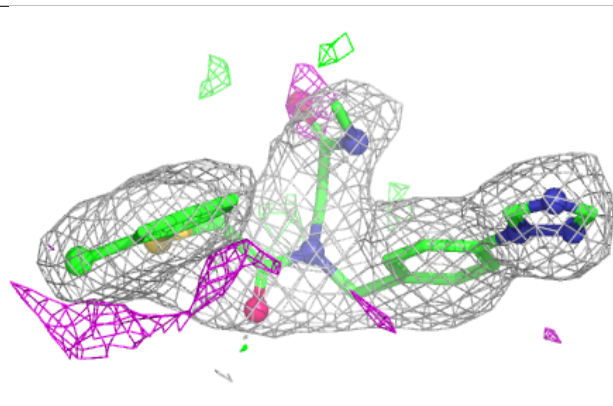
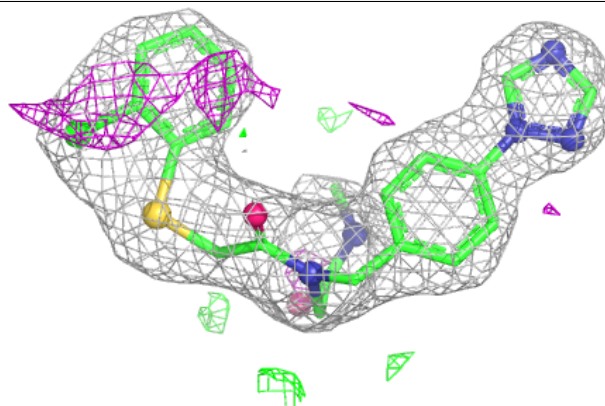


**Electron density around VFE K 1001:**

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and green (positive)

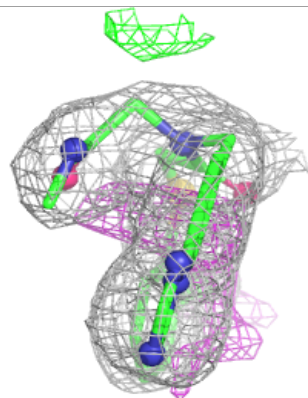
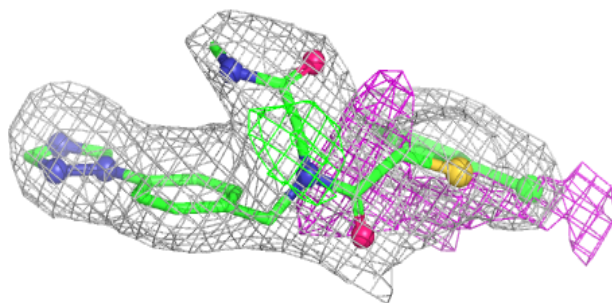
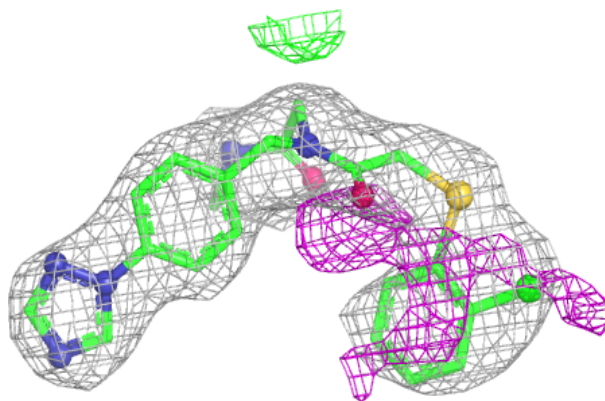
**Electron density around VFE L 1001:**

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

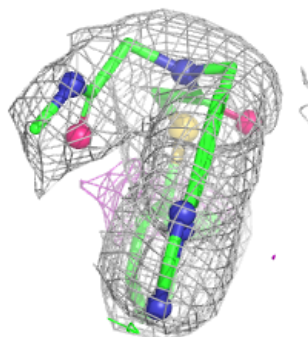
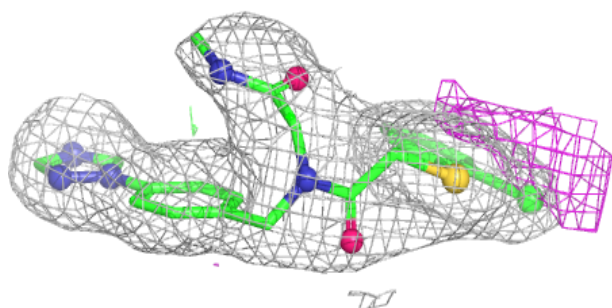
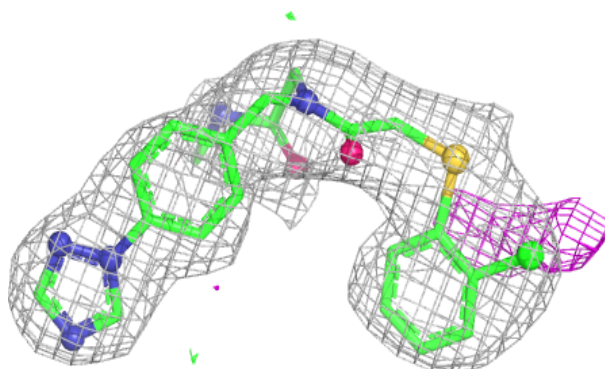


**Electron density around VFE Z 1001:**

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

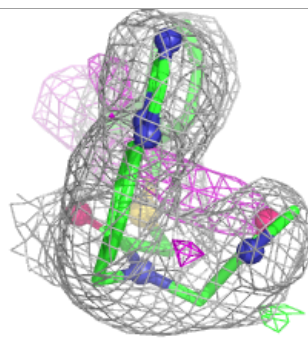
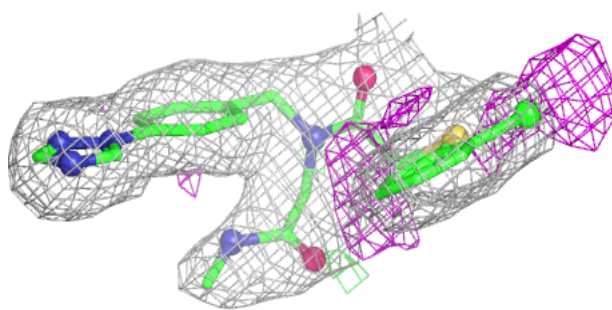
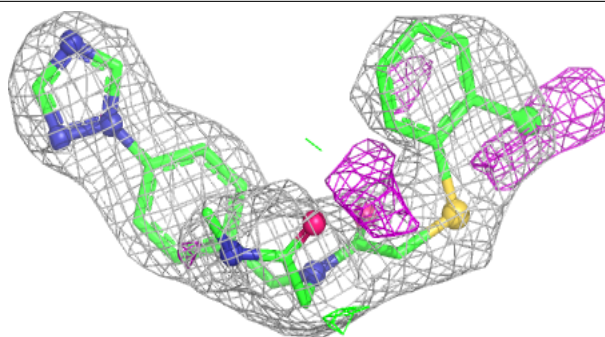
**Electron density around VFE a 1001:**

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

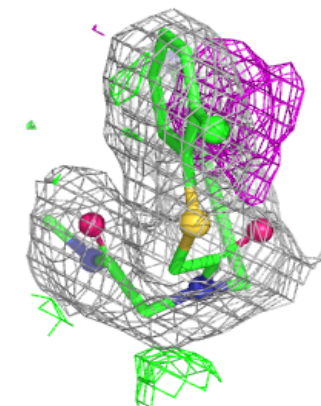
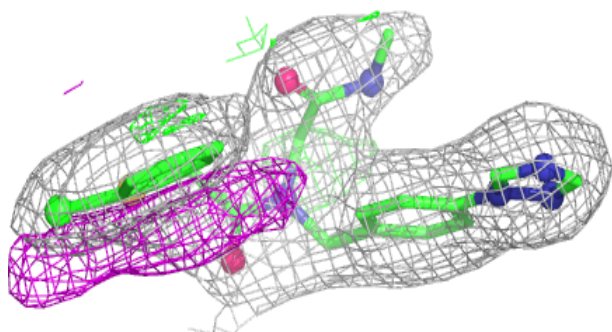
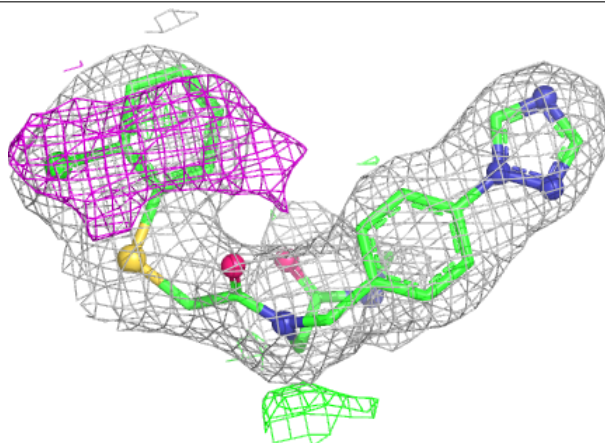


**Electron density around VFE c 1001:**

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

**Electron density around VFE D 1001:**

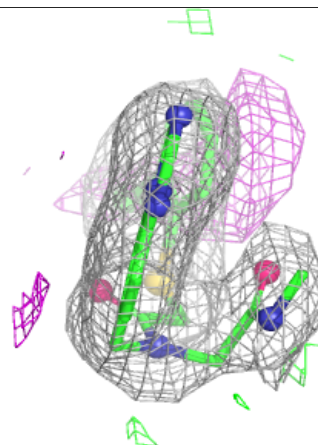
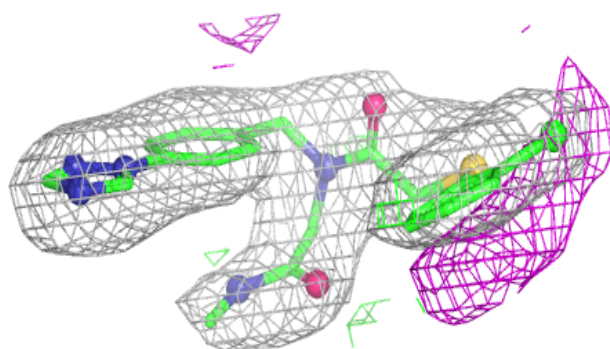
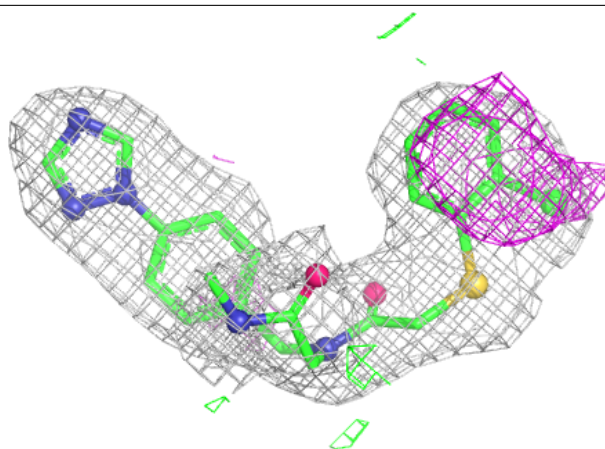
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



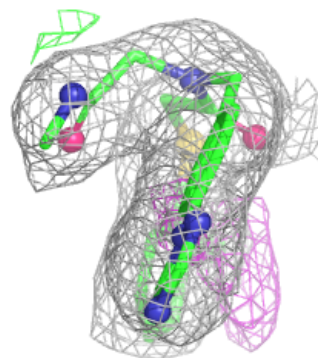
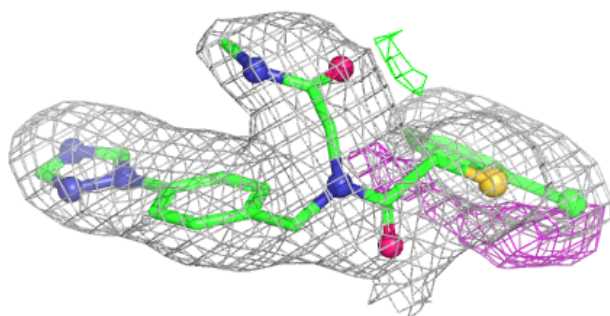
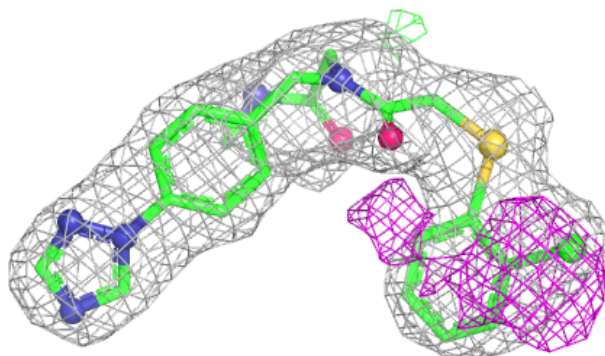


**Electron density around VFE B 1001:**

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

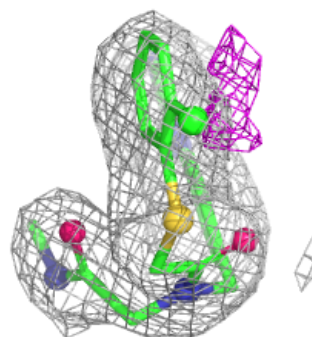
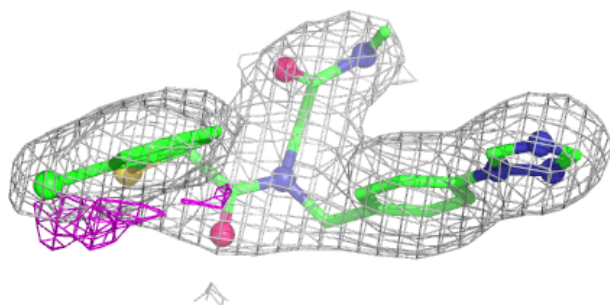
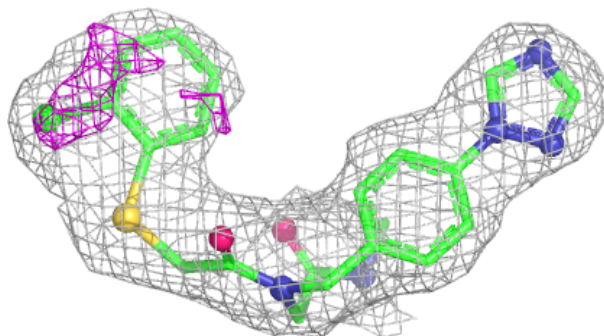
**Electron density around VFE V 1001:**

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

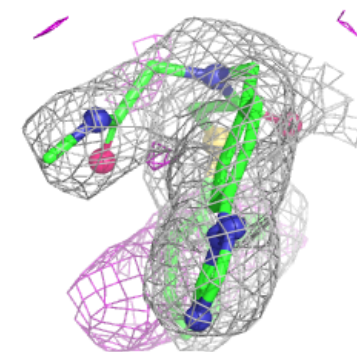
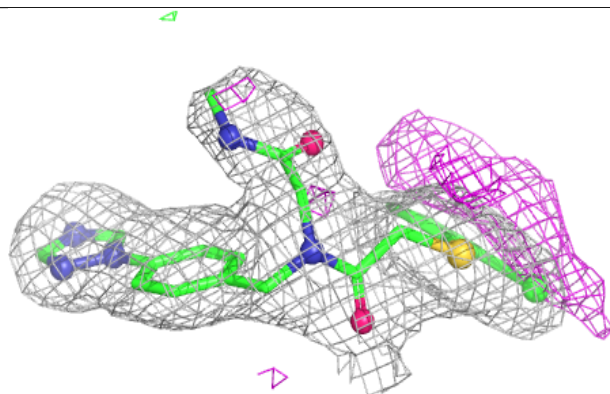
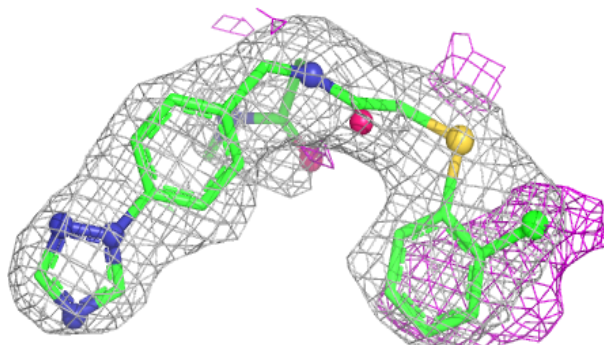


**Electron density around VFE O 1001:**

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

**Electron density around VFE Y 1001:**

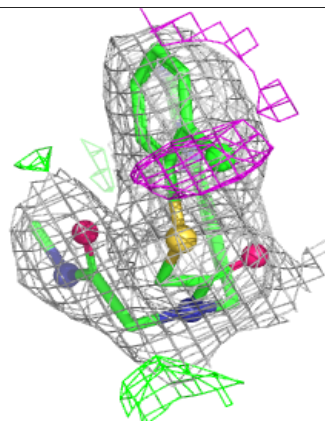
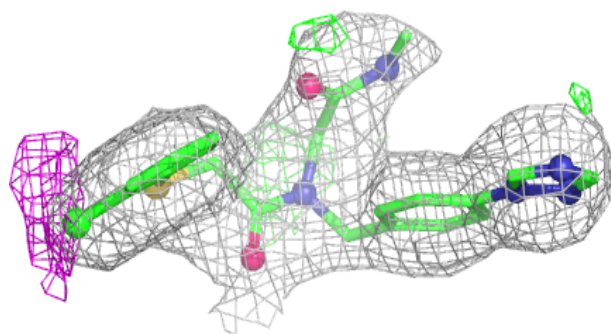
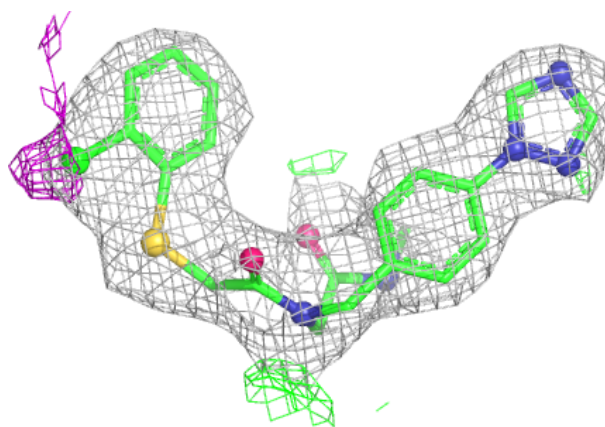
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



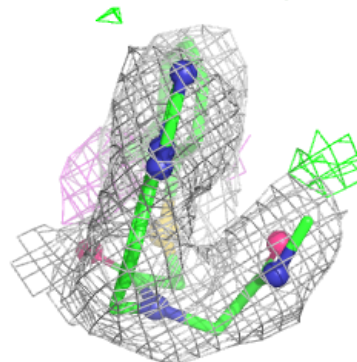
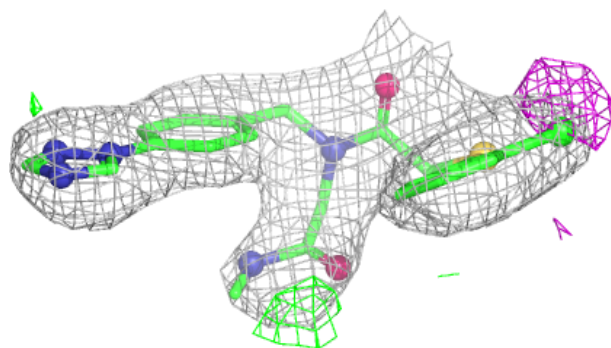
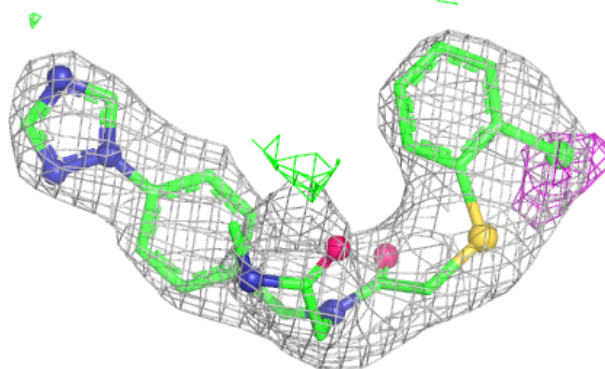


**Electron density around VFE E 1001:**

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

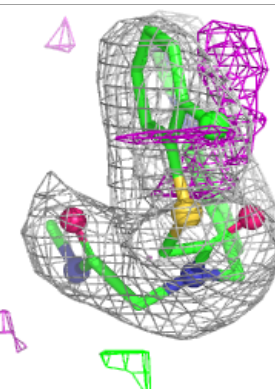
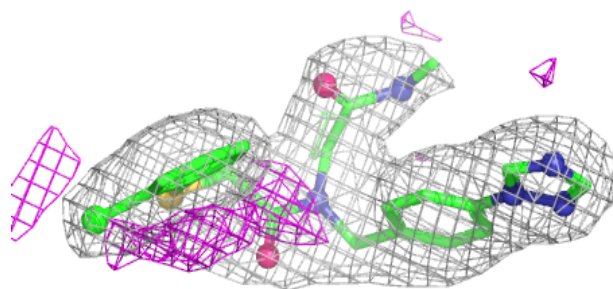
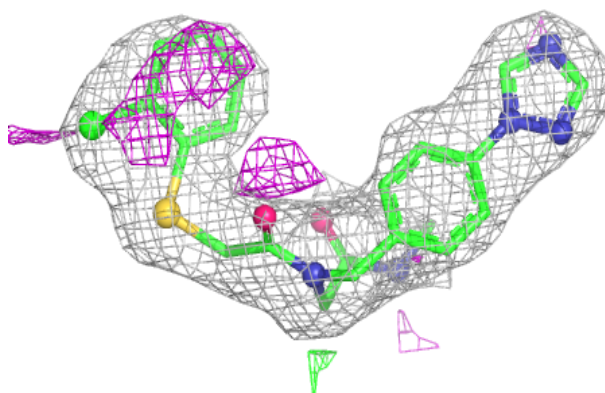
**Electron density around VFE Q 1001:**

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

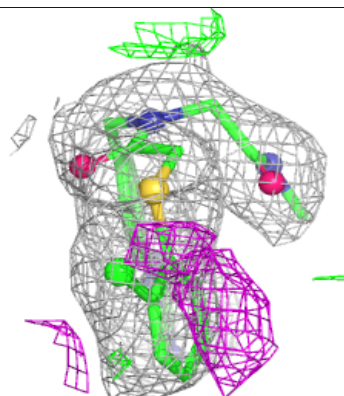
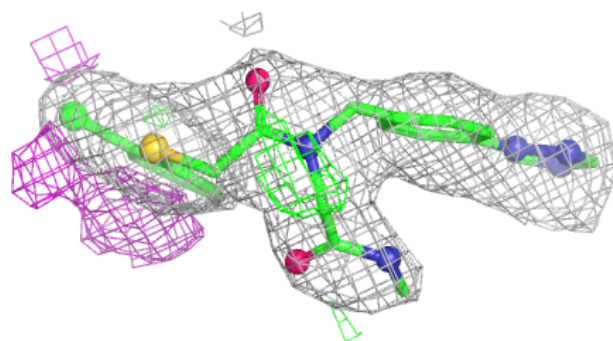
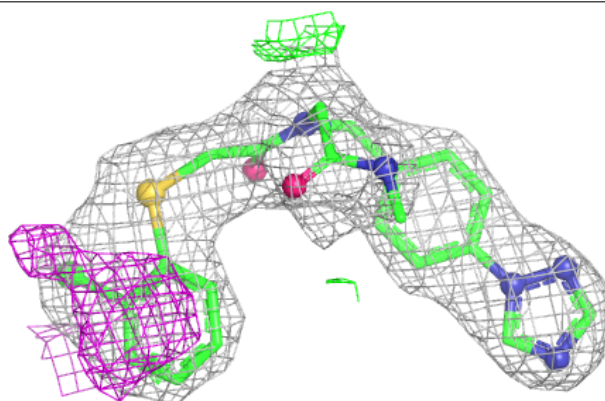


**Electron density around VFE b 1001:**

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

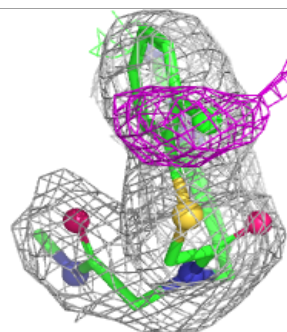
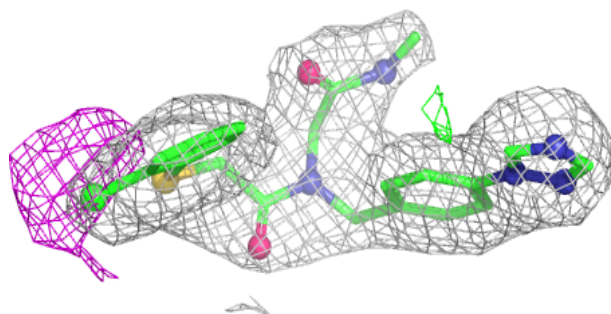
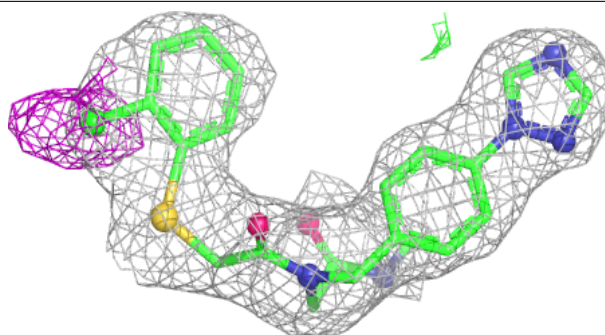
**Electron density around VFE G 1001:**

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

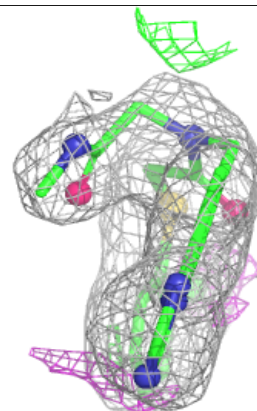
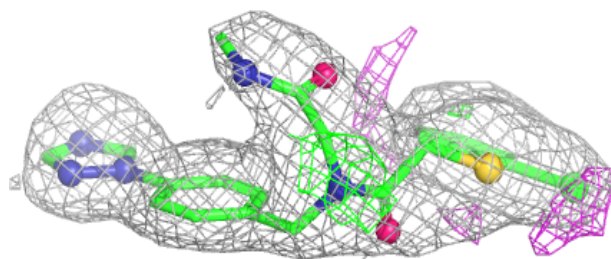
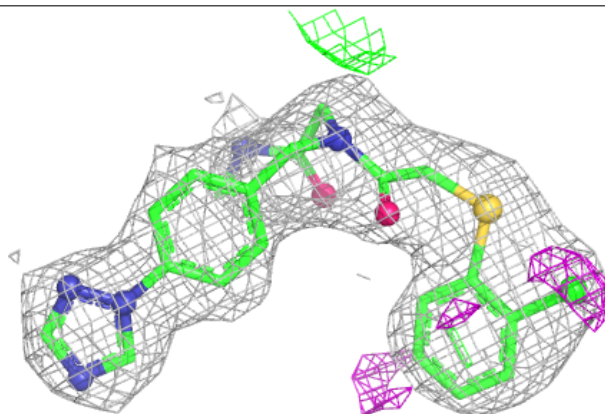


**Electron density around VFE A 1001:**

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

**Electron density around VFE W 1001:**

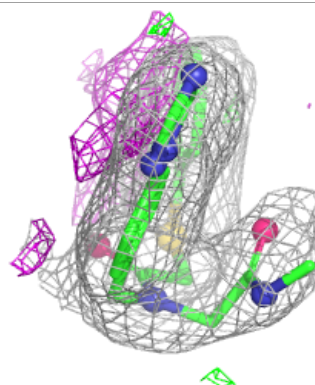
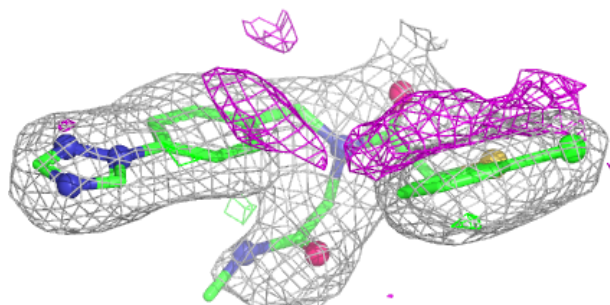
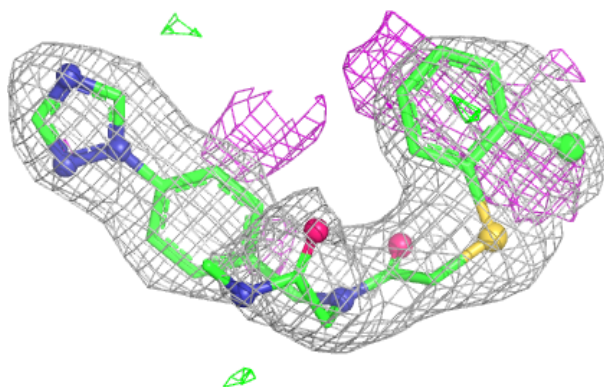
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



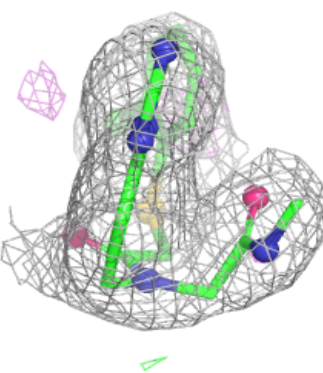
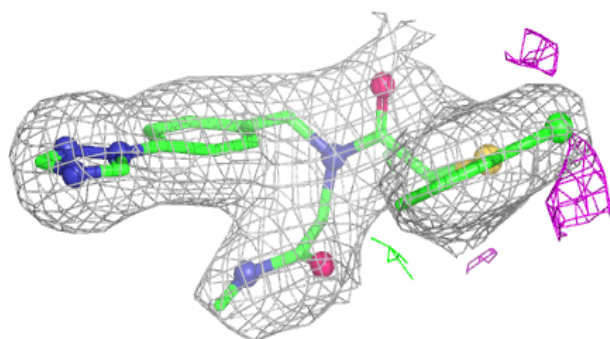
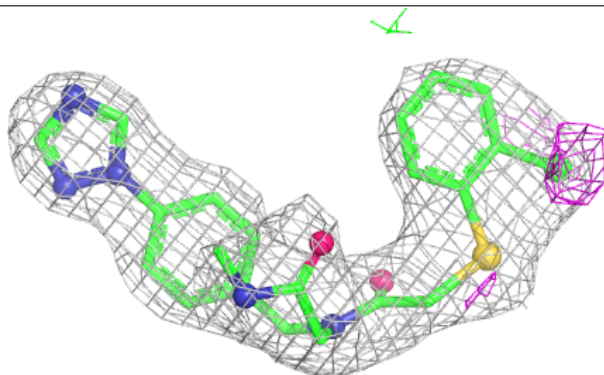


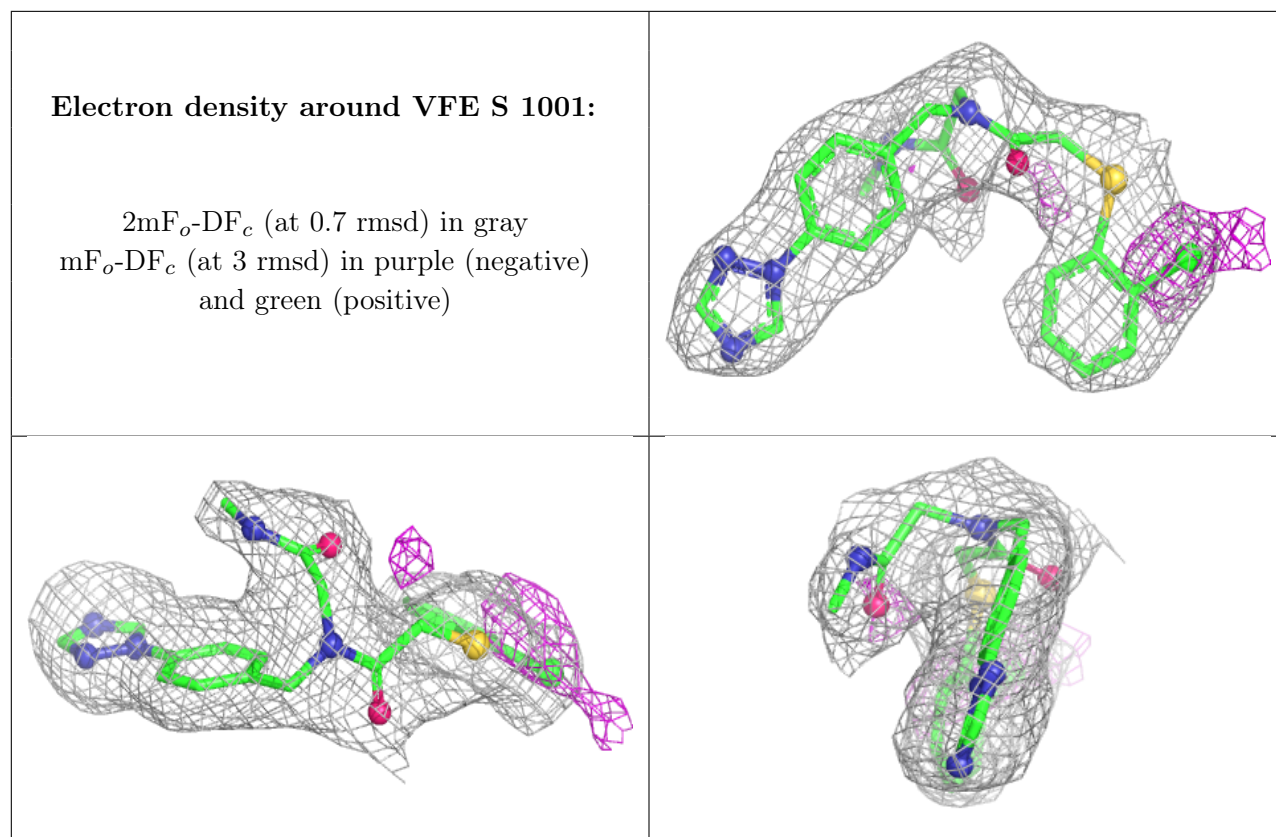
**Electron density around VFE F 1001:**

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

**Electron density around VFE N 1001:**

$2mF_o - DF_c$  (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.