



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:23 AM UTC

PDB ID : 5TS0 / pdb\_00005ts0  
Title : Structure of Mycobacterium tuberculosis proteasome in complex with N,C-capped dipeptide PKS2208  
Authors : Hsu, H.-C.; Fan, H.; Singh, P.K.; Wang, R.; Sukenick, G.; Nathan, C.; Lin, G.; Li, H.  
Deposited on : 2016-10-27  
Resolution : 2.85 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:

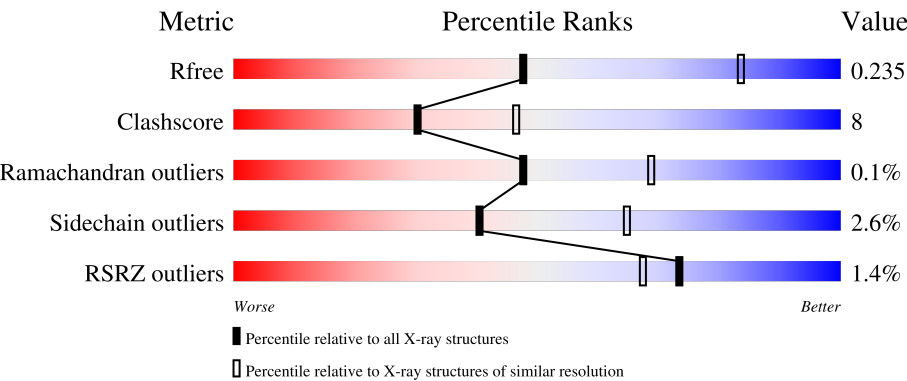
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 2.85 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     | 240    | <div><div>2%</div><div><div></div><div>72%</div><div>19%</div><div>9%</div></div></div>  |
| 1   | B     | 240    | <div><div>%</div><div><div></div><div>68%</div><div>21%</div><div>10%</div></div></div>  |
| 1   | C     | 240    | <div><div>2%</div><div><div></div><div>64%</div><div>25%</div><div>10%</div></div></div> |
| 1   | D     | 240    | <div><div>3%</div><div><div></div><div>67%</div><div>23%</div><div>10%</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 240    |                  |
| 1   | F     | 240    |                  |
| 1   | G     | 240    |                  |
| 1   | O     | 240    |                  |
| 1   | P     | 240    |                  |
| 1   | Q     | 240    |                  |
| 1   | R     | 240    |                  |
| 1   | S     | 240    |                  |
| 1   | T     | 240    |                  |
| 1   | U     | 240    |                  |
| 2   | H     | 240    |                  |
| 2   | I     | 240    |                  |
| 2   | J     | 240    |                  |
| 2   | K     | 240    |                  |
| 2   | L     | 240    |                  |
| 2   | M     | 240    |                  |
| 2   | N     | 240    |                  |
| 2   | V     | 240    |                  |
| 2   | W     | 240    |                  |
| 2   | X     | 240    |                  |
| 2   | Y     | 240    |                  |
| 2   | Z     | 240    |                  |
| 2   | a     | 240    |                  |
| 2   | b     | 240    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47311 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 Proteasome subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1677  | 1050 | 306 | 317 | 4 |         |         |       |
| 1   | B     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1668  | 1045 | 304 | 315 | 4 |         |         |       |
| 1   | C     | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1672  | 1047 | 305 | 316 | 4 |         |         |       |
| 1   | D     | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1670  | 1046 | 305 | 315 | 4 |         |         |       |
| 1   | E     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1677  | 1050 | 306 | 317 | 4 |         |         |       |
| 1   | F     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1655  | 1035 | 303 | 313 | 4 |         |         |       |
| 1   | G     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1690  | 1057 | 308 | 321 | 4 |         |         |       |
| 1   | O     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1664  | 1043 | 304 | 313 | 4 |         |         |       |
| 1   | P     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1677  | 1050 | 306 | 317 | 4 |         |         |       |
| 1   | Q     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1678  | 1050 | 306 | 318 | 4 |         |         |       |
| 1   | R     | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1670  | 1046 | 305 | 315 | 4 |         |         |       |
| 1   | S     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1678  | 1050 | 306 | 318 | 4 |         |         |       |
| 1   | T     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1679  | 1051 | 306 | 318 | 4 |         |         |       |
| 1   | U     | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1670  | 1046 | 305 | 315 | 4 |         |         |       |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| C     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| D     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| E     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| F     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| G     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| O     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| P     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| Q     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| R     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| S     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| T     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |
| U     | 9       | MET      | -      | initiating methionine | UNP A5U4D5 |

- Molecule 2 is a protein called Proteasome subunit beta.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | H     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | I     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | J     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | K     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | L     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | M     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | N     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | V     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | W     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | X     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | Y     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | Z     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | a     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | b     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |

There are 84 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| H     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| H     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| H     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| H     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| H     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| I     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| I     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| I     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| I     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| I     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| I     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| J     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| J     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| J     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| J     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| J     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| J     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| K     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| K     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| K     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| K     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| K     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| K     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| L     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| L     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| L     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| L     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| L     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| L     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| M     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| M     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| M     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| M     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| M     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| M     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |

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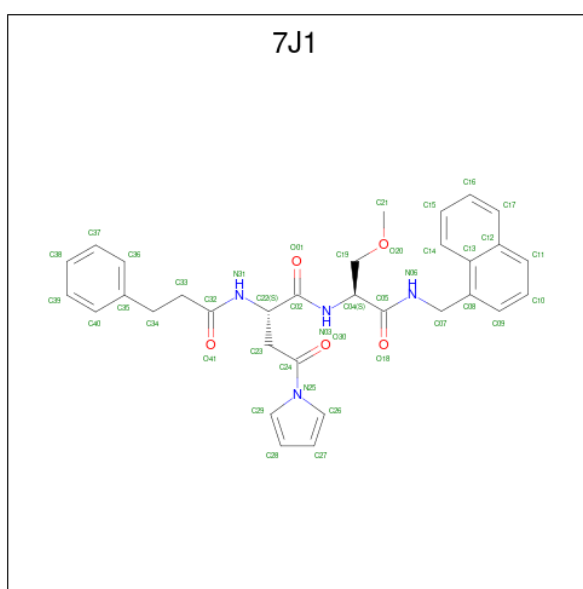
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| N     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| N     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| N     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| N     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| N     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| N     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| V     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| V     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| V     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| V     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| V     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| V     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| W     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| W     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| W     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| W     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| W     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| W     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| X     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| X     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| X     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| X     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| X     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| X     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| Y     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| Y     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| Y     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| Y     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| Y     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| Y     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| Z     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| Z     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| Z     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| Z     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| Z     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| Z     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |
| a     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| a     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| a     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| a     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| a     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| a     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| b     | 235     | HIS      | -      | expression tag | UNP A5U4D6 |
| b     | 236     | HIS      | -      | expression tag | UNP A5U4D6 |
| b     | 237     | HIS      | -      | expression tag | UNP A5U4D6 |
| b     | 238     | HIS      | -      | expression tag | UNP A5U4D6 |
| b     | 239     | HIS      | -      | expression tag | UNP A5U4D6 |
| b     | 240     | HIS      | -      | expression tag | UNP A5U4D6 |

- Molecule 3 is (2S)-N-{(2S)-3-methoxy-1-[(naphthalen-1-ylmethyl)amino]-1-oxopropan-2-yl}-4-oxo-2-[(3-phenylpropanoyl)amino]-4-(1H-pyrrol-1-yl)butanamide (non-preferred name) (CCD ID: 7J1) (formula: C<sub>32</sub>H<sub>34</sub>N<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | V     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | W     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | X     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | Y     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | Z     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | a     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |
| 3   | b     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 41    | 32 | 4 | 5 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 4   | B     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 4   | C     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 4   | D     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 4   | E     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 4   | F     | 8        | Total | O  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |
| 4   | G     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 4   | H     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 4   | I     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |
| 4   | J     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 4   | K     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 4   | L     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |

*Continued on next page...*

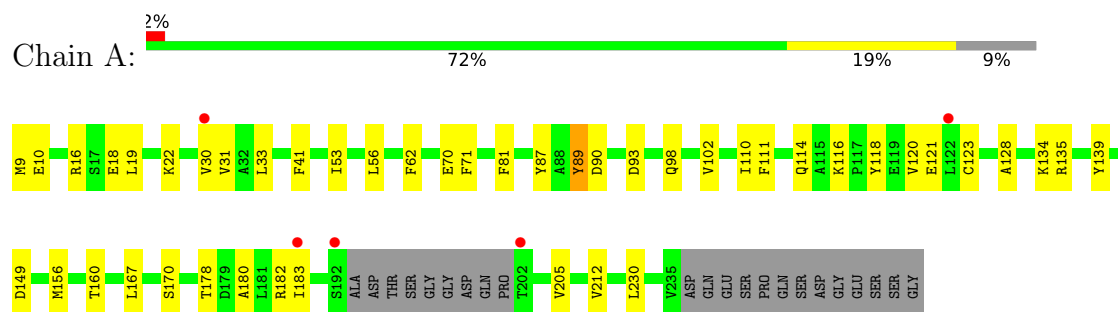
*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | M     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | N     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 4   | O     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 4   | P     | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 4   | Q     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 4   | R     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 4   | S     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 4   | T     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 4   | U     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 4   | V     | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 4   | W     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | X     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 4   | Y     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 4   | Z     | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 4   | a     | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 4   | b     | 16       | Total<br>16 | O<br>16 | 0       | 0       |

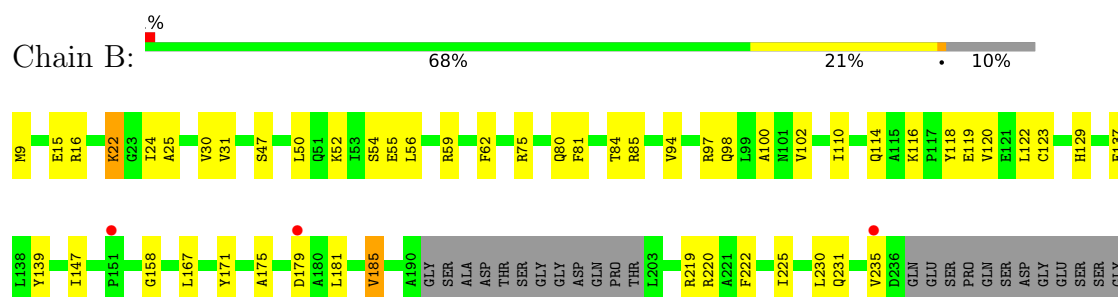
### 3 Residue-property plots

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.

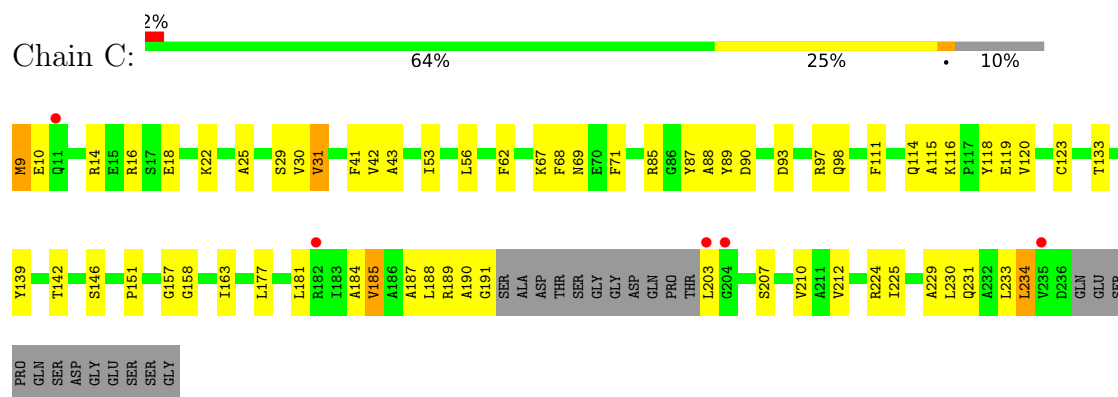
#### • Molecule 1: Proteasome subunit alpha



#### • Molecule 1: Proteasome subunit alpha



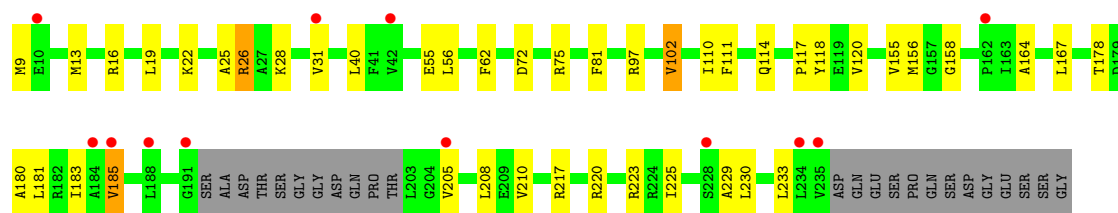
#### • Molecule 1: Proteasome subunit alpha



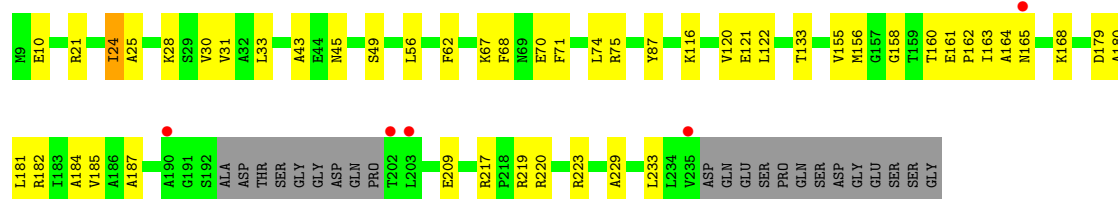
#### • Molecule 1: Proteasome subunit alpha



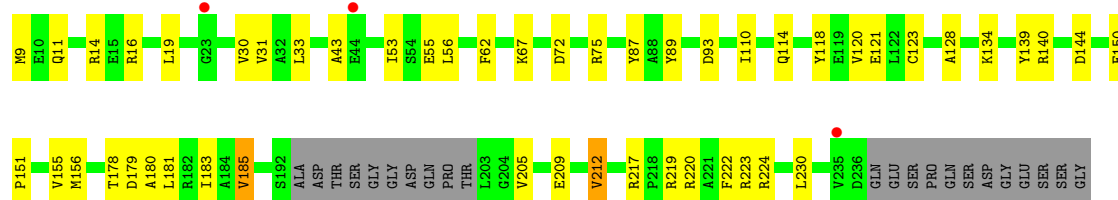




• Molecule 1: Proteasome subunit alpha



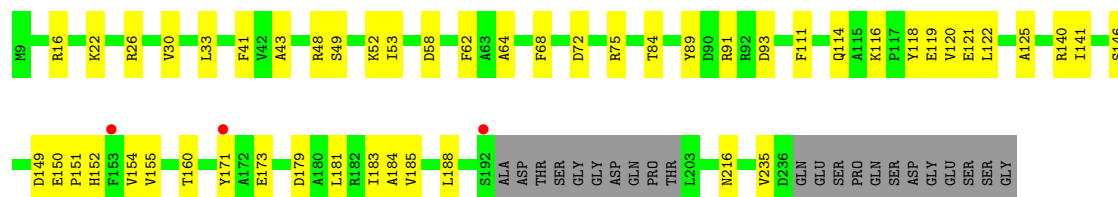
• Molecule 1: Proteasome subunit alpha



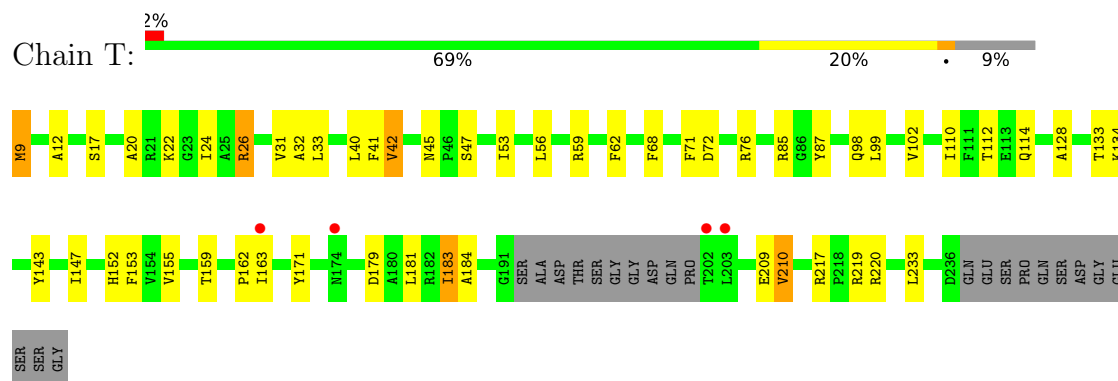
• Molecule 1: Proteasome subunit alpha



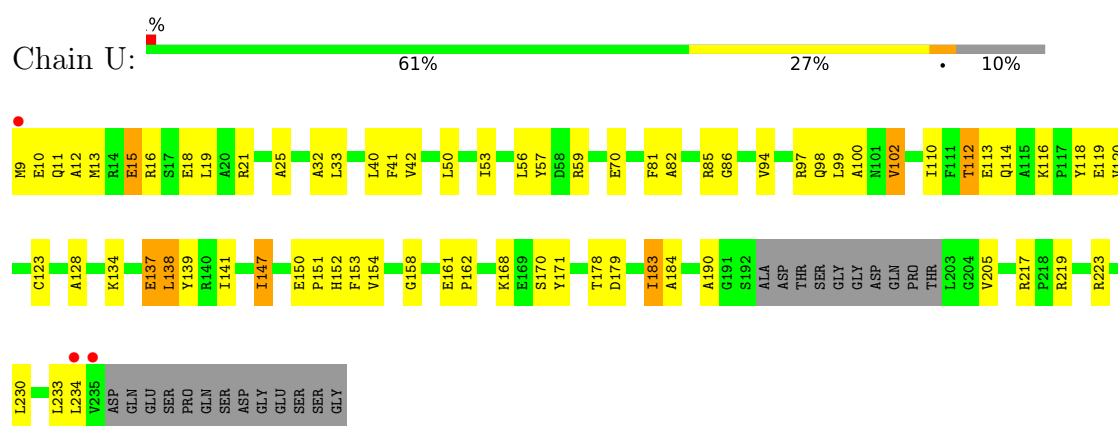
• Molecule 1: Proteasome subunit alpha



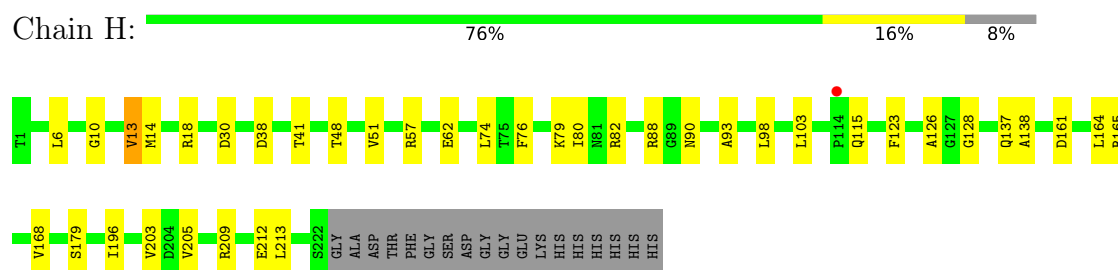
- Molecule 1: Proteasome subunit alpha



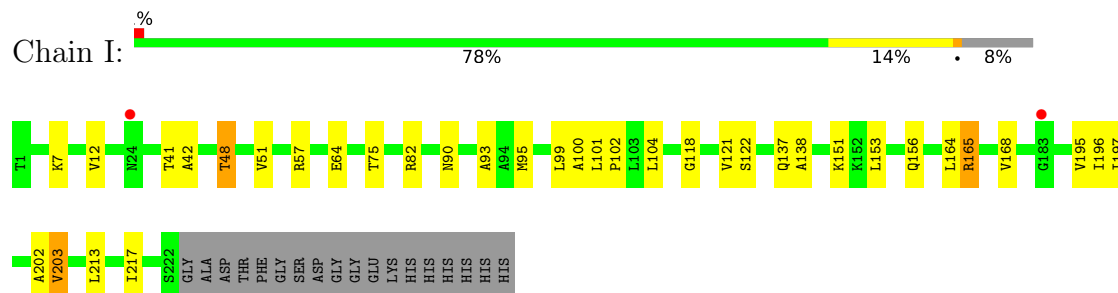
- Molecule 1: Proteasome subunit alpha



- Molecule 2: Proteasome subunit beta

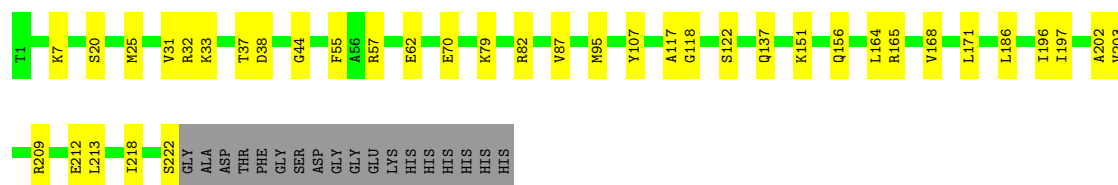


- Molecule 2: Proteasome subunit beta



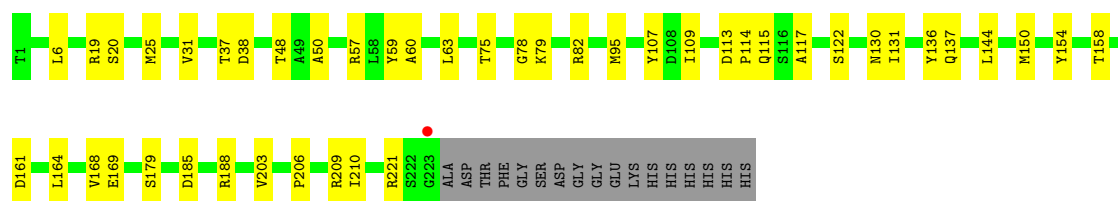
- Molecule 2: Proteasome subunit beta

Chain J:  77% 16% 8%



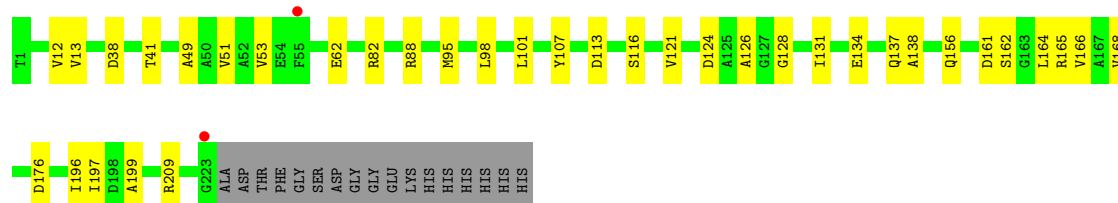
• Molecule 2: Proteasome subunit beta

Chain K:  74% 19% 7%



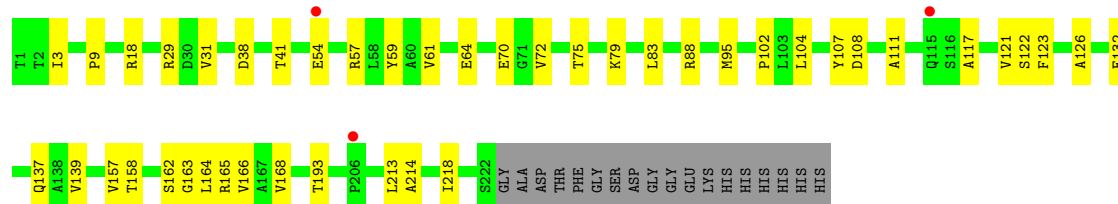
• Molecule 2: Proteasome subunit beta

Chain L:  78% 15% 7%



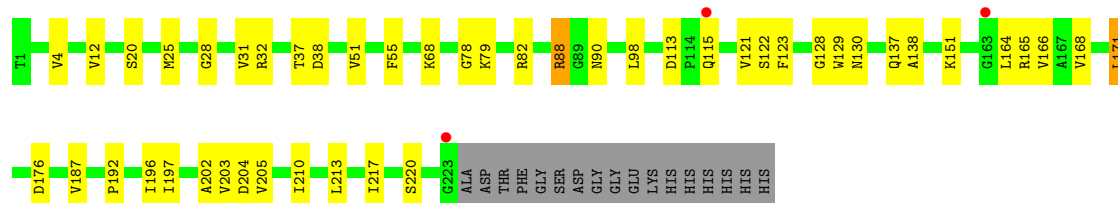
• Molecule 2: Proteasome subunit beta

Chain M:  74% 18% 8%

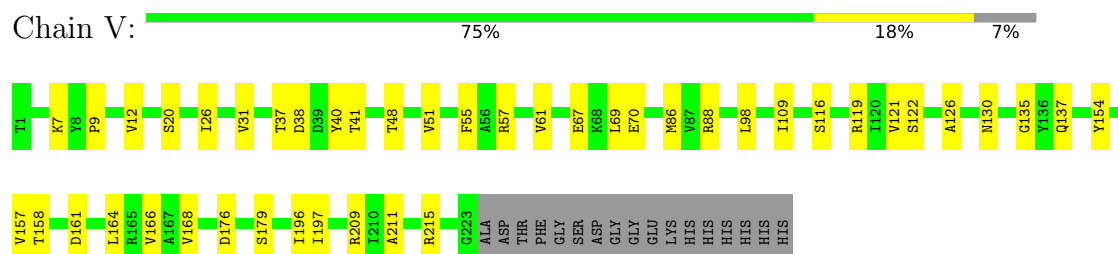


• Molecule 2: Proteasome subunit beta

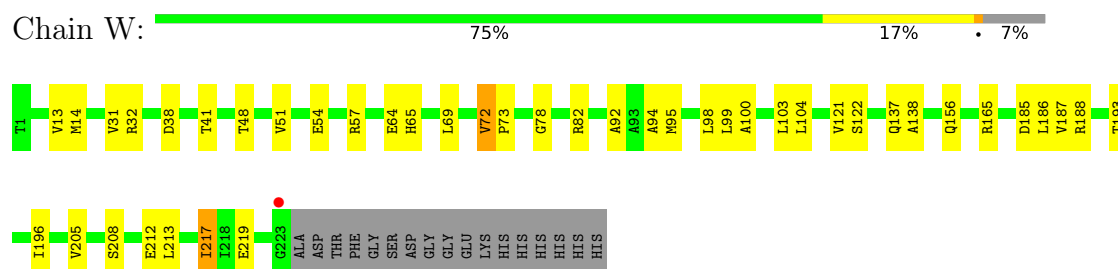
Chain N:  73% 19% 7%



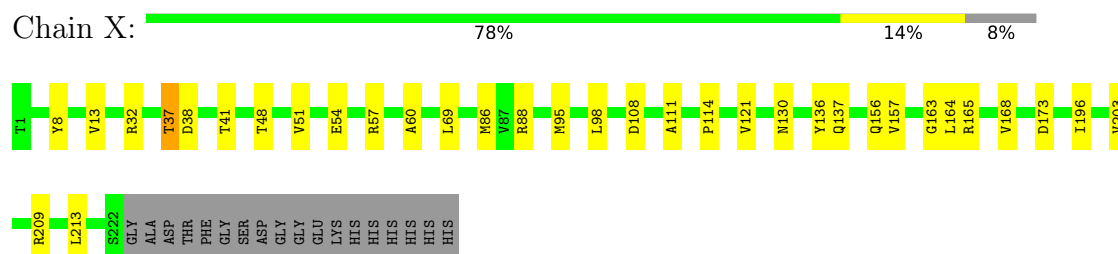
- Molecule 2: Proteasome subunit beta



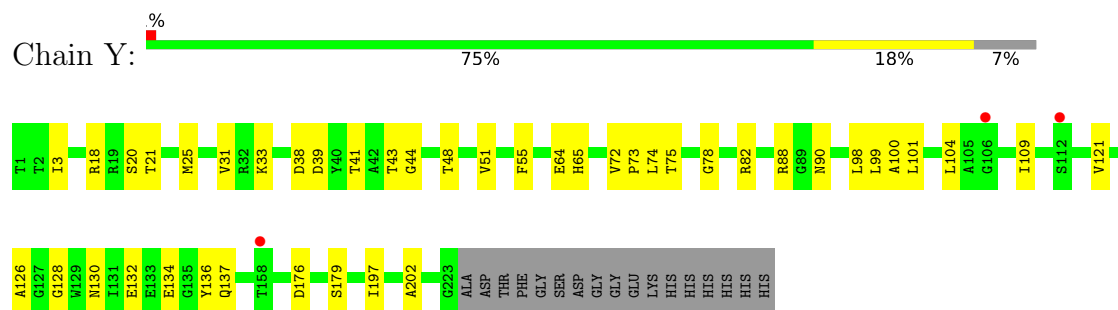
- Molecule 2: Proteasome subunit beta



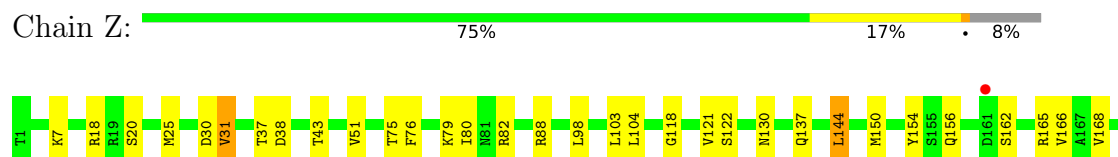
- Molecule 2: Proteasome subunit beta

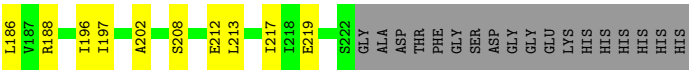


- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

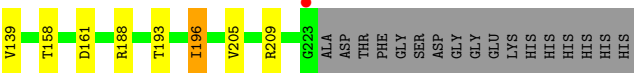
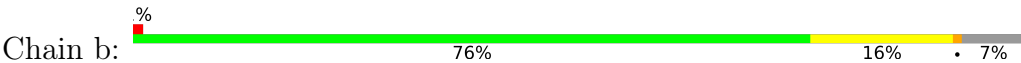




• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 120.55Å 198.54Å 165.72Å<br>90.00° 103.24° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 49.61 – 2.85<br>49.61 – 2.85                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.9 (49.61-2.85)<br>94.2 (49.61-2.85)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.17 (at 2.86Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.10.1_2155                                          | Depositor        |
| R, $R_{free}$                                                           | 0.177 , 0.235<br>0.179 , 0.235                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 8304 reflections (4.69%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 48.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.092                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 42.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 47311                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 52.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7J1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.50         | 1/1701 (0.1%)  | 0.72        | 0/2297         |
| 1   | B     | 0.46         | 0/1692         | 0.71        | 0/2285         |
| 1   | C     | 0.42         | 0/1696         | 0.68        | 0/2290         |
| 1   | D     | 0.46         | 0/1694         | 0.71        | 0/2287         |
| 1   | E     | 0.44         | 0/1701         | 0.72        | 0/2297         |
| 1   | F     | 0.45         | 0/1679         | 0.72        | 0/2266         |
| 1   | G     | 0.43         | 0/1714         | 0.71        | 0/2315         |
| 1   | O     | 0.45         | 0/1688         | 0.71        | 0/2279         |
| 1   | P     | 0.45         | 0/1701         | 0.73        | 0/2297         |
| 1   | Q     | 0.46         | 0/1702         | 0.71        | 0/2298         |
| 1   | R     | 0.46         | 0/1694         | 0.73        | 0/2287         |
| 1   | S     | 0.47         | 0/1702         | 0.72        | 0/2298         |
| 1   | T     | 0.49         | 0/1703         | 0.77        | 4/2300 (0.2%)  |
| 1   | U     | 0.52         | 0/1694         | 0.81        | 3/2287 (0.1%)  |
| 2   | H     | 0.45         | 0/1662         | 0.69        | 0/2254         |
| 2   | I     | 0.49         | 0/1662         | 0.71        | 0/2254         |
| 2   | J     | 0.45         | 0/1662         | 0.70        | 0/2254         |
| 2   | K     | 0.46         | 0/1666         | 0.74        | 0/2259         |
| 2   | L     | 0.46         | 0/1666         | 0.68        | 0/2259         |
| 2   | M     | 0.43         | 0/1662         | 0.67        | 0/2254         |
| 2   | N     | 0.45         | 0/1666         | 0.73        | 0/2259         |
| 2   | V     | 0.44         | 0/1666         | 0.69        | 0/2259         |
| 2   | W     | 0.48         | 0/1666         | 0.69        | 0/2259         |
| 2   | X     | 0.49         | 0/1662         | 0.72        | 0/2254         |
| 2   | Y     | 0.48         | 0/1666         | 0.73        | 0/2259         |
| 2   | Z     | 0.48         | 0/1662         | 0.72        | 0/2254         |
| 2   | a     | 0.44         | 0/1666         | 0.67        | 0/2259         |
| 2   | b     | 0.49         | 0/1666         | 0.72        | 0/2259         |
| All | All   | 0.46         | 1/47061 (0.0%) | 0.72        | 7/63679 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | Y     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 89  | TYR  | CA-C  | -6.43 | 1.49        | 1.52     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | U     | 15  | GLU  | CA-CB-CG | -10.73 | 92.64       | 114.10   |
| 1   | T     | 9   | MET  | CB-CG-SD | 6.60   | 132.49      | 112.70   |
| 1   | T     | 9   | MET  | N-CA-C   | 6.43   | 129.00      | 111.00   |
| 1   | T     | 9   | MET  | CA-C-N   | -5.70  | 112.07      | 120.28   |
| 1   | T     | 9   | MET  | C-N-CA   | -5.70  | 112.07      | 120.28   |
| 1   | U     | 137 | GLU  | CA-C-N   | -5.27  | 115.04      | 122.94   |
| 1   | U     | 137 | GLU  | C-N-CA   | -5.27  | 115.04      | 122.94   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | Y     | 128 | GLY  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1677  | 0        | 1680     | 32      | 0            |
| 1   | B     | 1668  | 0        | 1669     | 33      | 0            |
| 1   | C     | 1672  | 0        | 1672     | 42      | 0            |
| 1   | D     | 1670  | 0        | 1673     | 39      | 0            |
| 1   | E     | 1677  | 0        | 1680     | 32      | 0            |
| 1   | F     | 1655  | 0        | 1653     | 37      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | G     | 1690  | 0        | 1689     | 37      | 0            |
| 1   | O     | 1664  | 0        | 1668     | 34      | 0            |
| 1   | P     | 1677  | 0        | 1680     | 28      | 0            |
| 1   | Q     | 1678  | 0        | 1677     | 35      | 0            |
| 1   | R     | 1670  | 0        | 1673     | 38      | 0            |
| 1   | S     | 1678  | 0        | 1677     | 29      | 0            |
| 1   | T     | 1679  | 0        | 1679     | 33      | 0            |
| 1   | U     | 1670  | 0        | 1673     | 53      | 0            |
| 2   | H     | 1638  | 0        | 1633     | 23      | 0            |
| 2   | I     | 1638  | 0        | 1633     | 23      | 0            |
| 2   | J     | 1638  | 0        | 1633     | 24      | 0            |
| 2   | K     | 1642  | 0        | 1636     | 34      | 0            |
| 2   | L     | 1642  | 0        | 1636     | 23      | 0            |
| 2   | M     | 1638  | 0        | 1633     | 27      | 0            |
| 2   | N     | 1642  | 0        | 1636     | 27      | 0            |
| 2   | V     | 1642  | 0        | 1636     | 26      | 0            |
| 2   | W     | 1642  | 0        | 1636     | 27      | 0            |
| 2   | X     | 1638  | 0        | 1633     | 24      | 0            |
| 2   | Y     | 1642  | 0        | 1636     | 32      | 0            |
| 2   | Z     | 1638  | 0        | 1633     | 30      | 0            |
| 2   | a     | 1642  | 0        | 1636     | 21      | 0            |
| 2   | b     | 1642  | 0        | 1636     | 23      | 0            |
| 3   | H     | 41    | 0        | 0        | 0       | 0            |
| 3   | I     | 41    | 0        | 0        | 0       | 0            |
| 3   | J     | 41    | 0        | 0        | 0       | 0            |
| 3   | K     | 41    | 0        | 0        | 0       | 0            |
| 3   | L     | 41    | 0        | 0        | 0       | 0            |
| 3   | M     | 41    | 0        | 0        | 0       | 0            |
| 3   | N     | 41    | 0        | 0        | 0       | 0            |
| 3   | V     | 41    | 0        | 0        | 0       | 0            |
| 3   | W     | 41    | 0        | 0        | 0       | 0            |
| 3   | X     | 41    | 0        | 0        | 1       | 0            |
| 3   | Y     | 41    | 0        | 0        | 1       | 0            |
| 3   | Z     | 41    | 0        | 0        | 0       | 0            |
| 3   | a     | 41    | 0        | 0        | 0       | 0            |
| 3   | b     | 41    | 0        | 0        | 0       | 0            |
| 4   | A     | 12    | 0        | 0        | 1       | 0            |
| 4   | B     | 7     | 0        | 0        | 0       | 0            |
| 4   | C     | 9     | 0        | 0        | 0       | 0            |
| 4   | D     | 5     | 0        | 0        | 0       | 0            |
| 4   | E     | 7     | 0        | 0        | 1       | 0            |
| 4   | F     | 8     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | G     | 4     | 0        | 0        | 0       | 0            |
| 4   | H     | 14    | 0        | 0        | 0       | 0            |
| 4   | I     | 25    | 0        | 0        | 0       | 0            |
| 4   | J     | 13    | 0        | 0        | 2       | 0            |
| 4   | K     | 19    | 0        | 0        | 2       | 0            |
| 4   | L     | 14    | 0        | 0        | 0       | 0            |
| 4   | M     | 20    | 0        | 0        | 0       | 0            |
| 4   | N     | 11    | 0        | 0        | 1       | 0            |
| 4   | O     | 10    | 0        | 0        | 0       | 0            |
| 4   | P     | 4     | 0        | 0        | 0       | 0            |
| 4   | Q     | 5     | 0        | 0        | 0       | 0            |
| 4   | R     | 9     | 0        | 0        | 1       | 0            |
| 4   | S     | 15    | 0        | 0        | 1       | 0            |
| 4   | T     | 6     | 0        | 0        | 0       | 0            |
| 4   | U     | 10    | 0        | 0        | 2       | 0            |
| 4   | V     | 19    | 0        | 0        | 0       | 0            |
| 4   | W     | 12    | 0        | 0        | 0       | 0            |
| 4   | X     | 13    | 0        | 0        | 1       | 0            |
| 4   | Y     | 26    | 0        | 0        | 1       | 0            |
| 4   | Z     | 19    | 0        | 0        | 1       | 0            |
| 4   | a     | 16    | 0        | 0        | 0       | 0            |
| 4   | b     | 16    | 0        | 0        | 1       | 0            |
| All | All   | 47311 | 0        | 46329    | 783     | 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 8.

All (783) 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:P:24:ILE:HD11  | 1:P:121:GLU:HB2 | 1.50                     | 0.94              |
| 1:R:112:THR:HG22 | 1:R:113:GLU:HG3 | 1.55                     | 0.89              |
| 1:T:9:MET:HA     | 1:T:12:ALA:HB3  | 1.52                     | 0.88              |
| 1:D:16:ARG:NH2   | 1:D:114:GLN:O   | 2.06                     | 0.88              |
| 1:G:16:ARG:NH1   | 1:G:111:PHE:O   | 2.08                     | 0.86              |
| 2:H:38:ASP:HB3   | 2:H:41:THR:HB   | 1.57                     | 0.86              |
| 1:D:87:TYR:O     | 2:K:57:ARG:NH2  | 2.09                     | 0.85              |
| 1:F:9:MET:N      | 1:G:15:GLU:OE2  | 2.10                     | 0.85              |
| 1:R:16:ARG:NH1   | 1:R:111:PHE:O   | 2.10                     | 0.85              |
| 1:Q:9:MET:N      | 1:R:15:GLU:OE1  | 2.09                     | 0.84              |
| 1:U:85:ARG:NH2   | 1:U:98:GLN:OE1  | 2.12                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:54:GLU:OE2   | 2:N:88:ARG:NH2   | 2.14                     | 0.80              |
| 2:X:156:GLN:OE1  | 2:X:165:ARG:NH2  | 2.15                     | 0.80              |
| 1:P:155:VAL:HG21 | 1:P:164:ALA:HB2  | 1.64                     | 0.80              |
| 1:R:16:ARG:NH2   | 1:R:114:GLN:O    | 2.15                     | 0.79              |
| 1:G:16:ARG:NH2   | 1:G:114:GLN:O    | 2.16                     | 0.79              |
| 2:K:38:ASP:OD2   | 2:K:79:LYS:NZ    | 2.16                     | 0.78              |
| 1:S:179:ASP:O    | 1:S:183:ILE:HG12 | 1.82                     | 0.78              |
| 1:U:59:ARG:NH2   | 1:U:217:ARG:O    | 2.16                     | 0.78              |
| 1:C:41:PHE:HB3   | 1:C:53:ILE:HD12  | 1.67                     | 0.76              |
| 1:C:18:GLU:HG3   | 1:C:22:LYS:HE3   | 1.67                     | 0.76              |
| 2:W:156:GLN:OE1  | 2:W:165:ARG:NH1  | 2.18                     | 0.76              |
| 1:O:110:ILE:HG23 | 1:O:114:GLN:HG3  | 1.69                     | 0.75              |
| 1:Q:33:LEU:HD11  | 1:Q:180:ALA:HB1  | 1.67                     | 0.75              |
| 1:D:223:ARG:HE   | 1:D:224:ARG:H    | 1.34                     | 0.75              |
| 1:O:72:ASP:OD1   | 1:O:75:ARG:NH1   | 2.19                     | 0.75              |
| 1:C:87:TYR:O     | 2:J:57:ARG:NH2   | 2.20                     | 0.74              |
| 1:U:18:GLU:OE1   | 1:U:21:ARG:NH2   | 2.21                     | 0.74              |
| 2:M:38:ASP:OD2   | 2:M:79:LYS:NZ    | 2.21                     | 0.74              |
| 1:T:128:ALA:HB2  | 1:T:134:LYS:HB3  | 1.68                     | 0.73              |
| 2:Y:109:ILE:HD12 | 2:Y:109:ILE:H    | 1.53                     | 0.73              |
| 2:K:130:ASN:ND2  | 4:K:401:HOH:O    | 2.21                     | 0.73              |
| 1:C:9:MET:N      | 1:D:15:GLU:OE1   | 2.21                     | 0.73              |
| 1:O:205:VAL:HG13 | 1:O:230:LEU:HD23 | 1.69                     | 0.73              |
| 2:b:161:ASP:OD2  | 2:b:209:ARG:NH2  | 2.21                     | 0.73              |
| 1:U:118:TYR:HB3  | 1:U:120:VAL:HG22 | 1.70                     | 0.72              |
| 1:A:90:ASP:OD1   | 4:A:301:HOH:O    | 2.07                     | 0.72              |
| 1:P:33:LEU:HD11  | 1:P:180:ALA:HB1  | 1.72                     | 0.72              |
| 1:T:59:ARG:NH2   | 1:T:217:ARG:O    | 2.23                     | 0.72              |
| 1:C:30:VAL:HG13  | 1:C:43:ALA:HB2   | 1.71                     | 0.72              |
| 1:F:219:ARG:HH21 | 1:F:220:ARG:HD2  | 1.52                     | 0.72              |
| 2:J:156:GLN:OE1  | 2:J:165:ARG:NH1  | 2.22                     | 0.72              |
| 1:S:16:ARG:NH1   | 1:S:111:PHE:O    | 2.23                     | 0.72              |
| 2:J:38:ASP:OD2   | 2:J:79:LYS:NZ    | 2.23                     | 0.71              |
| 1:D:210:VAL:HG21 | 1:D:230:LEU:HD13 | 1.71                     | 0.71              |
| 1:G:98:GLN:O     | 1:G:102:VAL:HG23 | 1.91                     | 0.71              |
| 1:G:118:TYR:HB3  | 1:G:120:VAL:HG22 | 1.72                     | 0.71              |
| 1:U:33:LEU:HD13  | 1:U:153:PHE:HB3  | 1.73                     | 0.70              |
| 1:Q:205:VAL:HG13 | 1:Q:230:LEU:HD23 | 1.71                     | 0.70              |
| 1:F:118:TYR:HB3  | 1:F:120:VAL:HG22 | 1.73                     | 0.70              |
| 2:I:122:SER:HB3  | 2:I:137:GLN:HG2  | 1.74                     | 0.70              |
| 1:P:179:ASP:OD1  | 1:P:182:ARG:NH1  | 2.24                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:162:PRO:HB2  | 1:F:191:GLY:HA2  | 1.73                     | 0.69              |
| 2:W:92:ALA:HA    | 2:W:95:MET:HE2   | 1.73                     | 0.69              |
| 1:Q:121:GLU:OE1  | 1:Q:140:ARG:NH2  | 2.26                     | 0.69              |
| 2:X:54:GLU:OE1   | 2:Y:88:ARG:NH2   | 2.25                     | 0.69              |
| 1:T:45:ASN:ND2   | 1:T:209:GLU:OE1  | 2.26                     | 0.69              |
| 1:U:141:ILE:HG13 | 1:U:147:ILE:HD12 | 1.73                     | 0.69              |
| 2:b:57:ARG:NH1   | 4:b:401:HOH:O    | 2.25                     | 0.69              |
| 1:U:112:THR:HG22 | 1:U:113:GLU:HG3  | 1.75                     | 0.69              |
| 1:E:210:VAL:HG21 | 1:E:230:LEU:HD13 | 1.74                     | 0.68              |
| 1:G:128:ALA:HB2  | 1:G:134:LYS:HB3  | 1.75                     | 0.68              |
| 2:H:164:LEU:HD11 | 2:H:205:VAL:HG11 | 1.75                     | 0.68              |
| 2:I:51:VAL:HG23  | 2:I:100:ALA:HB2  | 1.76                     | 0.68              |
| 1:F:219:ARG:HH22 | 2:M:64:GLU:CD    | 2.01                     | 0.68              |
| 1:F:112:THR:HG22 | 1:F:113:GLU:HG3  | 1.76                     | 0.68              |
| 1:U:205:VAL:HG13 | 1:U:230:LEU:HD23 | 1.76                     | 0.68              |
| 2:Z:156:GLN:OE1  | 2:Z:165:ARG:NH1  | 2.27                     | 0.68              |
| 1:O:31:VAL:HG21  | 1:O:167:LEU:HD11 | 1.74                     | 0.68              |
| 1:O:19:LEU:HD13  | 1:U:9:MET:HE2    | 1.76                     | 0.67              |
| 2:N:187:VAL:O    | 4:N:401:HOH:O    | 2.11                     | 0.67              |
| 1:D:42:VAL:HG22  | 1:D:210:VAL:HG12 | 1.75                     | 0.67              |
| 2:N:122:SER:HB3  | 2:N:137:GLN:HG2  | 1.77                     | 0.67              |
| 1:T:219:ARG:HD3  | 1:T:220:ARG:HG3  | 1.75                     | 0.67              |
| 2:K:188:ARG:NH1  | 2:V:176:ASP:OD2  | 2.28                     | 0.67              |
| 1:Q:128:ALA:HB2  | 1:Q:134:LYS:HB3  | 1.75                     | 0.67              |
| 2:Z:7:LYS:NZ     | 2:Z:118:GLY:O    | 2.28                     | 0.67              |
| 1:C:42:VAL:HG11  | 1:C:184:ALA:HB1  | 1.77                     | 0.67              |
| 1:T:9:MET:HA     | 1:T:12:ALA:CB    | 2.22                     | 0.66              |
| 1:U:138:LEU:HD13 | 1:U:154:VAL:HG23 | 1.77                     | 0.66              |
| 1:Q:16:ARG:NH2   | 1:Q:114:GLN:O    | 2.28                     | 0.66              |
| 1:R:219:ARG:NH2  | 2:Y:64:GLU:OE1   | 2.27                     | 0.66              |
| 2:L:161:ASP:CG   | 2:L:209:ARG:HH22 | 2.04                     | 0.66              |
| 1:D:163:ILE:HG23 | 1:D:187:ALA:HB1  | 1.76                     | 0.66              |
| 2:X:8:TYR:CE2    | 2:X:196:ILE:HD11 | 2.30                     | 0.66              |
| 1:C:163:ILE:HD13 | 1:C:188:LEU:HD23 | 1.77                     | 0.66              |
| 2:Z:122:SER:HB3  | 2:Z:137:GLN:HG2  | 1.78                     | 0.66              |
| 1:C:31:VAL:HG13  | 1:C:42:VAL:HG13  | 1.79                     | 0.66              |
| 1:F:41:PHE:HB3   | 1:F:53:ILE:HD13  | 1.78                     | 0.66              |
| 1:F:110:ILE:HG23 | 1:F:114:GLN:HG3  | 1.78                     | 0.66              |
| 1:U:116:LYS:NZ   | 1:U:119:GLU:OE2  | 2.29                     | 0.65              |
| 1:E:140:ARG:NH2  | 1:E:155:VAL:O    | 2.29                     | 0.65              |
| 2:K:20:SER:HB2   | 2:K:31:VAL:HG21  | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:162:PRO:HB2  | 1:E:191:GLY:HA2  | 1.77                     | 0.65              |
| 1:G:181:LEU:O    | 1:G:185:VAL:HG23 | 1.97                     | 0.65              |
| 2:W:38:ASP:HB3   | 2:W:41:THR:CG2   | 2.27                     | 0.65              |
| 1:R:177:LEU:HD22 | 1:R:233:LEU:HD23 | 1.79                     | 0.64              |
| 1:A:30:VAL:HG23  | 1:A:156:MET:HE3  | 1.80                     | 0.64              |
| 2:I:213:LEU:O    | 2:I:217:ILE:HD12 | 1.98                     | 0.64              |
| 1:A:33:LEU:HD11  | 1:A:180:ALA:HB1  | 1.79                     | 0.64              |
| 1:T:179:ASP:O    | 1:T:183:ILE:HG22 | 1.97                     | 0.64              |
| 2:W:213:LEU:O    | 2:W:217:ILE:HD12 | 1.98                     | 0.64              |
| 2:X:38:ASP:HB3   | 2:X:41:THR:HB    | 1.79                     | 0.64              |
| 1:B:219:ARG:NH1  | 2:I:64:GLU:OE2   | 2.31                     | 0.64              |
| 1:T:9:MET:HE3    | 1:U:19:LEU:HD13  | 1.80                     | 0.64              |
| 1:E:30:VAL:HG13  | 1:E:43:ALA:HB2   | 1.80                     | 0.63              |
| 1:R:210:VAL:HG21 | 1:R:230:LEU:HD13 | 1.81                     | 0.63              |
| 1:U:42:VAL:HG11  | 1:U:184:ALA:HB1  | 1.80                     | 0.63              |
| 2:X:8:TYR:HE2    | 2:X:196:ILE:HD11 | 1.62                     | 0.63              |
| 1:B:16:ARG:NH2   | 1:B:114:GLN:O    | 2.23                     | 0.63              |
| 2:V:40:TYR:CE2   | 2:V:109:ILE:HD11 | 2.34                     | 0.63              |
| 2:b:122:SER:HB3  | 2:b:137:GLN:HG2  | 1.80                     | 0.63              |
| 2:Z:88:ARG:NH1   | 4:Z:401:HOH:O    | 2.31                     | 0.63              |
| 1:C:93:ASP:OD2   | 2:K:75:THR:HG22  | 1.99                     | 0.63              |
| 1:A:87:TYR:O     | 2:H:57:ARG:NH2   | 2.32                     | 0.62              |
| 1:E:81:PHE:CZ    | 1:E:102:VAL:HG21 | 2.34                     | 0.62              |
| 1:P:10:GLU:HG2   | 1:Q:19:LEU:HD12  | 1.79                     | 0.62              |
| 1:E:209:GLU:OE2  | 1:E:224:ARG:NH1  | 2.32                     | 0.62              |
| 1:B:118:TYR:HB3  | 1:B:120:VAL:HG22 | 1.81                     | 0.62              |
| 2:K:188:ARG:NH2  | 2:L:134:GLU:OE2  | 2.32                     | 0.62              |
| 1:D:110:ILE:HA   | 1:D:114:GLN:HG3  | 1.81                     | 0.62              |
| 2:V:122:SER:HB3  | 2:V:137:GLN:HG2  | 1.80                     | 0.62              |
| 1:C:85:ARG:NH1   | 1:C:98:GLN:OE1   | 2.32                     | 0.62              |
| 1:C:210:VAL:HG21 | 1:C:230:LEU:HD13 | 1.80                     | 0.62              |
| 2:L:95:MET:HE2   | 2:L:95:MET:HA    | 1.81                     | 0.62              |
| 1:F:76:ARG:NH2   | 2:M:70:GLU:OE1   | 2.32                     | 0.61              |
| 2:X:48:THR:HB    | 2:X:51:VAL:HG12  | 1.82                     | 0.61              |
| 1:F:42:VAL:HG11  | 1:F:184:ALA:HB1  | 1.82                     | 0.61              |
| 1:U:223:ARG:NH2  | 4:U:303:HOH:O    | 2.33                     | 0.61              |
| 1:D:223:ARG:HE   | 1:D:224:ARG:N    | 1.99                     | 0.61              |
| 1:G:179:ASP:O    | 1:G:183:ILE:HG23 | 2.01                     | 0.61              |
| 1:S:30:VAL:HG13  | 1:S:43:ALA:HB2   | 1.82                     | 0.61              |
| 1:S:151:PRO:HD2  | 4:S:303:HOH:O    | 2.01                     | 0.61              |
| 1:E:18:GLU:OE2   | 1:E:22:LYS:NZ    | 2.27                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:140:ARG:NH1  | 1:G:155:VAL:O    | 2.34                     | 0.61              |
| 2:H:51:VAL:HG21  | 2:H:98:LEU:HB3   | 1.83                     | 0.60              |
| 1:T:85:ARG:NH2   | 1:T:98:GLN:OE1   | 2.34                     | 0.60              |
| 1:A:30:VAL:CG2   | 1:A:156:MET:HE3  | 2.30                     | 0.60              |
| 1:O:217:ARG:HD3  | 1:O:223:ARG:HH11 | 1.64                     | 0.60              |
| 1:B:59:ARG:HG3   | 1:B:129:HIS:CD2  | 2.36                     | 0.60              |
| 1:R:210:VAL:HG23 | 1:R:225:ILE:HB   | 1.82                     | 0.60              |
| 1:S:149:ASP:OD2  | 1:T:47:SER:OG    | 2.19                     | 0.60              |
| 1:U:162:PRO:HB2  | 1:U:190:ALA:O    | 2.02                     | 0.59              |
| 1:G:30:VAL:HG13  | 1:G:43:ALA:HB2   | 1.83                     | 0.59              |
| 2:W:94:ALA:HB1   | 2:W:99:LEU:HD23  | 1.83                     | 0.59              |
| 2:V:161:ASP:CG   | 2:V:209:ARG:HH21 | 2.10                     | 0.59              |
| 2:K:75:THR:HG23  | 2:K:78:GLY:H     | 1.67                     | 0.59              |
| 2:K:122:SER:HB3  | 2:K:137:GLN:HG2  | 1.84                     | 0.59              |
| 1:Q:31:VAL:HG22  | 1:Q:155:VAL:HG22 | 1.83                     | 0.59              |
| 1:S:33:LEU:HD21  | 1:S:184:ALA:HB2  | 1.84                     | 0.59              |
| 1:C:181:LEU:O    | 1:C:185:VAL:HG23 | 2.02                     | 0.58              |
| 1:G:41:PHE:HB3   | 1:G:53:ILE:HD13  | 1.85                     | 0.58              |
| 1:E:128:ALA:HB2  | 1:E:134:LYS:HB3  | 1.83                     | 0.58              |
| 2:a:88:ARG:HD3   | 2:a:126:ALA:O    | 2.02                     | 0.58              |
| 1:C:89:TYR:CE2   | 2:K:82:ARG:HD2   | 2.39                     | 0.58              |
| 2:J:95:MET:HA    | 2:J:95:MET:HE2   | 1.86                     | 0.58              |
| 1:S:41:PHE:HB3   | 1:S:53:ILE:HD13  | 1.85                     | 0.58              |
| 1:A:118:TYR:HB3  | 1:A:120:VAL:HG22 | 1.85                     | 0.58              |
| 2:L:38:ASP:HB3   | 2:L:41:THR:OG1   | 2.04                     | 0.58              |
| 2:I:7:LYS:NZ     | 2:I:118:GLY:O    | 2.36                     | 0.57              |
| 1:O:217:ARG:HD3  | 1:O:223:ARG:NH1  | 2.18                     | 0.57              |
| 2:W:196:ILE:HD12 | 2:W:205:VAL:HG22 | 1.86                     | 0.57              |
| 2:Y:51:VAL:HG21  | 2:Y:98:LEU:HB3   | 1.87                     | 0.57              |
| 1:T:42:VAL:HG11  | 1:T:184:ALA:HB1  | 1.87                     | 0.57              |
| 2:J:122:SER:HB3  | 2:J:137:GLN:HG2  | 1.85                     | 0.57              |
| 2:M:9:PRO:HG2    | 2:M:158:THR:O    | 2.05                     | 0.57              |
| 1:U:110:ILE:HA   | 1:U:114:GLN:HG3  | 1.85                     | 0.57              |
| 1:Q:75:ARG:NH2   | 2:X:69:LEU:O     | 2.37                     | 0.57              |
| 1:U:56:LEU:HD13  | 1:U:99:LEU:HD22  | 1.87                     | 0.57              |
| 2:X:165:ARG:HG3  | 2:X:213:LEU:HD22 | 1.87                     | 0.57              |
| 2:M:3:ILE:HB     | 2:M:139:VAL:HG12 | 1.87                     | 0.57              |
| 1:U:82:ALA:HB2   | 1:U:99:LEU:HD21  | 1.87                     | 0.57              |
| 1:D:98:GLN:O     | 1:D:102:VAL:HG23 | 2.05                     | 0.56              |
| 2:M:54:GLU:CD    | 2:N:88:ARG:HH22  | 2.10                     | 0.56              |
| 1:Q:140:ARG:NH2  | 1:Q:155:VAL:O    | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:181:LEU:O    | 1:Q:185:VAL:HG23 | 2.04                     | 0.56              |
| 1:O:31:VAL:HG23  | 1:O:155:VAL:HG12 | 1.87                     | 0.56              |
| 2:J:222:SER:HB3  | 2:W:187:VAL:HG13 | 1.87                     | 0.56              |
| 1:T:112:THR:HG21 | 1:U:116:LYS:HE2  | 1.86                     | 0.56              |
| 1:F:181:LEU:O    | 1:F:185:VAL:HG23 | 2.04                     | 0.56              |
| 1:B:181:LEU:O    | 1:B:185:VAL:HG23 | 2.05                     | 0.56              |
| 2:Y:99:LEU:HD22  | 2:Y:100:ALA:N    | 2.21                     | 0.56              |
| 1:D:25:ALA:O     | 1:D:158:GLY:HA2  | 2.05                     | 0.56              |
| 1:A:98:GLN:O     | 1:A:102:VAL:HG23 | 2.05                     | 0.56              |
| 1:G:205:VAL:HG13 | 1:G:230:LEU:HD23 | 1.88                     | 0.56              |
| 2:J:62:GLU:OE2   | 2:J:82:ARG:NH2   | 2.39                     | 0.55              |
| 1:T:56:LEU:HG    | 1:T:62:PHE:HB2   | 1.87                     | 0.55              |
| 1:U:81:PHE:CE2   | 1:U:102:VAL:HG21 | 2.41                     | 0.55              |
| 2:W:72:VAL:HG12  | 2:W:73:PRO:HD2   | 1.88                     | 0.55              |
| 1:O:81:PHE:CE1   | 1:O:102:VAL:HG21 | 2.41                     | 0.55              |
| 1:A:31:VAL:HG21  | 1:A:167:LEU:HD11 | 1.87                     | 0.55              |
| 1:D:22:LYS:O     | 1:D:26:ARG:HG3   | 2.06                     | 0.55              |
| 1:O:210:VAL:HG21 | 1:O:230:LEU:HD13 | 1.86                     | 0.55              |
| 2:Y:38:ASP:HB3   | 2:Y:41:THR:OG1   | 2.05                     | 0.55              |
| 1:E:28:LYS:HB3   | 1:E:44:GLU:HB2   | 1.88                     | 0.55              |
| 1:F:180:ALA:HA   | 1:F:183:ILE:HG22 | 1.89                     | 0.55              |
| 1:T:159:THR:O    | 1:T:163:ILE:HD12 | 2.06                     | 0.55              |
| 2:V:51:VAL:HG21  | 2:V:98:LEU:HB3   | 1.88                     | 0.55              |
| 2:a:213:LEU:O    | 2:a:217:ILE:HD12 | 2.06                     | 0.55              |
| 2:M:95:MET:HA    | 2:M:95:MET:HE2   | 1.88                     | 0.55              |
| 2:M:214:ALA:O    | 2:M:218:ILE:HG12 | 2.06                     | 0.55              |
| 1:O:220:ARG:HH22 | 2:V:67:GLU:CD    | 2.13                     | 0.55              |
| 1:S:118:TYR:HB3  | 1:S:120:VAL:HG22 | 1.89                     | 0.55              |
| 2:W:54:GLU:OE2   | 2:X:88:ARG:NH2   | 2.40                     | 0.55              |
| 1:T:181:LEU:HD13 | 1:T:233:LEU:HD22 | 1.88                     | 0.55              |
| 1:D:118:TYR:HB3  | 1:D:120:VAL:HG22 | 1.87                     | 0.55              |
| 1:C:25:ALA:O     | 1:C:158:GLY:HA2  | 2.07                     | 0.55              |
| 1:G:56:LEU:HG    | 1:G:62:PHE:HB2   | 1.88                     | 0.55              |
| 1:G:121:GLU:HG2  | 1:G:142:THR:HA   | 1.89                     | 0.54              |
| 1:O:75:ARG:NH2   | 2:V:69:LEU:O     | 2.36                     | 0.54              |
| 1:O:118:TYR:HB3  | 1:O:120:VAL:HG22 | 1.88                     | 0.54              |
| 1:B:9:MET:HE1    | 1:C:115:ALA:O    | 2.07                     | 0.54              |
| 2:Z:38:ASP:OD2   | 2:Z:79:LYS:HE2   | 2.06                     | 0.54              |
| 2:M:157:VAL:HG22 | 2:M:163:GLY:HA2  | 1.89                     | 0.54              |
| 2:V:20:SER:HB2   | 2:V:31:VAL:HG21  | 1.89                     | 0.54              |
| 2:N:38:ASP:OD2   | 2:N:79:LYS:NZ    | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:16:ARG:NH1   | 1:C:111:PHE:O    | 2.41                     | 0.54              |
| 2:V:88:ARG:HD3   | 2:V:126:ALA:O    | 2.07                     | 0.54              |
| 2:a:121:VAL:HA   | 2:a:130:ASN:O    | 2.07                     | 0.54              |
| 2:N:192:PRO:O    | 2:N:210:ILE:HD13 | 2.08                     | 0.54              |
| 1:D:13:MET:HE2   | 1:E:116:LYS:HD3  | 1.90                     | 0.54              |
| 1:F:56:LEU:HG    | 1:F:62:PHE:HB2   | 1.89                     | 0.54              |
| 2:W:38:ASP:HB3   | 2:W:41:THR:HG23  | 1.90                     | 0.54              |
| 1:O:155:VAL:HG21 | 1:O:164:ALA:HB2  | 1.90                     | 0.54              |
| 1:G:11:GLN:HG3   | 1:G:12:ALA:H     | 1.74                     | 0.53              |
| 1:G:33:LEU:HD11  | 1:G:180:ALA:HB1  | 1.89                     | 0.53              |
| 1:A:10:GLU:HG3   | 1:B:15:GLU:HG3   | 1.90                     | 0.53              |
| 1:R:219:ARG:NH2  | 1:R:220:ARG:HD2  | 2.24                     | 0.53              |
| 1:Q:118:TYR:HB3  | 1:Q:120:VAL:HG22 | 1.90                     | 0.53              |
| 2:X:48:THR:HB    | 2:X:51:VAL:CG1   | 2.38                     | 0.53              |
| 2:X:157:VAL:HG22 | 2:X:163:GLY:HA2  | 1.90                     | 0.53              |
| 1:C:88:ALA:O     | 2:K:82:ARG:NH2   | 2.42                     | 0.53              |
| 2:K:95:MET:HE2   | 2:K:95:MET:HA    | 1.91                     | 0.53              |
| 1:O:55:GLU:OE2   | 1:O:220:ARG:HD2  | 2.08                     | 0.53              |
| 1:D:89:TYR:CE1   | 2:L:82:ARG:HD2   | 2.44                     | 0.53              |
| 1:D:68:PHE:HA    | 1:D:71:PHE:CE2   | 2.43                     | 0.53              |
| 2:b:95:MET:HE2   | 2:b:95:MET:HA    | 1.91                     | 0.53              |
| 2:J:20:SER:HB2   | 2:J:31:VAL:HG21  | 1.90                     | 0.53              |
| 2:Y:99:LEU:HD22  | 2:Y:100:ALA:H    | 1.73                     | 0.53              |
| 2:a:162:SER:O    | 2:a:166:VAL:HG23 | 2.09                     | 0.53              |
| 2:K:179:SER:HB3  | 2:V:26:ILE:HD11  | 1.91                     | 0.52              |
| 1:G:68:PHE:HA    | 1:G:71:PHE:CE2   | 2.44                     | 0.52              |
| 2:K:131:ILE:O    | 4:K:401:HOH:O    | 2.19                     | 0.52              |
| 1:O:117:PRO:HD2  | 1:U:9:MET:HE1    | 1.91                     | 0.52              |
| 1:Q:30:VAL:HG13  | 1:Q:156:MET:HE3  | 1.91                     | 0.52              |
| 1:R:30:VAL:HG13  | 1:R:156:MET:HE3  | 1.91                     | 0.52              |
| 1:B:81:PHE:CE2   | 1:B:102:VAL:HG11 | 2.45                     | 0.52              |
| 2:H:123:PHE:HA   | 2:H:128:GLY:O    | 2.10                     | 0.52              |
| 2:K:150:MET:O    | 2:K:154:TYR:HB2  | 2.09                     | 0.52              |
| 1:Q:53:ILE:O     | 1:Q:224:ARG:NH2  | 2.39                     | 0.52              |
| 1:S:72:ASP:OD1   | 1:S:75:ARG:NH1   | 2.43                     | 0.52              |
| 1:U:9:MET:O      | 1:U:13:MET:HG2   | 2.10                     | 0.52              |
| 1:A:110:ILE:HA   | 1:A:114:GLN:HG3  | 1.91                     | 0.52              |
| 2:I:48:THR:HB    | 2:I:51:VAL:HG22  | 1.91                     | 0.52              |
| 2:M:132:GLU:OE2  | 2:M:137:GLN:NE2  | 2.42                     | 0.52              |
| 1:P:30:VAL:HG13  | 1:P:43:ALA:HB2   | 1.91                     | 0.52              |
| 2:H:161:ASP:OD2  | 2:H:209:ARG:NH1  | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:161:ASP:OD2  | 2:K:209:ARG:NH2  | 2.43                     | 0.52              |
| 1:B:110:ILE:HA   | 1:B:114:GLN:HG3  | 1.91                     | 0.52              |
| 1:E:181:LEU:O    | 1:E:185:VAL:HG23 | 2.10                     | 0.52              |
| 1:U:151:PRO:HD2  | 4:U:305:HOH:O    | 2.09                     | 0.52              |
| 1:T:32:ALA:HA    | 1:T:40:LEU:O     | 2.10                     | 0.51              |
| 1:T:31:VAL:HG12  | 1:T:155:VAL:HG22 | 1.92                     | 0.51              |
| 1:U:179:ASP:O    | 1:U:183:ILE:HG22 | 2.10                     | 0.51              |
| 2:L:156:GLN:OE1  | 2:L:165:ARG:NH2  | 2.43                     | 0.51              |
| 1:P:45:ASN:OD1   | 1:P:209:GLU:HB2  | 2.10                     | 0.51              |
| 1:U:70:GLU:HB3   | 1:U:118:TYR:CD2  | 2.45                     | 0.51              |
| 2:Z:156:GLN:HG3  | 2:Z:165:ARG:HH12 | 1.76                     | 0.51              |
| 1:D:223:ARG:HA   | 1:D:223:ARG:NE   | 2.25                     | 0.51              |
| 2:M:164:LEU:O    | 2:M:168:VAL:HG23 | 2.11                     | 0.51              |
| 1:O:56:LEU:HG    | 1:O:62:PHE:HB2   | 1.93                     | 0.51              |
| 1:R:118:TYR:HB3  | 1:R:120:VAL:HG22 | 1.91                     | 0.51              |
| 1:U:59:ARG:HD2   | 1:U:128:ALA:O    | 2.09                     | 0.51              |
| 1:F:110:ILE:HA   | 1:F:114:GLN:HG2  | 1.93                     | 0.51              |
| 2:I:151:LYS:NZ   | 2:Y:176:ASP:OD2  | 2.34                     | 0.51              |
| 1:P:217:ARG:HG3  | 1:P:223:ARG:CZ   | 2.40                     | 0.51              |
| 1:C:56:LEU:HG    | 1:C:62:PHE:HB2   | 1.92                     | 0.51              |
| 2:X:108:ASP:HB3  | 2:X:111:ALA:HB2  | 1.91                     | 0.51              |
| 1:A:170:SER:HB2  | 1:A:183:ILE:HD12 | 1.92                     | 0.51              |
| 1:F:123:CYS:SG   | 1:F:154:VAL:HG21 | 2.50                     | 0.51              |
| 2:I:104:LEU:HB3  | 2:I:121:VAL:HB   | 1.93                     | 0.51              |
| 1:A:205:VAL:HG13 | 1:A:230:LEU:HD23 | 1.91                     | 0.51              |
| 1:B:56:LEU:HG    | 1:B:62:PHE:HB2   | 1.92                     | 0.51              |
| 1:E:230:LEU:O    | 1:E:234:LEU:HD22 | 2.10                     | 0.51              |
| 2:W:32:ARG:HD2   | 2:W:193:THR:HG21 | 1.92                     | 0.51              |
| 2:Z:168:VAL:HG23 | 2:Z:217:ILE:HD11 | 1.92                     | 0.51              |
| 2:a:3:ILE:HB     | 2:a:139:VAL:HG12 | 1.92                     | 0.51              |
| 2:a:150:MET:O    | 2:a:154:TYR:HB2  | 2.11                     | 0.51              |
| 1:B:62:PHE:CE2   | 1:B:122:LEU:HD22 | 2.46                     | 0.51              |
| 2:H:10:GLY:HA2   | 2:H:115:GLN:HA   | 1.92                     | 0.51              |
| 2:N:121:VAL:HA   | 2:N:130:ASN:O    | 2.11                     | 0.51              |
| 1:R:205:VAL:HG13 | 1:R:230:LEU:HD23 | 1.92                     | 0.51              |
| 2:b:5:ALA:HA     | 2:b:13:VAL:O     | 2.11                     | 0.51              |
| 2:b:49:ALA:O     | 2:b:53:VAL:HG23  | 2.11                     | 0.51              |
| 2:b:121:VAL:HG22 | 2:b:131:ILE:HG12 | 1.92                     | 0.51              |
| 1:D:163:ILE:HG12 | 1:D:187:ALA:O    | 2.12                     | 0.50              |
| 1:R:177:LEU:HD22 | 1:R:233:LEU:CD2  | 2.41                     | 0.50              |
| 1:S:121:GLU:OE2  | 1:S:140:ARG:NH2  | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:48:THR:HG21  | 2:V:98:LEU:HD22  | 1.93                     | 0.50              |
| 2:V:57:ARG:O     | 2:V:61:VAL:HG23  | 2.12                     | 0.50              |
| 1:D:205:VAL:HG23 | 1:D:230:LEU:HD23 | 1.92                     | 0.50              |
| 1:E:219:ARG:NH1  | 1:E:220:ARG:HD2  | 2.26                     | 0.50              |
| 1:F:32:ALA:HA    | 1:F:40:LEU:O     | 2.11                     | 0.50              |
| 1:Q:93:ASP:OD1   | 2:Y:75:THR:HG23  | 2.12                     | 0.50              |
| 1:F:141:ILE:HG13 | 1:F:147:ILE:HD12 | 1.93                     | 0.50              |
| 2:K:37:THR:HG23  | 2:K:60:ALA:HA    | 1.92                     | 0.50              |
| 1:Q:179:ASP:O    | 1:Q:183:ILE:HG23 | 2.12                     | 0.50              |
| 1:A:93:ASP:OD1   | 2:I:75:THR:HG23  | 2.12                     | 0.50              |
| 1:F:89:TYR:CD1   | 2:N:82:ARG:HD3   | 2.46                     | 0.50              |
| 1:T:33:LEU:HD13  | 1:T:153:PHE:HB3  | 1.94                     | 0.50              |
| 1:Q:9:MET:HE3    | 1:R:19:LEU:HD13  | 1.94                     | 0.50              |
| 1:A:149:ASP:OD2  | 1:B:47:SER:OG    | 2.20                     | 0.50              |
| 1:D:56:LEU:HG    | 1:D:62:PHE:HB2   | 1.94                     | 0.50              |
| 2:M:57:ARG:O     | 2:M:61:VAL:HG23  | 2.11                     | 0.50              |
| 1:P:219:ARG:NH2  | 2:W:64:GLU:OE2   | 2.20                     | 0.50              |
| 1:A:128:ALA:HB2  | 1:A:134:LYS:HB3  | 1.94                     | 0.50              |
| 1:B:116:LYS:NZ   | 1:B:119:GLU:OE2  | 2.36                     | 0.50              |
| 1:B:97:ARG:NH2   | 2:J:70:GLU:OE2   | 2.45                     | 0.50              |
| 1:D:72:ASP:OD1   | 1:D:75:ARG:NH1   | 2.45                     | 0.50              |
| 1:E:54:SER:CB    | 1:E:75:ARG:HD2   | 2.42                     | 0.50              |
| 1:O:181:LEU:O    | 1:O:185:VAL:HG23 | 2.12                     | 0.50              |
| 2:L:62:GLU:OE2   | 2:L:82:ARG:HD3   | 2.11                     | 0.49              |
| 2:I:137:GLN:HG3  | 2:I:138:ALA:N    | 2.27                     | 0.49              |
| 2:N:20:SER:HB2   | 2:N:31:VAL:HG21  | 1.94                     | 0.49              |
| 1:O:19:LEU:HD12  | 1:U:10:GLU:HG2   | 1.93                     | 0.49              |
| 1:E:93:ASP:OD1   | 2:M:75:THR:HG23  | 2.12                     | 0.49              |
| 1:Q:123:CYS:HA   | 1:Q:139:TYR:O    | 2.12                     | 0.49              |
| 1:F:150:GLU:HG3  | 1:F:154:VAL:HG12 | 1.95                     | 0.49              |
| 2:I:48:THR:HG22  | 4:J:408:HOH:O    | 2.10                     | 0.49              |
| 1:S:150:GLU:HG3  | 1:S:154:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:177:LEU:HD22 | 1:C:233:LEU:HD23 | 1.95                     | 0.49              |
| 1:D:116:LYS:NZ   | 1:D:119:GLU:OE2  | 2.43                     | 0.49              |
| 1:G:220:ARG:HG3  | 1:G:220:ARG:HH11 | 1.76                     | 0.49              |
| 2:W:104:LEU:HB3  | 2:W:121:VAL:HB   | 1.95                     | 0.49              |
| 2:a:137:GLN:HG3  | 2:a:138:ALA:N    | 2.27                     | 0.49              |
| 2:L:12:VAL:HG12  | 2:L:197:ILE:HB   | 1.94                     | 0.49              |
| 2:N:55:PHE:HZ    | 2:N:90:ASN:HB2   | 1.77                     | 0.49              |
| 1:C:10:GLU:O     | 1:C:14:ARG:HG3   | 2.13                     | 0.49              |
| 1:D:97:ARG:HD2   | 1:E:49:SER:HB2   | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:121:VAL:HG22 | 2:L:131:ILE:HG12 | 1.94                     | 0.49              |
| 2:L:162:SER:O    | 2:L:166:VAL:HG23 | 2.13                     | 0.49              |
| 1:P:25:ALA:O     | 1:P:158:GLY:HA2  | 2.13                     | 0.49              |
| 2:I:153:LEU:O    | 2:I:156:GLN:HG2  | 2.13                     | 0.49              |
| 2:M:88:ARG:HD3   | 2:M:126:ALA:O    | 2.12                     | 0.49              |
| 1:P:74:LEU:HD12  | 1:P:120:VAL:HG11 | 1.94                     | 0.49              |
| 1:Q:55:GLU:HB2   | 1:Q:222:PHE:CG   | 2.48                     | 0.49              |
| 1:U:25:ALA:O     | 1:U:158:GLY:HA2  | 2.13                     | 0.49              |
| 1:U:100:ALA:HB1  | 1:U:147:ILE:HD11 | 1.95                     | 0.49              |
| 2:Y:121:VAL:HA   | 2:Y:130:ASN:O    | 2.13                     | 0.49              |
| 2:Z:18:ARG:NH2   | 2:Z:30:ASP:O     | 2.45                     | 0.49              |
| 1:C:116:LYS:NZ   | 1:C:119:GLU:OE1  | 2.38                     | 0.48              |
| 2:M:104:LEU:HB3  | 2:M:121:VAL:HB   | 1.95                     | 0.48              |
| 1:P:33:LEU:HD21  | 1:P:184:ALA:HB2  | 1.95                     | 0.48              |
| 1:T:99:LEU:O     | 1:T:102:VAL:HG12 | 2.13                     | 0.48              |
| 1:B:167:LEU:O    | 1:B:171:TYR:N    | 2.46                     | 0.48              |
| 2:I:99:LEU:HD21  | 2:I:101:LEU:HD13 | 1.94                     | 0.48              |
| 2:K:161:ASP:CG   | 2:K:209:ARG:HH21 | 2.21                     | 0.48              |
| 1:T:110:ILE:HA   | 1:T:114:GLN:HG3  | 1.94                     | 0.48              |
| 2:Y:132:GLU:OE2  | 2:Y:134:GLU:HB2  | 2.13                     | 0.48              |
| 1:B:94:VAL:HA    | 1:B:98:GLN:NE2   | 2.28                     | 0.48              |
| 1:G:33:LEU:HD21  | 1:G:184:ALA:HB2  | 1.95                     | 0.48              |
| 1:B:54:SER:CB    | 1:B:75:ARG:HD2   | 2.43                     | 0.48              |
| 1:E:62:PHE:CZ    | 1:E:75:ARG:HB2   | 2.48                     | 0.48              |
| 2:K:169:GLU:OE2  | 2:K:221:ARG:NH2  | 2.43                     | 0.48              |
| 1:R:42:VAL:HG11  | 1:R:184:ALA:HB1  | 1.96                     | 0.48              |
| 1:S:155:VAL:HG22 | 1:S:160:THR:HG22 | 1.94                     | 0.48              |
| 1:T:181:LEU:CD1  | 1:T:210:VAL:HG11 | 2.43                     | 0.48              |
| 1:F:81:PHE:CE1   | 1:F:102:VAL:HG21 | 2.48                     | 0.48              |
| 2:H:76:PHE:CE2   | 2:H:80:ILE:HD11  | 2.48                     | 0.48              |
| 2:H:209:ARG:NH2  | 2:H:212:GLU:OE1  | 2.45                     | 0.48              |
| 2:K:164:LEU:O    | 2:K:168:VAL:HG23 | 2.14                     | 0.48              |
| 1:O:16:ARG:NH2   | 1:O:111:PHE:O    | 2.47                     | 0.48              |
| 1:Q:144:ASP:O    | 1:R:67:LYS:NZ    | 2.28                     | 0.48              |
| 2:L:164:LEU:O    | 2:L:168:VAL:HG23 | 2.14                     | 0.48              |
| 1:P:87:TYR:O     | 2:W:57:ARG:NH2   | 2.47                     | 0.48              |
| 1:F:55:GLU:CD    | 1:F:220:ARG:HH21 | 2.21                     | 0.48              |
| 1:D:74:LEU:HD13  | 1:D:122:LEU:HD11 | 1.96                     | 0.48              |
| 1:R:189:ARG:HG3  | 1:R:203:LEU:HD12 | 1.94                     | 0.48              |
| 2:V:38:ASP:HB3   | 2:V:41:THR:OG1   | 2.14                     | 0.48              |
| 2:Y:20:SER:HB2   | 2:Y:31:VAL:HG11  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:18:ARG:HD3   | 2:M:193:THR:HG23 | 1.96                     | 0.48              |
| 1:T:68:PHE:HA    | 1:T:71:PHE:CE2   | 2.49                     | 0.48              |
| 1:U:33:LEU:HD12  | 1:U:171:TYR:CD1  | 2.49                     | 0.48              |
| 2:M:38:ASP:OD1   | 2:M:41:THR:N     | 2.47                     | 0.47              |
| 1:S:16:ARG:NH2   | 1:S:114:GLN:O    | 2.33                     | 0.47              |
| 2:V:116:SER:O    | 2:V:119:ARG:NH1  | 2.40                     | 0.47              |
| 2:b:51:VAL:HG21  | 2:b:98:LEU:HB3   | 1.96                     | 0.47              |
| 1:S:89:TYR:CE1   | 2:a:82:ARG:HD3   | 2.49                     | 0.47              |
| 2:b:196:ILE:HG13 | 2:b:205:VAL:HG22 | 1.96                     | 0.47              |
| 1:B:22:LYS:HB2   | 1:B:22:LYS:HE2   | 1.59                     | 0.47              |
| 1:T:72:ASP:O     | 1:T:76:ARG:HG3   | 2.15                     | 0.47              |
| 1:B:219:ARG:NH1  | 1:B:220:ARG:HD2  | 2.29                     | 0.47              |
| 1:F:100:ALA:HB1  | 1:F:147:ILE:HD11 | 1.96                     | 0.47              |
| 2:J:186:LEU:HD11 | 2:J:218:ILE:HD12 | 1.96                     | 0.47              |
| 1:O:229:ALA:O    | 1:O:233:LEU:HG   | 2.14                     | 0.47              |
| 2:V:7:LYS:O      | 2:V:154:TYR:OH   | 2.30                     | 0.47              |
| 2:Y:33:LYS:O     | 2:Y:44:GLY:HA2   | 2.13                     | 0.47              |
| 2:Z:51:VAL:HG21  | 2:Z:98:LEU:HB3   | 1.96                     | 0.47              |
| 2:H:161:ASP:CG   | 2:H:209:ARG:HH11 | 2.22                     | 0.47              |
| 1:O:225:ILE:HG21 | 1:O:233:LEU:HD12 | 1.95                     | 0.47              |
| 1:F:70:GLU:OE2   | 1:F:116:LYS:NZ   | 2.47                     | 0.47              |
| 2:Z:168:VAL:HG23 | 2:Z:217:ILE:CD1  | 2.45                     | 0.47              |
| 2:b:121:VAL:HA   | 2:b:130:ASN:O    | 2.14                     | 0.47              |
| 1:B:100:ALA:HB1  | 1:B:147:ILE:HD11 | 1.96                     | 0.47              |
| 1:C:163:ILE:HG12 | 1:C:187:ALA:O    | 2.14                     | 0.47              |
| 1:C:189:ARG:O    | 1:C:191:GLY:N    | 2.47                     | 0.47              |
| 1:E:16:ARG:NH2   | 1:E:114:GLN:O    | 2.30                     | 0.47              |
| 1:Q:11:GLN:OE1   | 1:Q:14:ARG:NH2   | 2.48                     | 0.47              |
| 1:R:56:LEU:HG    | 1:R:62:PHE:HB2   | 1.95                     | 0.47              |
| 2:Z:88:ARG:HD2   | 2:Z:88:ARG:O     | 2.14                     | 0.47              |
| 2:b:3:ILE:HB     | 2:b:139:VAL:HG12 | 1.97                     | 0.47              |
| 1:A:16:ARG:HA    | 1:G:9:MET:HE1    | 1.97                     | 0.47              |
| 1:P:67:LYS:HD3   | 1:P:70:GLU:CD    | 2.39                     | 0.47              |
| 1:R:147:ILE:HG21 | 1:S:68:PHE:CD2   | 2.50                     | 0.47              |
| 1:U:12:ALA:O     | 1:U:16:ARG:HG3   | 2.14                     | 0.47              |
| 1:D:70:GLU:HB3   | 1:D:118:TYR:CD2  | 2.50                     | 0.47              |
| 1:D:89:TYR:HE1   | 2:L:82:ARG:HD2   | 1.79                     | 0.47              |
| 1:F:33:LEU:HD21  | 1:F:184:ALA:HB2  | 1.96                     | 0.47              |
| 2:H:137:GLN:HG3  | 2:H:138:ALA:N    | 2.29                     | 0.47              |
| 2:N:123:PHE:CE1  | 2:N:129:TRP:HB3  | 2.50                     | 0.47              |
| 1:R:151:PRO:HD2  | 4:R:305:HOH:O    | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:20:ALA:O     | 1:T:24:ILE:HD12  | 2.14                     | 0.47              |
| 1:C:210:VAL:HG23 | 1:C:225:ILE:HB   | 1.96                     | 0.47              |
| 1:D:182:ARG:HA   | 1:D:185:VAL:HG22 | 1.96                     | 0.47              |
| 1:E:118:TYR:HB3  | 1:E:120:VAL:HG22 | 1.98                     | 0.47              |
| 1:R:89:TYR:CD1   | 2:Z:82:ARG:HD3   | 2.50                     | 0.47              |
| 1:U:94:VAL:HA    | 1:U:98:GLN:NE2   | 2.30                     | 0.47              |
| 1:U:97:ARG:NH1   | 2:V:70:GLU:O     | 2.48                     | 0.47              |
| 2:Z:20:SER:HB2   | 2:Z:31:VAL:HG11  | 1.97                     | 0.47              |
| 2:Z:162:SER:O    | 2:Z:166:VAL:HG23 | 2.15                     | 0.47              |
| 2:Z:165:ARG:HG3  | 2:Z:213:LEU:HD22 | 1.97                     | 0.47              |
| 1:B:123:CYS:HA   | 1:B:139:TYR:O    | 2.15                     | 0.46              |
| 1:F:163:ILE:HD13 | 1:F:188:LEU:HD12 | 1.96                     | 0.46              |
| 1:B:137:GLU:OE1  | 1:B:139:TYR:OH   | 2.33                     | 0.46              |
| 1:E:229:ALA:O    | 1:E:233:LEU:HD13 | 2.15                     | 0.46              |
| 2:J:197:ILE:HG12 | 2:J:202:ALA:CB   | 2.45                     | 0.46              |
| 1:R:141:ILE:HG13 | 1:R:147:ILE:HD12 | 1.97                     | 0.46              |
| 1:T:22:LYS:NZ    | 1:T:26:ARG:HD2   | 2.30                     | 0.46              |
| 1:T:181:LEU:HD12 | 1:T:210:VAL:HG11 | 1.96                     | 0.46              |
| 2:H:88:ARG:HD3   | 2:H:126:ALA:O    | 2.14                     | 0.46              |
| 2:J:107:TYR:CE2  | 2:J:117:ALA:HB3  | 2.50                     | 0.46              |
| 2:W:38:ASP:HB3   | 2:W:41:THR:HG22  | 1.96                     | 0.46              |
| 2:W:185:ASP:OD2  | 2:W:188:ARG:HD2  | 2.14                     | 0.46              |
| 2:Z:43:THR:HG22  | 2:Z:104:LEU:HD12 | 1.98                     | 0.46              |
| 2:K:179:SER:HB2  | 2:V:179:SER:HB2  | 1.98                     | 0.46              |
| 1:R:22:LYS:O     | 1:R:26:ARG:HG3   | 2.15                     | 0.46              |
| 2:X:121:VAL:HA   | 2:X:130:ASN:O    | 2.15                     | 0.46              |
| 1:E:110:ILE:HA   | 1:E:114:GLN:HG3  | 1.98                     | 0.46              |
| 1:O:13:MET:HE2   | 1:P:116:LYS:HD3  | 1.97                     | 0.46              |
| 1:O:40:LEU:HD21  | 1:O:181:LEU:HA   | 1.98                     | 0.46              |
| 1:P:163:ILE:HG12 | 1:P:187:ALA:O    | 2.15                     | 0.46              |
| 2:Z:121:VAL:HA   | 2:Z:130:ASN:O    | 2.16                     | 0.46              |
| 2:H:179:SER:HB2  | 2:Y:179:SER:HB2  | 1.98                     | 0.46              |
| 1:O:185:VAL:HG13 | 1:O:208:LEU:HD11 | 1.97                     | 0.46              |
| 2:V:121:VAL:HA   | 2:V:130:ASN:O    | 2.15                     | 0.46              |
| 2:X:164:LEU:O    | 2:X:168:VAL:HG23 | 2.16                     | 0.46              |
| 2:J:7:LYS:NZ     | 2:J:118:GLY:O    | 2.49                     | 0.46              |
| 2:N:176:ASP:OD2  | 2:Z:188:ARG:NH1  | 2.48                     | 0.46              |
| 2:X:95:MET:HE2   | 2:X:95:MET:HA    | 1.96                     | 0.46              |
| 2:b:137:GLN:HG3  | 2:b:138:ALA:N    | 2.30                     | 0.46              |
| 1:B:225:ILE:HG22 | 1:B:230:LEU:HB2  | 1.98                     | 0.46              |
| 1:D:128:ALA:HB2  | 1:D:134:LYS:HB3  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:52:LYS:NZ    | 1:S:64:ALA:O     | 2.46                     | 0.46              |
| 1:T:41:PHE:HB3   | 1:T:53:ILE:HD13  | 1.97                     | 0.46              |
| 2:b:43:THR:HG22  | 2:b:104:LEU:CD1  | 2.45                     | 0.46              |
| 1:B:25:ALA:O     | 1:B:158:GLY:HA2  | 2.16                     | 0.46              |
| 1:B:81:PHE:CZ    | 1:B:102:VAL:HG11 | 2.51                     | 0.46              |
| 1:C:16:ARG:NH2   | 1:C:114:GLN:O    | 2.40                     | 0.46              |
| 1:G:9:MET:HE2    | 1:G:9:MET:HB3    | 1.71                     | 0.46              |
| 2:J:209:ARG:NH1  | 2:J:212:GLU:OE2  | 2.39                     | 0.46              |
| 2:M:38:ASP:OD1   | 2:M:38:ASP:C     | 2.59                     | 0.46              |
| 2:M:122:SER:HB3  | 2:M:137:GLN:HG2  | 1.98                     | 0.46              |
| 1:O:180:ALA:HA   | 1:O:183:ILE:HD12 | 1.98                     | 0.46              |
| 1:U:138:LEU:HD12 | 1:U:150:GLU:HB2  | 1.97                     | 0.46              |
| 2:a:49:ALA:O     | 2:a:53:VAL:HG23  | 2.15                     | 0.46              |
| 1:B:231:GLN:O    | 1:B:235:VAL:HG12 | 2.16                     | 0.45              |
| 1:G:166:ALA:O    | 1:G:170:SER:HB3  | 2.16                     | 0.45              |
| 1:Q:110:ILE:HA   | 1:Q:114:GLN:HG3  | 1.98                     | 0.45              |
| 2:W:51:VAL:HG21  | 2:W:98:LEU:HB3   | 1.97                     | 0.45              |
| 1:C:29:SER:OG    | 1:C:157:GLY:O    | 2.23                     | 0.45              |
| 1:E:64:ALA:HA    | 1:E:156:MET:HE1  | 1.97                     | 0.45              |
| 1:P:31:VAL:HG22  | 1:P:155:VAL:HG12 | 1.98                     | 0.45              |
| 1:P:68:PHE:HA    | 1:P:71:PHE:CE2   | 2.51                     | 0.45              |
| 1:S:22:LYS:O     | 1:S:26:ARG:HG3   | 2.16                     | 0.45              |
| 1:T:59:ARG:HD2   | 1:T:128:ALA:O    | 2.16                     | 0.45              |
| 1:C:203:LEU:HB3  | 1:C:207:SER:OG   | 2.16                     | 0.45              |
| 1:D:210:VAL:HG23 | 1:D:225:ILE:HB   | 1.97                     | 0.45              |
| 1:O:97:ARG:HD2   | 1:P:49:SER:HB2   | 1.98                     | 0.45              |
| 1:U:94:VAL:HA    | 1:U:98:GLN:HE22  | 1.80                     | 0.45              |
| 1:U:123:CYS:HA   | 1:U:139:TYR:O    | 2.16                     | 0.45              |
| 2:b:20:SER:HB2   | 2:b:31:VAL:HG11  | 1.99                     | 0.45              |
| 2:K:37:THR:HG22  | 2:K:63:LEU:HD12  | 1.98                     | 0.45              |
| 2:K:37:THR:HG21  | 2:K:59:TYR:CD2   | 2.51                     | 0.45              |
| 1:Q:93:ASP:CG    | 2:Y:75:THR:HG23  | 2.41                     | 0.45              |
| 1:Q:212:VAL:HG22 | 1:Q:223:ARG:HG3  | 1.98                     | 0.45              |
| 1:S:181:LEU:O    | 1:S:185:VAL:HG23 | 2.16                     | 0.45              |
| 1:C:68:PHE:HA    | 1:C:71:PHE:CE2   | 2.52                     | 0.45              |
| 2:I:196:ILE:HG22 | 2:I:203:VAL:HG13 | 1.98                     | 0.45              |
| 2:J:165:ARG:HG3  | 2:J:213:LEU:HD22 | 1.99                     | 0.45              |
| 2:N:113:ASP:OD2  | 2:N:115:GLN:HB3  | 2.17                     | 0.45              |
| 1:A:170:SER:OG   | 1:A:183:ILE:HG23 | 2.16                     | 0.45              |
| 1:D:105:GLN:HG3  | 1:D:106:THR:N    | 2.32                     | 0.45              |
| 2:I:95:MET:HE2   | 2:I:95:MET:HA    | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:185:ASP:OD2  | 2:K:188:ARG:HD2  | 2.17                     | 0.45              |
| 1:E:38:GLY:HA3   | 1:E:213:LEU:O    | 2.17                     | 0.45              |
| 1:U:9:MET:HG3    | 1:U:10:GLU:N     | 2.31                     | 0.45              |
| 1:U:41:PHE:HB3   | 1:U:53:ILE:HD13  | 1.98                     | 0.45              |
| 1:U:233:LEU:O    | 1:U:233:LEU:HD23 | 2.17                     | 0.45              |
| 1:E:56:LEU:HG    | 1:E:62:PHE:HB2   | 1.99                     | 0.45              |
| 1:G:225:ILE:HG21 | 1:G:233:LEU:HD12 | 1.99                     | 0.45              |
| 2:L:51:VAL:HG21  | 2:L:98:LEU:HB3   | 1.99                     | 0.45              |
| 1:S:122:LEU:HD23 | 1:S:122:LEU:HA   | 1.69                     | 0.45              |
| 2:Y:101:LEU:HA   | 2:Y:101:LEU:HD12 | 1.73                     | 0.45              |
| 1:B:175:ALA:HB1  | 1:B:179:ASP:HB3  | 1.99                     | 0.45              |
| 2:N:4:VAL:HG22   | 2:N:171:LEU:HD13 | 1.99                     | 0.45              |
| 1:D:205:VAL:HG13 | 1:D:206:ALA:H    | 1.82                     | 0.45              |
| 1:F:219:ARG:NH2  | 1:F:220:ARG:HD2  | 2.28                     | 0.45              |
| 1:R:68:PHE:HA    | 1:R:71:PHE:CE2   | 2.51                     | 0.45              |
| 2:b:99:LEU:HD22  | 2:b:100:ALA:N    | 2.32                     | 0.45              |
| 1:C:56:LEU:HD23  | 1:C:56:LEU:HA    | 1.78                     | 0.44              |
| 1:C:142:THR:OG1  | 1:C:146:SER:HB2  | 2.17                     | 0.44              |
| 1:E:33:LEU:HD11  | 1:E:180:ALA:HB1  | 2.00                     | 0.44              |
| 1:F:72:ASP:O     | 1:F:76:ARG:HG3   | 2.16                     | 0.44              |
| 2:M:165:ARG:HG3  | 2:M:213:LEU:HD22 | 1.98                     | 0.44              |
| 1:Q:219:ARG:NH2  | 1:Q:220:ARG:HD2  | 2.32                     | 0.44              |
| 1:S:152:HIS:HB3  | 1:S:171:TYR:CE2  | 2.52                     | 0.44              |
| 1:G:123:CYS:HA   | 1:G:139:TYR:O    | 2.17                     | 0.44              |
| 2:N:217:ILE:O    | 2:N:220:SER:OG   | 2.24                     | 0.44              |
| 1:P:56:LEU:HG    | 1:P:62:PHE:HB2   | 1.99                     | 0.44              |
| 1:S:116:LYS:NZ   | 1:S:119:GLU:OE2  | 2.46                     | 0.44              |
| 2:Y:21:THR:O     | 3:Y:301:7J1:N03  | 2.50                     | 0.44              |
| 1:A:89:TYR:CD1   | 2:I:82:ARG:HD3   | 2.51                     | 0.44              |
| 1:R:219:ARG:HH21 | 1:R:220:ARG:HD2  | 1.83                     | 0.44              |
| 2:X:48:THR:HG21  | 2:X:98:LEU:HD22  | 1.98                     | 0.44              |
| 2:K:206:PRO:O    | 2:K:210:ILE:HD12 | 2.17                     | 0.44              |
| 2:L:176:ASP:OD2  | 2:b:188:ARG:NH1  | 2.50                     | 0.44              |
| 1:A:71:PHE:HB3   | 1:A:120:VAL:CG1  | 2.47                     | 0.44              |
| 1:B:30:VAL:CG2   | 1:B:52:LYS:HE3   | 2.46                     | 0.44              |
| 2:H:38:ASP:OD2   | 2:H:79:LYS:NZ    | 2.49                     | 0.44              |
| 2:L:137:GLN:HG3  | 2:L:138:ALA:N    | 2.32                     | 0.44              |
| 1:Q:89:TYR:CD1   | 2:Y:74:LEU:HD21  | 2.52                     | 0.44              |
| 2:W:13:VAL:HG22  | 2:W:196:ILE:HG12 | 1.98                     | 0.44              |
| 2:X:32:ARG:NH1   | 4:X:402:HOH:O    | 2.50                     | 0.44              |
| 1:C:53:ILE:O     | 1:C:224:ARG:NH2  | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:90:ASN:OD1   | 2:I:93:ALA:HB3   | 2.17                     | 0.44              |
| 2:K:50:ALA:HB2   | 2:L:128:GLY:H    | 1.82                     | 0.44              |
| 2:L:88:ARG:HD3   | 2:L:126:ALA:O    | 2.18                     | 0.44              |
| 2:b:7:LYS:HE3    | 2:b:135:GLY:HA2  | 2.00                     | 0.44              |
| 2:b:38:ASP:OD2   | 2:b:79:LYS:NZ    | 2.41                     | 0.44              |
| 1:E:163:ILE:HG13 | 1:E:191:GLY:HA3  | 1.99                     | 0.44              |
| 1:E:203:LEU:HD23 | 1:E:203:LEU:HA   | 1.85                     | 0.44              |
| 1:G:56:LEU:O     | 2:N:68:LYS:HE3   | 2.18                     | 0.44              |
| 1:A:56:LEU:HG    | 1:A:62:PHE:HB2   | 2.00                     | 0.44              |
| 1:C:229:ALA:O    | 1:C:233:LEU:HD13 | 2.18                     | 0.44              |
| 1:R:83:ASP:OD2   | 2:Y:65:HIS:ND1   | 2.43                     | 0.44              |
| 1:R:161:GLU:HB2  | 1:R:162:PRO:HD3  | 1.98                     | 0.44              |
| 2:Y:55:PHE:HZ    | 2:Y:90:ASN:HB2   | 1.82                     | 0.44              |
| 1:E:70:GLU:HB3   | 1:E:118:TYR:CD2  | 2.53                     | 0.43              |
| 1:F:54:SER:CB    | 1:F:75:ARG:HD2   | 2.48                     | 0.43              |
| 1:F:137:GLU:HB3  | 1:G:48:ARG:NH1   | 2.33                     | 0.43              |
| 2:N:197:ILE:HG12 | 2:N:202:ALA:CB   | 2.48                     | 0.43              |
| 1:P:161:GLU:N    | 1:P:162:PRO:HD2  | 2.33                     | 0.43              |
| 1:G:54:SER:CB    | 1:G:75:ARG:HD2   | 2.48                     | 0.43              |
| 2:I:156:GLN:NE2  | 2:I:165:ARG:NH1  | 2.66                     | 0.43              |
| 1:R:18:GLU:O     | 1:R:22:LYS:HG2   | 2.19                     | 0.43              |
| 1:R:31:VAL:HG23  | 1:R:42:VAL:HG13  | 2.00                     | 0.43              |
| 1:U:152:HIS:HB3  | 1:U:171:TYR:CE2  | 2.54                     | 0.43              |
| 2:Y:109:ILE:H    | 2:Y:109:ILE:CD1  | 2.24                     | 0.43              |
| 2:J:33:LYS:O     | 2:J:44:GLY:HA2   | 2.18                     | 0.43              |
| 2:L:101:LEU:HD23 | 2:L:101:LEU:HA   | 1.75                     | 0.43              |
| 1:U:134:LYS:NZ   | 1:U:137:GLU:OE1  | 2.50                     | 0.43              |
| 2:W:78:GLY:O     | 2:W:82:ARG:HG2   | 2.18                     | 0.43              |
| 2:Y:78:GLY:O     | 2:Y:82:ARG:HG2   | 2.17                     | 0.43              |
| 2:Z:197:ILE:HG12 | 2:Z:202:ALA:CB   | 2.48                     | 0.43              |
| 2:I:42:ALA:HB2   | 2:I:195:VAL:HG11 | 2.00                     | 0.43              |
| 1:O:25:ALA:O     | 1:O:158:GLY:HA2  | 2.19                     | 0.43              |
| 2:a:48:THR:HG21  | 2:a:98:LEU:HA    | 1.99                     | 0.43              |
| 1:B:55:GLU:HB2   | 1:B:222:PHE:CG   | 2.53                     | 0.43              |
| 1:C:71:PHE:HB3   | 1:C:120:VAL:HG12 | 2.00                     | 0.43              |
| 1:Q:128:ALA:CB   | 1:Q:134:LYS:HB3  | 2.44                     | 0.43              |
| 2:V:7:LYS:HE3    | 2:V:135:GLY:HA2  | 2.00                     | 0.43              |
| 2:W:69:LEU:HD23  | 2:W:69:LEU:HA    | 1.85                     | 0.43              |
| 2:X:86:MET:HE3   | 2:X:86:MET:HB2   | 1.85                     | 0.43              |
| 1:A:19:LEU:HD13  | 1:G:9:MET:HE3    | 2.00                     | 0.43              |
| 1:A:56:LEU:HA    | 1:A:56:LEU:HD23  | 1.76                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:181:LEU:O    | 1:P:185:VAL:HG23 | 2.18                     | 0.43              |
| 1:S:93:ASP:OD1   | 2:a:75:THR:HG23  | 2.19                     | 0.43              |
| 2:Y:132:GLU:HG3  | 2:Y:134:GLU:H    | 1.83                     | 0.43              |
| 1:U:32:ALA:O     | 1:U:153:PHE:HA   | 2.18                     | 0.43              |
| 1:U:57:TYR:OH    | 1:U:86:GLY:HA3   | 2.18                     | 0.43              |
| 2:Z:150:MET:O    | 2:Z:154:TYR:HB2  | 2.18                     | 0.43              |
| 1:A:16:ARG:NH2   | 1:A:111:PHE:O    | 2.51                     | 0.43              |
| 1:F:28:LYS:HB3   | 1:F:44:GLU:HB3   | 2.00                     | 0.43              |
| 2:L:13:VAL:HG22  | 2:L:196:ILE:HG13 | 2.00                     | 0.43              |
| 2:M:59:TYR:CE1   | 2:M:83:LEU:HB2   | 2.54                     | 0.43              |
| 2:W:137:GLN:HG3  | 2:W:138:ALA:N    | 2.34                     | 0.43              |
| 2:Z:38:ASP:OD1   | 2:Z:38:ASP:C     | 2.61                     | 0.43              |
| 1:G:70:GLU:HB3   | 1:G:118:TYR:CD2  | 2.54                     | 0.43              |
| 2:M:102:PRO:HD2  | 2:M:123:PHE:HB2  | 1.99                     | 0.43              |
| 2:N:151:LYS:NZ   | 2:a:173:ASP:OD1  | 2.49                     | 0.43              |
| 1:P:229:ALA:O    | 1:P:233:LEU:HD13 | 2.19                     | 0.43              |
| 1:Q:9:MET:HB3    | 1:Q:9:MET:HE2    | 1.50                     | 0.43              |
| 2:b:9:PRO:HG2    | 2:b:158:THR:O    | 2.19                     | 0.43              |
| 1:D:164:ALA:O    | 1:D:168:LYS:HG2  | 2.19                     | 0.43              |
| 2:J:171:LEU:HD23 | 2:J:171:LEU:HA   | 1.79                     | 0.43              |
| 1:O:156:MET:HE3  | 1:O:156:MET:HB2  | 1.98                     | 0.43              |
| 2:V:164:LEU:O    | 2:V:168:VAL:HG23 | 2.19                     | 0.43              |
| 2:W:208:SER:O    | 2:W:212:GLU:HG3  | 2.19                     | 0.43              |
| 2:X:37:THR:HG22  | 2:X:60:ALA:HB2   | 2.01                     | 0.43              |
| 2:a:9:PRO:HG2    | 2:a:158:THR:O    | 2.19                     | 0.43              |
| 1:C:177:LEU:CD2  | 1:C:233:LEU:HD23 | 2.48                     | 0.42              |
| 2:H:14:MET:HE2   | 2:H:103:LEU:HD23 | 2.00                     | 0.42              |
| 1:Q:30:VAL:HG23  | 1:Q:43:ALA:HB2   | 2.00                     | 0.42              |
| 1:B:31:VAL:HG21  | 1:B:167:LEU:HD11 | 2.01                     | 0.42              |
| 2:K:19:ARG:NH1   | 2:K:179:SER:O    | 2.48                     | 0.42              |
| 2:N:78:GLY:O     | 2:N:82:ARG:HG2   | 2.20                     | 0.42              |
| 1:F:205:VAL:O    | 1:F:206:ALA:HB3  | 2.20                     | 0.42              |
| 2:H:18:ARG:NH2   | 2:H:30:ASP:O     | 2.47                     | 0.42              |
| 1:S:62:PHE:CE2   | 1:S:122:LEU:HD22 | 2.55                     | 0.42              |
| 2:a:196:ILE:HG22 | 2:a:203:VAL:HG13 | 2.02                     | 0.42              |
| 1:E:138:LEU:HB2  | 1:E:150:GLU:O    | 2.20                     | 0.42              |
| 1:P:165:ASN:O    | 1:P:168:LYS:HB3  | 2.19                     | 0.42              |
| 1:P:219:ARG:NH2  | 1:P:220:ARG:HD2  | 2.34                     | 0.42              |
| 1:Q:56:LEU:HG    | 1:Q:62:PHE:HB2   | 2.02                     | 0.42              |
| 1:Q:209:GLU:OE2  | 1:Q:224:ARG:NH2  | 2.50                     | 0.42              |
| 1:U:234:LEU:HD23 | 1:U:234:LEU:HA   | 1.86                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:9:PRO:HG2    | 2:V:158:THR:O    | 2.20                     | 0.42              |
| 2:Y:38:ASP:OD1   | 2:Y:39:ASP:N     | 2.52                     | 0.42              |
| 1:A:123:CYS:HA   | 1:A:139:TYR:O    | 2.19                     | 0.42              |
| 1:G:100:ALA:HB1  | 1:G:147:ILE:HD11 | 2.01                     | 0.42              |
| 2:N:32:ARG:NH1   | 2:N:204:ASP:OD2  | 2.52                     | 0.42              |
| 2:N:51:VAL:HG21  | 2:N:98:LEU:HB3   | 2.01                     | 0.42              |
| 1:T:17:SER:HG    | 1:T:143:TYR:HH   | 1.67                     | 0.42              |
| 2:a:101:LEU:HD23 | 2:a:101:LEU:HA   | 1.91                     | 0.42              |
| 2:H:164:LEU:O    | 2:H:168:VAL:HG23 | 2.19                     | 0.42              |
| 1:Q:128:ALA:HA   | 1:Q:134:LYS:HD3  | 2.02                     | 0.42              |
| 1:R:31:VAL:CG2   | 1:R:42:VAL:HG13  | 2.50                     | 0.42              |
| 1:U:150:GLU:HA   | 1:U:151:PRO:HD3  | 1.91                     | 0.42              |
| 1:U:219:ARG:NH2  | 2:b:64:GLU:OE2   | 2.38                     | 0.42              |
| 2:V:86:MET:HE3   | 2:V:86:MET:HB2   | 1.90                     | 0.42              |
| 2:Y:72:VAL:HG12  | 2:Y:73:PRO:O     | 2.19                     | 0.42              |
| 2:Z:25:MET:HE1   | 2:a:144:LEU:HD21 | 2.01                     | 0.42              |
| 2:Z:186:LEU:HD12 | 2:Z:186:LEU:H    | 1.83                     | 0.42              |
| 1:A:121:GLU:HG2  | 1:A:156:MET:HG2  | 2.01                     | 0.42              |
| 1:C:67:LYS:NZ    | 1:C:69:ASN:OD1   | 2.46                     | 0.42              |
| 2:H:62:GLU:OE2   | 2:H:82:ARG:HB3   | 2.20                     | 0.42              |
| 2:I:12:VAL:HG12  | 2:I:197:ILE:HB   | 2.02                     | 0.42              |
| 2:J:55:PHE:HE2   | 2:J:87:VAL:HG22  | 1.84                     | 0.42              |
| 1:O:110:ILE:HA   | 1:O:114:GLN:HG2  | 2.00                     | 0.42              |
| 1:P:62:PHE:CE1   | 1:P:75:ARG:HB2   | 2.55                     | 0.42              |
| 1:U:161:GLU:N    | 1:U:162:PRO:HD2  | 2.35                     | 0.42              |
| 2:V:211:ALA:O    | 2:V:215:ARG:HG3  | 2.19                     | 0.42              |
| 2:Z:104:LEU:HB3  | 2:Z:121:VAL:HB   | 2.02                     | 0.42              |
| 2:a:165:ARG:HB2  | 2:a:213:LEU:HD22 | 2.02                     | 0.42              |
| 2:L:113:ASP:HB3  | 2:L:116:SER:OG   | 2.19                     | 0.42              |
| 2:Y:43:THR:HG22  | 2:Y:104:LEU:CD1  | 2.49                     | 0.42              |
| 1:C:230:LEU:O    | 1:C:234:LEU:HD12 | 2.19                     | 0.42              |
| 1:D:30:VAL:HG13  | 1:D:156:MET:HE3  | 2.02                     | 0.42              |
| 1:E:150:GLU:HA   | 1:E:151:PRO:HD3  | 1.67                     | 0.42              |
| 2:J:209:ARG:HA   | 2:J:209:ARG:HD2  | 1.87                     | 0.42              |
| 2:L:49:ALA:O     | 2:L:53:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:81:PHE:CZ    | 1:A:102:VAL:HG21 | 2.55                     | 0.42              |
| 1:D:34:ALA:O     | 1:D:171:TYR:OH   | 2.27                     | 0.42              |
| 2:K:107:TYR:CE1  | 2:K:117:ALA:HB3  | 2.55                     | 0.42              |
| 2:N:25:MET:HE2   | 2:N:25:MET:HB3   | 1.77                     | 0.42              |
| 1:O:22:LYS:O     | 1:O:26:ARG:HD2   | 2.19                     | 0.42              |
| 1:P:156:MET:HE3  | 1:P:156:MET:HB2  | 1.90                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:118:TYR:HB3  | 1:C:120:VAL:HG22 | 2.02                     | 0.41              |
| 1:G:78:GLY:HA3   | 1:G:103:TYR:OH   | 2.19                     | 0.41              |
| 2:J:32:ARG:NH1   | 4:J:402:HOH:O    | 2.52                     | 0.41              |
| 2:K:209:ARG:NH1  | 2:K:209:ARG:HG2  | 2.35                     | 0.41              |
| 2:N:165:ARG:HA   | 2:N:213:LEU:HD13 | 2.02                     | 0.41              |
| 1:R:42:VAL:HB    | 1:R:210:VAL:HG12 | 2.02                     | 0.41              |
| 1:R:45:ASN:ND2   | 1:R:209:GLU:OE1  | 2.43                     | 0.41              |
| 2:a:186:LEU:HD11 | 2:a:218:ILE:CD1  | 2.50                     | 0.41              |
| 1:A:31:VAL:CG2   | 1:A:167:LEU:HD11 | 2.48                     | 0.41              |
| 2:L:124:ASP:OD1  | 2:L:124:ASP:C    | 2.63                     | 0.41              |
| 2:M:70:GLU:O     | 2:M:72:VAL:HG12  | 2.21                     | 0.41              |
| 2:N:164:LEU:O    | 2:N:168:VAL:HG23 | 2.20                     | 0.41              |
| 2:V:157:VAL:HG23 | 2:V:166:VAL:HG21 | 2.02                     | 0.41              |
| 2:a:38:ASP:OD1   | 2:a:38:ASP:C     | 2.64                     | 0.41              |
| 2:I:101:LEU:HA   | 2:I:102:PRO:HD3  | 1.91                     | 0.41              |
| 2:I:164:LEU:O    | 2:I:168:VAL:HG23 | 2.20                     | 0.41              |
| 1:R:149:ASP:OD2  | 1:S:48:ARG:HG2   | 2.20                     | 0.41              |
| 1:T:147:ILE:HG12 | 1:U:50:LEU:HD11  | 2.03                     | 0.41              |
| 2:X:13:VAL:HG22  | 2:X:196:ILE:CD1  | 2.51                     | 0.41              |
| 2:Z:156:GLN:CD   | 2:Z:165:ARG:HH12 | 2.26                     | 0.41              |
| 1:E:159:THR:OG1  | 1:E:191:GLY:O    | 2.37                     | 0.41              |
| 1:F:28:LYS:HD2   | 1:F:44:GLU:CD    | 2.46                     | 0.41              |
| 1:G:217:ARG:HA   | 1:G:217:ARG:HD2  | 1.83                     | 0.41              |
| 2:K:6:LEU:CD1    | 2:K:136:TYR:HB3  | 2.50                     | 0.41              |
| 2:L:107:TYR:OH   | 2:L:199:ALA:HB2  | 2.21                     | 0.41              |
| 2:M:162:SER:O    | 2:M:166:VAL:HG23 | 2.21                     | 0.41              |
| 1:Q:150:GLU:HA   | 1:Q:151:PRO:HD3  | 1.87                     | 0.41              |
| 1:R:93:ASP:OD1   | 2:Z:75:THR:HG23  | 2.19                     | 0.41              |
| 1:R:97:ARG:HD3   | 1:S:49:SER:HB2   | 2.02                     | 0.41              |
| 1:S:188:LEU:HD23 | 1:S:188:LEU:HA   | 1.84                     | 0.41              |
| 3:X:301:7J1:C36  | 2:Y:126:ALA:HB2  | 2.51                     | 0.41              |
| 1:D:32:ALA:HA    | 1:D:40:LEU:O     | 2.21                     | 0.41              |
| 1:G:89:TYR:CD2   | 2:H:74:LEU:HD21  | 2.55                     | 0.41              |
| 2:H:6:LEU:HG     | 2:H:13:VAL:HG12  | 2.03                     | 0.41              |
| 2:J:186:LEU:HD11 | 2:J:218:ILE:CD1  | 2.51                     | 0.41              |
| 2:N:20:SER:HB3   | 2:N:28:GLY:HA3   | 2.03                     | 0.41              |
| 2:N:137:GLN:HG3  | 2:N:138:ALA:N    | 2.36                     | 0.41              |
| 2:Y:18:ARG:HG2   | 4:Y:405:HOH:O    | 2.21                     | 0.41              |
| 1:A:116:LYS:HD3  | 1:G:112:THR:CG2  | 2.51                     | 0.41              |
| 1:C:71:PHE:HB3   | 1:C:120:VAL:CG1  | 2.50                     | 0.41              |
| 1:G:166:ALA:O    | 1:G:170:SER:CB   | 2.68                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Y:25:MET:HE1   | 2:Z:144:LEU:HD11 | 2.02                     | 0.41              |
| 2:b:18:ARG:HD3   | 2:b:193:THR:HG23 | 2.03                     | 0.41              |
| 1:B:80:GLN:O     | 1:B:84:THR:HG23  | 2.20                     | 0.41              |
| 1:D:156:MET:HE3  | 1:D:156:MET:HB2  | 1.98                     | 0.41              |
| 2:J:151:LYS:HE2  | 2:X:173:ASP:OD1  | 2.20                     | 0.41              |
| 2:K:144:LEU:HD12 | 2:K:144:LEU:N    | 2.35                     | 0.41              |
| 1:Q:72:ASP:OD1   | 1:Q:75:ARG:NH1   | 2.53                     | 0.41              |
| 1:T:87:TYR:CZ    | 2:a:58:LEU:HD13  | 2.55                     | 0.41              |
| 2:V:12:VAL:HG12  | 2:V:197:ILE:HB   | 2.01                     | 0.41              |
| 1:A:70:GLU:HB3   | 1:A:118:TYR:CD2  | 2.55                     | 0.41              |
| 1:D:72:ASP:O     | 1:D:76:ARG:HG3   | 2.21                     | 0.41              |
| 2:J:164:LEU:O    | 2:J:168:VAL:HG23 | 2.20                     | 0.41              |
| 2:N:123:PHE:HA   | 2:N:128:GLY:O    | 2.21                     | 0.41              |
| 2:W:99:LEU:HD22  | 2:W:100:ALA:H    | 1.86                     | 0.41              |
| 2:b:10:GLY:HA2   | 2:b:115:GLN:HA   | 2.02                     | 0.41              |
| 1:B:56:LEU:HA    | 1:B:56:LEU:HD23  | 1.68                     | 0.41              |
| 1:B:85:ARG:HD2   | 1:B:85:ARG:HA    | 1.94                     | 0.41              |
| 1:C:97:ARG:HD2   | 1:D:49:SER:HB2   | 2.03                     | 0.41              |
| 1:D:92:ARG:HA    | 1:D:92:ARG:HD2   | 1.95                     | 0.41              |
| 1:F:163:ILE:HG13 | 1:F:191:GLY:HA3  | 2.01                     | 0.41              |
| 2:M:107:TYR:CE2  | 2:M:117:ALA:HB3  | 2.56                     | 0.41              |
| 1:R:156:MET:HE3  | 1:R:156:MET:HB2  | 1.92                     | 0.41              |
| 2:W:14:MET:HE1   | 2:W:103:LEU:O    | 2.21                     | 0.41              |
| 2:Y:197:ILE:HG12 | 2:Y:202:ALA:CB   | 2.51                     | 0.41              |
| 2:Z:76:PHE:CE2   | 2:Z:80:ILE:HD11  | 2.56                     | 0.41              |
| 2:Z:103:LEU:HD12 | 2:Z:121:VAL:O    | 2.21                     | 0.41              |
| 2:Z:186:LEU:HD12 | 2:Z:186:LEU:N    | 2.36                     | 0.41              |
| 1:A:9:MET:HE3    | 1:A:9:MET:HB3    | 1.91                     | 0.41              |
| 1:C:231:GLN:HA   | 1:C:234:LEU:CD1  | 2.51                     | 0.41              |
| 2:K:6:LEU:HD12   | 2:K:136:TYR:HB3  | 2.02                     | 0.41              |
| 2:M:108:ASP:HB3  | 2:M:111:ALA:HB2  | 2.03                     | 0.41              |
| 1:O:28:LYS:HA    | 1:O:28:LYS:HD3   | 1.78                     | 0.41              |
| 1:P:217:ARG:HG3  | 1:P:223:ARG:NE   | 2.36                     | 0.41              |
| 1:S:141:ILE:HA   | 1:S:146:SER:O    | 2.21                     | 0.41              |
| 2:W:65:HIS:NE2   | 2:W:69:LEU:HD11  | 2.36                     | 0.41              |
| 2:W:122:SER:HB3  | 2:W:137:GLN:HG2  | 2.02                     | 0.41              |
| 2:X:136:TYR:O    | 2:X:137:GLN:HG2  | 2.21                     | 0.41              |
| 1:F:31:VAL:HG22  | 1:F:155:VAL:HG22 | 2.03                     | 0.40              |
| 1:F:55:GLU:HB2   | 1:F:222:PHE:CG   | 2.56                     | 0.40              |
| 1:G:11:GLN:HG3   | 1:G:12:ALA:N     | 2.35                     | 0.40              |
| 2:V:55:PHE:CE1   | 2:V:86:MET:HG2   | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Y:3:ILE:HG21   | 2:Y:44:GLY:HA3   | 2.03                     | 0.40              |
| 1:F:33:LEU:HD11  | 1:F:180:ALA:HB1  | 2.03                     | 0.40              |
| 1:F:217:ARG:NH1  | 1:F:223:ARG:HD3  | 2.36                     | 0.40              |
| 1:G:72:ASP:O     | 1:G:76:ARG:HG3   | 2.21                     | 0.40              |
| 2:H:164:LEU:O    | 2:H:164:LEU:HD23 | 2.21                     | 0.40              |
| 2:J:25:MET:HB3   | 2:J:25:MET:HE2   | 1.70                     | 0.40              |
| 1:O:9:MET:HE2    | 1:O:9:MET:HB3    | 1.75                     | 0.40              |
| 1:O:81:PHE:CZ    | 1:O:102:VAL:HG21 | 2.56                     | 0.40              |
| 1:U:170:SER:OG   | 1:U:183:ILE:HG13 | 2.20                     | 0.40              |
| 2:W:186:LEU:HA   | 2:W:186:LEU:HD23 | 1.70                     | 0.40              |
| 2:X:209:ARG:O    | 2:X:209:ARG:HD3  | 2.21                     | 0.40              |
| 2:a:32:ARG:HG3   | 2:a:193:THR:HG21 | 2.02                     | 0.40              |
| 2:b:38:ASP:OD1   | 2:b:39:ASP:N     | 2.53                     | 0.40              |
| 1:C:90:ASP:HB3   | 2:K:75:THR:HG21  | 2.02                     | 0.40              |
| 1:C:123:CYS:HA   | 1:C:139:TYR:O    | 2.21                     | 0.40              |
| 2:H:90:ASN:OD1   | 2:H:93:ALA:HB3   | 2.21                     | 0.40              |
| 2:K:113:ASP:C    | 2:K:115:GLN:H    | 2.29                     | 0.40              |
| 1:R:12:ALA:O     | 1:R:16:ARG:HG3   | 2.22                     | 0.40              |
| 1:U:85:ARG:HA    | 1:U:85:ARG:HD2   | 1.91                     | 0.40              |
| 2:Y:136:TYR:O    | 2:Y:137:GLN:HG2  | 2.22                     | 0.40              |
| 1:A:41:PHE:HB3   | 1:A:53:ILE:HD13  | 2.02                     | 0.40              |
| 1:R:32:ALA:C     | 1:R:33:LEU:HD12  | 2.46                     | 0.40              |
| 1:S:58:ASP:OD2   | 1:S:91:ARG:NH1   | 2.54                     | 0.40              |
| 1:T:152:HIS:HB3  | 1:T:171:TYR:CE2  | 2.56                     | 0.40              |
| 1:T:159:THR:HG22 | 1:T:162:PRO:HD2  | 2.02                     | 0.40              |
| 1:U:11:GLN:O     | 1:U:15:GLU:HB2   | 2.20                     | 0.40              |
| 1:U:178:THR:HA   | 1:U:233:LEU:HD21 | 2.03                     | 0.40              |
| 1:A:18:GLU:HG2   | 1:A:22:LYS:NZ    | 2.36                     | 0.40              |
| 1:E:105:GLN:NE2  | 4:E:301:HOH:O    | 2.24                     | 0.40              |
| 2:H:164:LEU:HD22 | 2:H:213:LEU:CD1  | 2.52                     | 0.40              |
| 2:I:197:ILE:HG12 | 2:I:202:ALA:CB   | 2.52                     | 0.40              |
| 1:Q:87:TYR:O     | 2:X:57:ARG:NH1   | 2.54                     | 0.40              |
| 1:S:41:PHE:HZ    | 1:S:125:ALA:HB3  | 1.87                     | 0.40              |
| 1:U:32:ALA:HA    | 1:U:40:LEU:O     | 2.21                     | 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     | 214/240 (89%) | 208 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | B     | 212/240 (88%) | 208 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | C     | 213/240 (89%) | 205 (96%) | 5 (2%)  | 3 (1%)   | 9           | 18  |
| 1   | D     | 213/240 (89%) | 204 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 1   | E     | 214/240 (89%) | 207 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 1   | F     | 211/240 (88%) | 204 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 1   | G     | 216/240 (90%) | 211 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | O     | 212/240 (88%) | 204 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | P     | 214/240 (89%) | 208 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Q     | 214/240 (89%) | 207 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 1   | R     | 213/240 (89%) | 209 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | S     | 214/240 (89%) | 205 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 1   | T     | 214/240 (89%) | 207 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 1   | U     | 213/240 (89%) | 205 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 2   | H     | 220/240 (92%) | 216 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 2   | I     | 220/240 (92%) | 216 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 2   | J     | 220/240 (92%) | 215 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 2   | K     | 221/240 (92%) | 217 (98%) | 3 (1%)  | 1 (0%)   | 24          | 43  |
| 2   | L     | 221/240 (92%) | 218 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 2   | M     | 220/240 (92%) | 215 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 2   | N     | 221/240 (92%) | 215 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 2   | V     | 221/240 (92%) | 218 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 2   | W     | 221/240 (92%) | 217 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 2   | X     | 220/240 (92%) | 213 (97%) | 6 (3%)  | 1 (0%)   | 24          | 43  |
| 2   | Y     | 221/240 (92%) | 217 (98%) | 4 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | Z     | 220/240 (92%)   | 218 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 2   | a     | 221/240 (92%)   | 216 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | b     | 221/240 (92%)   | 218 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| All | All   | 6075/6720 (90%) | 5921 (98%) | 149 (2%) | 5 (0%)   | 48          | 69  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 190 | ALA  |
| 1   | C     | 234 | LEU  |
| 1   | C     | 151 | PRO  |
| 2   | X     | 114 | PRO  |
| 2   | K     | 114 | PRO  |

### 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     | 167/184 (91%) | 162 (97%) | 5 (3%)   | 36          | 60 |
| 1   | B     | 166/184 (90%) | 162 (98%) | 4 (2%)   | 43          | 67 |
| 1   | C     | 166/184 (90%) | 161 (97%) | 5 (3%)   | 36          | 60 |
| 1   | D     | 166/184 (90%) | 163 (98%) | 3 (2%)   | 51          | 74 |
| 1   | E     | 167/184 (91%) | 159 (95%) | 8 (5%)   | 23          | 46 |
| 1   | F     | 164/184 (89%) | 158 (96%) | 6 (4%)   | 30          | 55 |
| 1   | G     | 168/184 (91%) | 165 (98%) | 3 (2%)   | 51          | 74 |
| 1   | O     | 165/184 (90%) | 161 (98%) | 4 (2%)   | 43          | 67 |
| 1   | P     | 167/184 (91%) | 161 (96%) | 6 (4%)   | 31          | 56 |
| 1   | Q     | 167/184 (91%) | 162 (97%) | 5 (3%)   | 36          | 60 |
| 1   | R     | 166/184 (90%) | 162 (98%) | 4 (2%)   | 43          | 67 |
| 1   | S     | 167/184 (91%) | 163 (98%) | 4 (2%)   | 43          | 67 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | T     | 167/184 (91%)   | 162 (97%)  | 5 (3%)   | 36          | 60  |
| 1   | U     | 166/184 (90%)   | 160 (96%)  | 6 (4%)   | 31          | 56  |
| 2   | H     | 165/178 (93%)   | 160 (97%)  | 5 (3%)   | 36          | 60  |
| 2   | I     | 165/178 (93%)   | 160 (97%)  | 5 (3%)   | 36          | 60  |
| 2   | J     | 165/178 (93%)   | 162 (98%)  | 3 (2%)   | 51          | 74  |
| 2   | K     | 165/178 (93%)   | 160 (97%)  | 5 (3%)   | 36          | 60  |
| 2   | L     | 165/178 (93%)   | 165 (100%) | 0        | 100         | 100 |
| 2   | M     | 165/178 (93%)   | 163 (99%)  | 2 (1%)   | 63          | 80  |
| 2   | N     | 165/178 (93%)   | 157 (95%)  | 8 (5%)   | 23          | 46  |
| 2   | V     | 165/178 (93%)   | 163 (99%)  | 2 (1%)   | 63          | 80  |
| 2   | W     | 165/178 (93%)   | 160 (97%)  | 5 (3%)   | 36          | 60  |
| 2   | X     | 165/178 (93%)   | 163 (99%)  | 2 (1%)   | 63          | 80  |
| 2   | Y     | 165/178 (93%)   | 164 (99%)  | 1 (1%)   | 78          | 89  |
| 2   | Z     | 165/178 (93%)   | 158 (96%)  | 7 (4%)   | 26          | 51  |
| 2   | a     | 165/178 (93%)   | 159 (96%)  | 6 (4%)   | 31          | 56  |
| 2   | b     | 165/178 (93%)   | 162 (98%)  | 3 (2%)   | 51          | 74  |
| All | All   | 4639/5068 (92%) | 4517 (97%) | 122 (3%) | 40          | 65  |

All (122) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 135 | ARG  |
| 1   | A     | 160 | THR  |
| 1   | A     | 178 | THR  |
| 1   | A     | 182 | ARG  |
| 1   | A     | 212 | VAL  |
| 1   | B     | 22  | LYS  |
| 1   | B     | 24  | ILE  |
| 1   | B     | 50  | LEU  |
| 1   | B     | 185 | VAL  |
| 1   | C     | 9   | MET  |
| 1   | C     | 31  | VAL  |
| 1   | C     | 133 | THR  |
| 1   | C     | 185 | VAL  |
| 1   | C     | 212 | VAL  |
| 1   | D     | 30  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 133 | THR  |
| 1   | D     | 183 | ILE  |
| 1   | E     | 9   | MET  |
| 1   | E     | 133 | THR  |
| 1   | E     | 178 | THR  |
| 1   | E     | 185 | VAL  |
| 1   | E     | 202 | THR  |
| 1   | E     | 225 | ILE  |
| 1   | E     | 226 | THR  |
| 1   | E     | 234 | LEU  |
| 1   | F     | 102 | VAL  |
| 1   | F     | 133 | THR  |
| 1   | F     | 173 | GLU  |
| 1   | F     | 178 | THR  |
| 1   | F     | 183 | ILE  |
| 1   | F     | 185 | VAL  |
| 1   | G     | 28  | LYS  |
| 1   | G     | 48  | ARG  |
| 1   | G     | 189 | ARG  |
| 2   | H     | 13  | VAL  |
| 2   | H     | 48  | THR  |
| 2   | H     | 165 | ARG  |
| 2   | H     | 196 | ILE  |
| 2   | H     | 203 | VAL  |
| 2   | I     | 41  | THR  |
| 2   | I     | 48  | THR  |
| 2   | I     | 57  | ARG  |
| 2   | I     | 165 | ARG  |
| 2   | I     | 203 | VAL  |
| 2   | J     | 37  | THR  |
| 2   | J     | 196 | ILE  |
| 2   | J     | 203 | VAL  |
| 2   | K     | 25  | MET  |
| 2   | K     | 48  | THR  |
| 2   | K     | 109 | ILE  |
| 2   | K     | 158 | THR  |
| 2   | K     | 203 | VAL  |
| 2   | M     | 29  | ARG  |
| 2   | M     | 31  | VAL  |
| 2   | N     | 12  | VAL  |
| 2   | N     | 37  | THR  |
| 2   | N     | 88  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 166 | VAL  |
| 2   | N     | 171 | LEU  |
| 2   | N     | 196 | ILE  |
| 2   | N     | 203 | VAL  |
| 2   | N     | 205 | VAL  |
| 1   | O     | 26  | ARG  |
| 1   | O     | 102 | VAL  |
| 1   | O     | 178 | THR  |
| 1   | O     | 185 | VAL  |
| 1   | P     | 21  | ARG  |
| 1   | P     | 24  | ILE  |
| 1   | P     | 28  | LYS  |
| 1   | P     | 122 | LEU  |
| 1   | P     | 133 | THR  |
| 1   | P     | 160 | THR  |
| 1   | Q     | 67  | LYS  |
| 1   | Q     | 178 | THR  |
| 1   | Q     | 185 | VAL  |
| 1   | Q     | 212 | VAL  |
| 1   | Q     | 217 | ARG  |
| 1   | R     | 30  | VAL  |
| 1   | R     | 42  | VAL  |
| 1   | R     | 133 | THR  |
| 1   | R     | 147 | ILE  |
| 1   | S     | 84  | THR  |
| 1   | S     | 173 | GLU  |
| 1   | S     | 216 | ASN  |
| 1   | S     | 235 | VAL  |
| 1   | T     | 26  | ARG  |
| 1   | T     | 42  | VAL  |
| 1   | T     | 133 | THR  |
| 1   | T     | 183 | ILE  |
| 1   | T     | 210 | VAL  |
| 1   | U     | 102 | VAL  |
| 1   | U     | 112 | THR  |
| 1   | U     | 138 | LEU  |
| 1   | U     | 147 | ILE  |
| 1   | U     | 168 | LYS  |
| 1   | U     | 183 | ILE  |
| 2   | V     | 37  | THR  |
| 2   | V     | 196 | ILE  |
| 2   | W     | 31  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | W     | 48  | THR  |
| 2   | W     | 72  | VAL  |
| 2   | W     | 217 | ILE  |
| 2   | W     | 219 | GLU  |
| 2   | X     | 37  | THR  |
| 2   | X     | 203 | VAL  |
| 2   | Y     | 48  | THR  |
| 2   | Z     | 31  | VAL  |
| 2   | Z     | 37  | THR  |
| 2   | Z     | 144 | LEU  |
| 2   | Z     | 196 | ILE  |
| 2   | Z     | 208 | SER  |
| 2   | Z     | 212 | GLU  |
| 2   | Z     | 219 | GLU  |
| 2   | a     | 31  | VAL  |
| 2   | a     | 37  | THR  |
| 2   | a     | 41  | THR  |
| 2   | a     | 48  | THR  |
| 2   | a     | 168 | VAL  |
| 2   | a     | 203 | VAL  |
| 2   | b     | 13  | VAL  |
| 2   | b     | 72  | VAL  |
| 2   | b     | 196 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | GLN  |
| 1   | A     | 231 | GLN  |
| 1   | B     | 98  | GLN  |
| 1   | B     | 129 | HIS  |
| 1   | D     | 105 | GLN  |
| 1   | D     | 174 | ASN  |
| 1   | E     | 152 | HIS  |
| 1   | F     | 11  | GLN  |
| 1   | G     | 231 | GLN  |
| 2   | H     | 110 | HIS  |
| 2   | H     | 130 | ASN  |
| 2   | I     | 65  | HIS  |
| 2   | I     | 81  | ASN  |
| 2   | K     | 81  | ASN  |
| 2   | K     | 110 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 90  | ASN  |
| 2   | M     | 130 | ASN  |
| 2   | N     | 137 | GLN  |
| 1   | O     | 105 | GLN  |
| 1   | O     | 129 | HIS  |
| 1   | O     | 231 | GLN  |
| 1   | P     | 98  | GLN  |
| 1   | P     | 152 | HIS  |
| 1   | Q     | 129 | HIS  |
| 1   | Q     | 231 | GLN  |
| 1   | S     | 129 | HIS  |
| 1   | T     | 51  | GLN  |
| 2   | W     | 137 | GLN  |
| 2   | X     | 65  | HIS  |
| 2   | Z     | 130 | ASN  |
| 2   | Z     | 137 | GLN  |
| 2   | a     | 110 | HIS  |
| 2   | a     | 130 | ASN  |
| 2   | b     | 96  | GLN  |
| 2   | b     | 137 | 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](#)

14 ligands are modelled in this entry.

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 |
| 3   | 7J1  | M     | 301 | -    | 44,44,44     | 2.05 | 9 (20%)  | 54,58,58    | 1.86 | 12 (22%) |
| 3   | 7J1  | V     | 301 | -    | 44,44,44     | 2.41 | 8 (18%)  | 54,58,58    | 1.31 | 8 (14%)  |
| 3   | 7J1  | Y     | 301 | -    | 44,44,44     | 2.05 | 9 (20%)  | 54,58,58    | 1.51 | 10 (18%) |
| 3   | 7J1  | H     | 301 | -    | 44,44,44     | 2.43 | 8 (18%)  | 54,58,58    | 1.37 | 9 (16%)  |
| 3   | 7J1  | W     | 301 | -    | 44,44,44     | 2.20 | 11 (25%) | 54,58,58    | 1.41 | 7 (12%)  |
| 3   | 7J1  | N     | 301 | -    | 44,44,44     | 2.22 | 8 (18%)  | 54,58,58    | 1.39 | 8 (14%)  |
| 3   | 7J1  | J     | 301 | -    | 44,44,44     | 2.16 | 9 (20%)  | 54,58,58    | 1.66 | 10 (18%) |
| 3   | 7J1  | X     | 301 | -    | 44,44,44     | 2.15 | 9 (20%)  | 54,58,58    | 1.31 | 8 (14%)  |
| 3   | 7J1  | b     | 301 | -    | 44,44,44     | 2.41 | 10 (22%) | 54,58,58    | 1.45 | 9 (16%)  |
| 3   | 7J1  | K     | 301 | -    | 44,44,44     | 2.56 | 9 (20%)  | 54,58,58    | 1.36 | 7 (12%)  |
| 3   | 7J1  | L     | 301 | -    | 44,44,44     | 2.39 | 9 (20%)  | 54,58,58    | 1.24 | 7 (12%)  |
| 3   | 7J1  | Z     | 301 | -    | 44,44,44     | 2.32 | 7 (15%)  | 54,58,58    | 1.26 | 6 (11%)  |
| 3   | 7J1  | a     | 301 | -    | 44,44,44     | 2.34 | 9 (20%)  | 54,58,58    | 1.22 | 5 (9%)   |
| 3   | 7J1  | I     | 301 | -    | 44,44,44     | 2.45 | 10 (22%) | 54,58,58    | 1.24 | 4 (7%)   |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | 7J1  | M     | 301 | -    | -       | 2/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | V     | 301 | -    | -       | 2/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | Y     | 301 | -    | -       | 2/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | H     | 301 | -    | -       | 5/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | W     | 301 | -    | -       | 5/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | N     | 301 | -    | -       | 4/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | J     | 301 | -    | -       | 3/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | X     | 301 | -    | -       | 3/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | b     | 301 | -    | -       | 2/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | K     | 301 | -    | -       | 5/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | L     | 301 | -    | -       | 2/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | Z     | 301 | -    | -       | 4/37/37/37 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | 7J1  | a     | 301 | -    | -       | 3/37/37/37 | 0/4/4/4 |
| 3   | 7J1  | I     | 301 | -    | -       | 3/37/37/37 | 0/4/4/4 |

All (125) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | I     | 301 | 7J1  | C26-C27 | 9.52 | 1.57        | 1.37     |
| 3   | K     | 301 | 7J1  | C29-C28 | 9.31 | 1.57        | 1.37     |
| 3   | K     | 301 | 7J1  | C26-C27 | 9.09 | 1.56        | 1.37     |
| 3   | Z     | 301 | 7J1  | C29-C28 | 8.70 | 1.55        | 1.37     |
| 3   | L     | 301 | 7J1  | C29-C28 | 8.54 | 1.55        | 1.37     |
| 3   | Z     | 301 | 7J1  | C26-C27 | 8.31 | 1.55        | 1.37     |
| 3   | V     | 301 | 7J1  | C29-C28 | 8.31 | 1.55        | 1.37     |
| 3   | H     | 301 | 7J1  | C29-C28 | 8.29 | 1.55        | 1.37     |
| 3   | b     | 301 | 7J1  | C29-C28 | 8.08 | 1.54        | 1.37     |
| 3   | I     | 301 | 7J1  | C29-C28 | 8.08 | 1.54        | 1.37     |
| 3   | N     | 301 | 7J1  | C26-C27 | 8.05 | 1.54        | 1.37     |
| 3   | W     | 301 | 7J1  | C29-C28 | 7.87 | 1.54        | 1.37     |
| 3   | H     | 301 | 7J1  | C26-C27 | 7.85 | 1.54        | 1.37     |
| 3   | Y     | 301 | 7J1  | C29-C28 | 7.80 | 1.54        | 1.37     |
| 3   | a     | 301 | 7J1  | C29-C28 | 7.76 | 1.53        | 1.37     |
| 3   | N     | 301 | 7J1  | C29-C28 | 7.76 | 1.53        | 1.37     |
| 3   | V     | 301 | 7J1  | C26-C27 | 7.75 | 1.53        | 1.37     |
| 3   | X     | 301 | 7J1  | C26-C27 | 7.74 | 1.53        | 1.37     |
| 3   | L     | 301 | 7J1  | C26-C27 | 7.62 | 1.53        | 1.37     |
| 3   | J     | 301 | 7J1  | C29-C28 | 7.52 | 1.53        | 1.37     |
| 3   | J     | 301 | 7J1  | C26-C27 | 7.47 | 1.53        | 1.37     |
| 3   | X     | 301 | 7J1  | C29-C28 | 7.34 | 1.53        | 1.37     |
| 3   | b     | 301 | 7J1  | C26-C27 | 7.27 | 1.52        | 1.37     |
| 3   | a     | 301 | 7J1  | C26-C27 | 7.00 | 1.52        | 1.37     |
| 3   | Y     | 301 | 7J1  | C26-C27 | 6.95 | 1.52        | 1.37     |
| 3   | W     | 301 | 7J1  | C26-C27 | 6.88 | 1.52        | 1.37     |
| 3   | M     | 301 | 7J1  | C29-C28 | 6.82 | 1.51        | 1.37     |
| 3   | a     | 301 | 7J1  | C26-N25 | 6.80 | 1.51        | 1.38     |
| 3   | H     | 301 | 7J1  | C26-N25 | 6.50 | 1.50        | 1.38     |
| 3   | M     | 301 | 7J1  | C26-C27 | 6.44 | 1.51        | 1.37     |
| 3   | K     | 301 | 7J1  | C26-N25 | 6.43 | 1.50        | 1.38     |
| 3   | V     | 301 | 7J1  | C26-N25 | 6.00 | 1.49        | 1.38     |
| 3   | b     | 301 | 7J1  | C26-N25 | 5.85 | 1.49        | 1.38     |
| 3   | L     | 301 | 7J1  | C26-N25 | 5.68 | 1.49        | 1.38     |
| 3   | I     | 301 | 7J1  | C29-N25 | 5.42 | 1.48        | 1.38     |
| 3   | W     | 301 | 7J1  | C26-N25 | 4.95 | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | Z     | 301 | 7J1  | C26-N25 | 4.94  | 1.47        | 1.38     |
| 3   | M     | 301 | 7J1  | C26-N25 | 4.82  | 1.47        | 1.38     |
| 3   | b     | 301 | 7J1  | C29-N25 | 4.61  | 1.47        | 1.38     |
| 3   | V     | 301 | 7J1  | C27-C28 | 4.42  | 1.55        | 1.41     |
| 3   | Y     | 301 | 7J1  | C26-N25 | 4.39  | 1.46        | 1.38     |
| 3   | a     | 301 | 7J1  | C27-C28 | 4.36  | 1.55        | 1.41     |
| 3   | X     | 301 | 7J1  | C26-N25 | 4.35  | 1.46        | 1.38     |
| 3   | V     | 301 | 7J1  | C29-N25 | 4.31  | 1.46        | 1.38     |
| 3   | N     | 301 | 7J1  | C29-N25 | 4.30  | 1.46        | 1.38     |
| 3   | H     | 301 | 7J1  | C29-N25 | 4.22  | 1.46        | 1.38     |
| 3   | J     | 301 | 7J1  | C26-N25 | 4.12  | 1.46        | 1.38     |
| 3   | I     | 301 | 7J1  | C26-N25 | 4.06  | 1.46        | 1.38     |
| 3   | b     | 301 | 7J1  | C27-C28 | 4.02  | 1.53        | 1.41     |
| 3   | H     | 301 | 7J1  | C27-C28 | 3.96  | 1.53        | 1.41     |
| 3   | L     | 301 | 7J1  | C27-C28 | 3.96  | 1.53        | 1.41     |
| 3   | W     | 301 | 7J1  | C27-C28 | 3.93  | 1.53        | 1.41     |
| 3   | K     | 301 | 7J1  | C27-C28 | 3.89  | 1.53        | 1.41     |
| 3   | N     | 301 | 7J1  | C26-N25 | 3.85  | 1.45        | 1.38     |
| 3   | N     | 301 | 7J1  | C27-C28 | 3.82  | 1.53        | 1.41     |
| 3   | H     | 301 | 7J1  | C04-N03 | -3.78 | 1.38        | 1.45     |
| 3   | K     | 301 | 7J1  | C29-N25 | 3.78  | 1.45        | 1.38     |
| 3   | Z     | 301 | 7J1  | C27-C28 | 3.69  | 1.52        | 1.41     |
| 3   | a     | 301 | 7J1  | C29-N25 | 3.64  | 1.45        | 1.38     |
| 3   | X     | 301 | 7J1  | C29-N25 | 3.57  | 1.45        | 1.38     |
| 3   | L     | 301 | 7J1  | C29-N25 | 3.57  | 1.45        | 1.38     |
| 3   | I     | 301 | 7J1  | C27-C28 | 3.56  | 1.52        | 1.41     |
| 3   | Z     | 301 | 7J1  | C04-N03 | -3.55 | 1.38        | 1.45     |
| 3   | J     | 301 | 7J1  | C33-C32 | 3.51  | 1.58        | 1.51     |
| 3   | Z     | 301 | 7J1  | C29-N25 | 3.48  | 1.45        | 1.38     |
| 3   | b     | 301 | 7J1  | C04-N03 | -3.45 | 1.38        | 1.45     |
| 3   | J     | 301 | 7J1  | C02-N03 | 3.41  | 1.41        | 1.34     |
| 3   | X     | 301 | 7J1  | C27-C28 | 3.32  | 1.51        | 1.41     |
| 3   | V     | 301 | 7J1  | C04-N03 | -3.26 | 1.39        | 1.45     |
| 3   | M     | 301 | 7J1  | C23-C24 | -3.18 | 1.45        | 1.51     |
| 3   | M     | 301 | 7J1  | C29-N25 | 3.16  | 1.44        | 1.38     |
| 3   | a     | 301 | 7J1  | C23-C22 | 3.15  | 1.60        | 1.53     |
| 3   | I     | 301 | 7J1  | C32-N31 | 3.12  | 1.40        | 1.34     |
| 3   | L     | 301 | 7J1  | C23-C22 | 3.11  | 1.60        | 1.53     |
| 3   | M     | 301 | 7J1  | C27-C28 | 3.10  | 1.51        | 1.41     |
| 3   | J     | 301 | 7J1  | C29-N25 | 3.10  | 1.44        | 1.38     |
| 3   | K     | 301 | 7J1  | C02-N03 | 3.08  | 1.40        | 1.34     |
| 3   | W     | 301 | 7J1  | C29-N25 | 3.07  | 1.44        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | X     | 301 | 7J1  | C04-C05 | -3.06 | 1.45        | 1.52     |
| 3   | b     | 301 | 7J1  | C19-C04 | 3.05  | 1.60        | 1.52     |
| 3   | L     | 301 | 7J1  | C22-C02 | 3.02  | 1.60        | 1.52     |
| 3   | a     | 301 | 7J1  | C32-N31 | 3.02  | 1.40        | 1.34     |
| 3   | J     | 301 | 7J1  | C27-C28 | 2.99  | 1.50        | 1.41     |
| 3   | J     | 301 | 7J1  | C32-N31 | 2.95  | 1.40        | 1.34     |
| 3   | b     | 301 | 7J1  | C10-C09 | 2.92  | 1.43        | 1.38     |
| 3   | Y     | 301 | 7J1  | C07-C08 | -2.91 | 1.44        | 1.51     |
| 3   | W     | 301 | 7J1  | C10-C09 | 2.87  | 1.43        | 1.38     |
| 3   | L     | 301 | 7J1  | C10-C09 | 2.80  | 1.43        | 1.38     |
| 3   | M     | 301 | 7J1  | C02-N03 | 2.76  | 1.39        | 1.34     |
| 3   | M     | 301 | 7J1  | C10-C09 | 2.75  | 1.43        | 1.38     |
| 3   | b     | 301 | 7J1  | C22-N31 | -2.74 | 1.40        | 1.45     |
| 3   | Z     | 301 | 7J1  | C32-N31 | 2.72  | 1.39        | 1.34     |
| 3   | K     | 301 | 7J1  | C33-C32 | 2.62  | 1.56        | 1.51     |
| 3   | X     | 301 | 7J1  | C10-C09 | 2.61  | 1.43        | 1.38     |
| 3   | I     | 301 | 7J1  | C02-N03 | 2.59  | 1.39        | 1.34     |
| 3   | Y     | 301 | 7J1  | C27-C28 | 2.55  | 1.49        | 1.41     |
| 3   | W     | 301 | 7J1  | C32-N31 | 2.55  | 1.39        | 1.34     |
| 3   | Y     | 301 | 7J1  | C29-N25 | 2.49  | 1.43        | 1.38     |
| 3   | N     | 301 | 7J1  | C04-N03 | -2.48 | 1.40        | 1.45     |
| 3   | I     | 301 | 7J1  | C23-C24 | -2.45 | 1.47        | 1.51     |
| 3   | a     | 301 | 7J1  | C04-C05 | -2.43 | 1.46        | 1.52     |
| 3   | a     | 301 | 7J1  | C02-N03 | 2.41  | 1.39        | 1.34     |
| 3   | V     | 301 | 7J1  | C05-N06 | 2.37  | 1.39        | 1.33     |
| 3   | H     | 301 | 7J1  | C04-C05 | 2.35  | 1.58        | 1.52     |
| 3   | I     | 301 | 7J1  | C10-C09 | 2.34  | 1.42        | 1.38     |
| 3   | W     | 301 | 7J1  | C19-C04 | 2.34  | 1.58        | 1.52     |
| 3   | H     | 301 | 7J1  | C05-N06 | 2.33  | 1.39        | 1.33     |
| 3   | N     | 301 | 7J1  | C32-N31 | 2.32  | 1.38        | 1.34     |
| 3   | Y     | 301 | 7J1  | C07-N06 | -2.31 | 1.41        | 1.46     |
| 3   | X     | 301 | 7J1  | C04-N03 | -2.28 | 1.41        | 1.45     |
| 3   | Y     | 301 | 7J1  | C32-N31 | 2.25  | 1.38        | 1.34     |
| 3   | N     | 301 | 7J1  | C05-N06 | 2.23  | 1.38        | 1.33     |
| 3   | M     | 301 | 7J1  | C05-N06 | 2.20  | 1.38        | 1.33     |
| 3   | V     | 301 | 7J1  | C04-C05 | 2.20  | 1.58        | 1.52     |
| 3   | I     | 301 | 7J1  | C05-N06 | 2.18  | 1.38        | 1.33     |
| 3   | L     | 301 | 7J1  | C16-C15 | 2.16  | 1.43        | 1.38     |
| 3   | b     | 301 | 7J1  | C07-N06 | -2.15 | 1.41        | 1.46     |
| 3   | W     | 301 | 7J1  | C02-N03 | 2.12  | 1.38        | 1.34     |
| 3   | K     | 301 | 7J1  | C16-C15 | 2.07  | 1.42        | 1.38     |
| 3   | W     | 301 | 7J1  | C13-C12 | -2.06 | 1.39        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | K     | 301 | 7J1  | C32-N31 | 2.06  | 1.38        | 1.34     |
| 3   | W     | 301 | 7J1  | C23-C24 | -2.05 | 1.47        | 1.51     |
| 3   | J     | 301 | 7J1  | C10-C09 | 2.05  | 1.42        | 1.38     |
| 3   | Y     | 301 | 7J1  | C04-N03 | -2.03 | 1.41        | 1.45     |
| 3   | X     | 301 | 7J1  | C32-N31 | 2.01  | 1.38        | 1.34     |

All (110) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | M     | 301 | 7J1  | C26-C27-C28 | -5.92 | 102.47      | 107.74   |
| 3   | J     | 301 | 7J1  | C26-C27-C28 | -5.92 | 102.47      | 107.74   |
| 3   | Y     | 301 | 7J1  | C26-C27-C28 | -5.30 | 103.02      | 107.74   |
| 3   | M     | 301 | 7J1  | C29-C28-C27 | -4.94 | 103.34      | 107.74   |
| 3   | b     | 301 | 7J1  | C26-C27-C28 | -4.92 | 103.36      | 107.74   |
| 3   | M     | 301 | 7J1  | C27-C26-N25 | -4.90 | 102.95      | 107.86   |
| 3   | M     | 301 | 7J1  | C28-C29-N25 | -4.72 | 103.13      | 107.86   |
| 3   | N     | 301 | 7J1  | C27-C26-N25 | -4.72 | 103.14      | 107.86   |
| 3   | J     | 301 | 7J1  | C28-C29-N25 | -4.35 | 103.50      | 107.86   |
| 3   | K     | 301 | 7J1  | C28-C29-N25 | -4.24 | 103.62      | 107.86   |
| 3   | W     | 301 | 7J1  | C26-N25-C29 | 4.15  | 112.59      | 108.41   |
| 3   | J     | 301 | 7J1  | C29-C28-C27 | -4.14 | 104.06      | 107.74   |
| 3   | Y     | 301 | 7J1  | C28-C29-N25 | -4.11 | 103.75      | 107.86   |
| 3   | W     | 301 | 7J1  | C33-C32-N31 | 3.98  | 122.88      | 115.86   |
| 3   | I     | 301 | 7J1  | C23-C22-C02 | -3.92 | 101.32      | 110.57   |
| 3   | b     | 301 | 7J1  | C27-C26-N25 | -3.92 | 103.93      | 107.86   |
| 3   | I     | 301 | 7J1  | C29-C28-C27 | -3.85 | 104.32      | 107.74   |
| 3   | X     | 301 | 7J1  | C19-C04-C05 | -3.82 | 102.33      | 110.39   |
| 3   | V     | 301 | 7J1  | C26-N25-C29 | 3.75  | 112.18      | 108.41   |
| 3   | a     | 301 | 7J1  | C26-N25-C29 | 3.73  | 112.16      | 108.41   |
| 3   | H     | 301 | 7J1  | C26-C27-C28 | -3.64 | 104.50      | 107.74   |
| 3   | Z     | 301 | 7J1  | C26-N25-C29 | 3.48  | 111.91      | 108.41   |
| 3   | H     | 301 | 7J1  | C33-C32-N31 | 3.44  | 121.93      | 115.86   |
| 3   | W     | 301 | 7J1  | C23-C22-C02 | -3.37 | 102.61      | 110.57   |
| 3   | Y     | 301 | 7J1  | C26-N25-C29 | 3.31  | 111.74      | 108.41   |
| 3   | J     | 301 | 7J1  | O41-C32-N31 | -3.29 | 117.38      | 122.95   |
| 3   | K     | 301 | 7J1  | O41-C32-N31 | -3.29 | 117.39      | 122.95   |
| 3   | N     | 301 | 7J1  | C26-C27-C28 | -3.28 | 104.82      | 107.74   |
| 3   | Z     | 301 | 7J1  | C23-C22-C02 | -3.28 | 102.84      | 110.57   |
| 3   | M     | 301 | 7J1  | C26-N25-C29 | 3.26  | 111.69      | 108.41   |
| 3   | M     | 301 | 7J1  | C19-C04-C05 | -3.24 | 103.55      | 110.39   |
| 3   | W     | 301 | 7J1  | O41-C32-N31 | -3.14 | 117.64      | 122.95   |
| 3   | J     | 301 | 7J1  | C33-C32-N31 | 3.10  | 121.33      | 115.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | H     | 301 | 7J1  | O41-C32-N31 | -3.10 | 117.70      | 122.95   |
| 3   | Z     | 301 | 7J1  | C33-C32-N31 | 3.10  | 121.32      | 115.86   |
| 3   | L     | 301 | 7J1  | C33-C32-N31 | 3.09  | 121.32      | 115.86   |
| 3   | N     | 301 | 7J1  | C23-C22-C02 | -3.08 | 103.32      | 110.57   |
| 3   | b     | 301 | 7J1  | C28-C29-N25 | -3.05 | 104.81      | 107.86   |
| 3   | K     | 301 | 7J1  | C29-C28-C27 | -2.99 | 105.08      | 107.74   |
| 3   | N     | 301 | 7J1  | C33-C32-N31 | 2.98  | 121.11      | 115.86   |
| 3   | H     | 301 | 7J1  | C19-C04-N03 | -2.97 | 104.75      | 111.31   |
| 3   | K     | 301 | 7J1  | C33-C32-N31 | 2.95  | 121.06      | 115.86   |
| 3   | Y     | 301 | 7J1  | C23-C22-C02 | -2.95 | 103.62      | 110.57   |
| 3   | V     | 301 | 7J1  | C33-C32-N31 | 2.94  | 121.04      | 115.86   |
| 3   | V     | 301 | 7J1  | O41-C32-N31 | -2.91 | 118.02      | 122.95   |
| 3   | L     | 301 | 7J1  | C26-N25-C29 | 2.88  | 111.31      | 108.41   |
| 3   | V     | 301 | 7J1  | C27-C26-N25 | -2.87 | 104.98      | 107.86   |
| 3   | X     | 301 | 7J1  | C26-N25-C29 | 2.86  | 111.29      | 108.41   |
| 3   | M     | 301 | 7J1  | C33-C32-N31 | 2.86  | 120.90      | 115.86   |
| 3   | H     | 301 | 7J1  | C26-N25-C29 | 2.83  | 111.26      | 108.41   |
| 3   | X     | 301 | 7J1  | O41-C32-N31 | -2.81 | 118.19      | 122.95   |
| 3   | K     | 301 | 7J1  | C26-C27-C28 | -2.81 | 105.24      | 107.74   |
| 3   | X     | 301 | 7J1  | C28-C29-N25 | -2.77 | 105.09      | 107.86   |
| 3   | M     | 301 | 7J1  | C23-C22-C02 | -2.75 | 104.08      | 110.57   |
| 3   | Y     | 301 | 7J1  | C27-C26-N25 | -2.75 | 105.11      | 107.86   |
| 3   | a     | 301 | 7J1  | C19-C04-C05 | -2.68 | 104.73      | 110.39   |
| 3   | Y     | 301 | 7J1  | C29-C28-C27 | -2.63 | 105.39      | 107.74   |
| 3   | L     | 301 | 7J1  | O01-C02-N03 | -2.63 | 118.26      | 122.96   |
| 3   | N     | 301 | 7J1  | C26-N25-C29 | 2.59  | 111.02      | 108.41   |
| 3   | M     | 301 | 7J1  | C04-N03-C02 | 2.59  | 127.20      | 121.65   |
| 3   | V     | 301 | 7J1  | C05-C04-N03 | -2.58 | 104.13      | 111.11   |
| 3   | N     | 301 | 7J1  | O41-C32-N31 | -2.57 | 118.61      | 122.95   |
| 3   | b     | 301 | 7J1  | C26-N25-C29 | 2.55  | 110.98      | 108.41   |
| 3   | W     | 301 | 7J1  | C28-C29-N25 | -2.55 | 105.31      | 107.86   |
| 3   | Y     | 301 | 7J1  | C33-C32-N31 | 2.51  | 120.29      | 115.86   |
| 3   | X     | 301 | 7J1  | C05-C04-N03 | -2.51 | 104.32      | 111.11   |
| 3   | H     | 301 | 7J1  | C23-C22-C02 | -2.51 | 104.65      | 110.57   |
| 3   | X     | 301 | 7J1  | C04-C05-N06 | 2.50  | 121.90      | 116.54   |
| 3   | V     | 301 | 7J1  | C26-C27-C28 | -2.49 | 105.52      | 107.74   |
| 3   | V     | 301 | 7J1  | C23-C22-C02 | -2.48 | 104.71      | 110.57   |
| 3   | J     | 301 | 7J1  | C23-C22-C02 | -2.48 | 104.73      | 110.57   |
| 3   | Z     | 301 | 7J1  | C19-C04-N03 | -2.45 | 105.91      | 111.31   |
| 3   | X     | 301 | 7J1  | C27-C26-N25 | -2.44 | 105.42      | 107.86   |
| 3   | a     | 301 | 7J1  | C33-C32-N31 | 2.44  | 120.16      | 115.86   |
| 3   | W     | 301 | 7J1  | C05-C04-N03 | -2.41 | 104.58      | 111.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | M     | 301 | 7J1  | C19-C04-N03 | -2.39 | 106.03      | 111.31   |
| 3   | H     | 301 | 7J1  | C27-C26-N25 | -2.38 | 105.48      | 107.86   |
| 3   | M     | 301 | 7J1  | O41-C32-N31 | -2.36 | 118.96      | 122.95   |
| 3   | J     | 301 | 7J1  | C26-N25-C29 | 2.36  | 110.78      | 108.41   |
| 3   | Y     | 301 | 7J1  | O20-C19-C04 | -2.36 | 102.83      | 109.25   |
| 3   | L     | 301 | 7J1  | C19-C04-C05 | -2.35 | 105.44      | 110.39   |
| 3   | b     | 301 | 7J1  | C05-C04-N03 | -2.35 | 104.76      | 111.11   |
| 3   | X     | 301 | 7J1  | C34-C33-C32 | 2.31  | 118.02      | 112.83   |
| 3   | N     | 301 | 7J1  | C28-C29-N25 | -2.29 | 105.56      | 107.86   |
| 3   | L     | 301 | 7J1  | C05-C04-N03 | -2.25 | 105.03      | 111.11   |
| 3   | Y     | 301 | 7J1  | C23-C22-N31 | 2.25  | 114.92      | 110.64   |
| 3   | I     | 301 | 7J1  | C33-C32-N31 | 2.24  | 119.80      | 115.86   |
| 3   | Z     | 301 | 7J1  | C02-C22-N31 | -2.23 | 105.07      | 111.11   |
| 3   | J     | 301 | 7J1  | C04-N03-C02 | 2.23  | 126.44      | 121.65   |
| 3   | b     | 301 | 7J1  | C29-C28-C27 | -2.22 | 105.77      | 107.74   |
| 3   | H     | 301 | 7J1  | C28-C29-N25 | -2.20 | 105.65      | 107.86   |
| 3   | Y     | 301 | 7J1  | O41-C32-N31 | -2.20 | 119.23      | 122.95   |
| 3   | W     | 301 | 7J1  | C19-C04-C05 | -2.16 | 105.83      | 110.39   |
| 3   | K     | 301 | 7J1  | C23-C22-C02 | -2.16 | 105.48      | 110.57   |
| 3   | N     | 301 | 7J1  | C29-C28-C27 | -2.16 | 105.82      | 107.74   |
| 3   | M     | 301 | 7J1  | C04-C05-N06 | 2.15  | 121.15      | 116.54   |
| 3   | L     | 301 | 7J1  | C23-C22-C02 | -2.13 | 105.53      | 110.57   |
| 3   | H     | 301 | 7J1  | C17-C12-C11 | -2.12 | 118.18      | 123.01   |
| 3   | J     | 301 | 7J1  | C27-C26-N25 | -2.09 | 105.77      | 107.86   |
| 3   | L     | 301 | 7J1  | C26-C27-C28 | -2.06 | 105.91      | 107.74   |
| 3   | I     | 301 | 7J1  | O01-C02-N03 | -2.06 | 119.27      | 122.96   |
| 3   | V     | 301 | 7J1  | C04-C05-N06 | 2.06  | 120.95      | 116.54   |
| 3   | K     | 301 | 7J1  | C27-C26-N25 | -2.06 | 105.80      | 107.86   |
| 3   | b     | 301 | 7J1  | O01-C02-N03 | -2.05 | 119.28      | 122.96   |
| 3   | Z     | 301 | 7J1  | O41-C32-C33 | -2.05 | 118.30      | 122.02   |
| 3   | J     | 301 | 7J1  | C19-C04-C05 | -2.04 | 106.10      | 110.39   |
| 3   | b     | 301 | 7J1  | C33-C32-N31 | 2.03  | 119.45      | 115.86   |
| 3   | a     | 301 | 7J1  | C23-C22-N31 | 2.02  | 114.48      | 110.64   |
| 3   | b     | 301 | 7J1  | C23-C22-C02 | -2.01 | 105.83      | 110.57   |
| 3   | a     | 301 | 7J1  | O41-C32-C33 | -2.01 | 118.38      | 122.02   |

There are no chirality outliers.

All (45) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | H     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | H     | 301 | 7J1  | C05-C04-C19-O20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | I     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | I     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | J     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | K     | 301 | 7J1  | N31-C22-C23-C24 |
| 3   | L     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | L     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | M     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | M     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | N     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | N     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | W     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | W     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | X     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | X     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | Y     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | Y     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | Z     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | Z     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | a     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | a     | 301 | 7J1  | C05-C04-C19-O20 |
| 3   | J     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | X     | 301 | 7J1  | C04-C19-O20-C21 |
| 3   | Z     | 301 | 7J1  | C04-C19-O20-C21 |
| 3   | b     | 301 | 7J1  | C04-C19-O20-C21 |
| 3   | I     | 301 | 7J1  | C04-C19-O20-C21 |
| 3   | W     | 301 | 7J1  | C04-C19-O20-C21 |
| 3   | N     | 301 | 7J1  | C32-C33-C34-C35 |
| 3   | K     | 301 | 7J1  | C02-C22-C23-C24 |
| 3   | K     | 301 | 7J1  | N03-C04-C19-O20 |
| 3   | J     | 301 | 7J1  | C04-C19-O20-C21 |
| 3   | K     | 301 | 7J1  | C33-C34-C35-C40 |
| 3   | K     | 301 | 7J1  | C33-C34-C35-C36 |
| 3   | W     | 301 | 7J1  | C33-C34-C35-C40 |
| 3   | H     | 301 | 7J1  | C04-C19-O20-C21 |
| 3   | W     | 301 | 7J1  | C33-C34-C35-C36 |
| 3   | V     | 301 | 7J1  | C22-C23-C24-O30 |
| 3   | N     | 301 | 7J1  | C22-C23-C24-N25 |
| 3   | V     | 301 | 7J1  | C22-C23-C24-N25 |
| 3   | Z     | 301 | 7J1  | C22-C23-C24-N25 |
| 3   | a     | 301 | 7J1  | C22-C23-C24-N25 |
| 3   | b     | 301 | 7J1  | C22-C23-C24-N25 |
| 3   | H     | 301 | 7J1  | C33-C34-C35-C40 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | H     | 301 | 7J1  | C33-C34-C35-C36 |

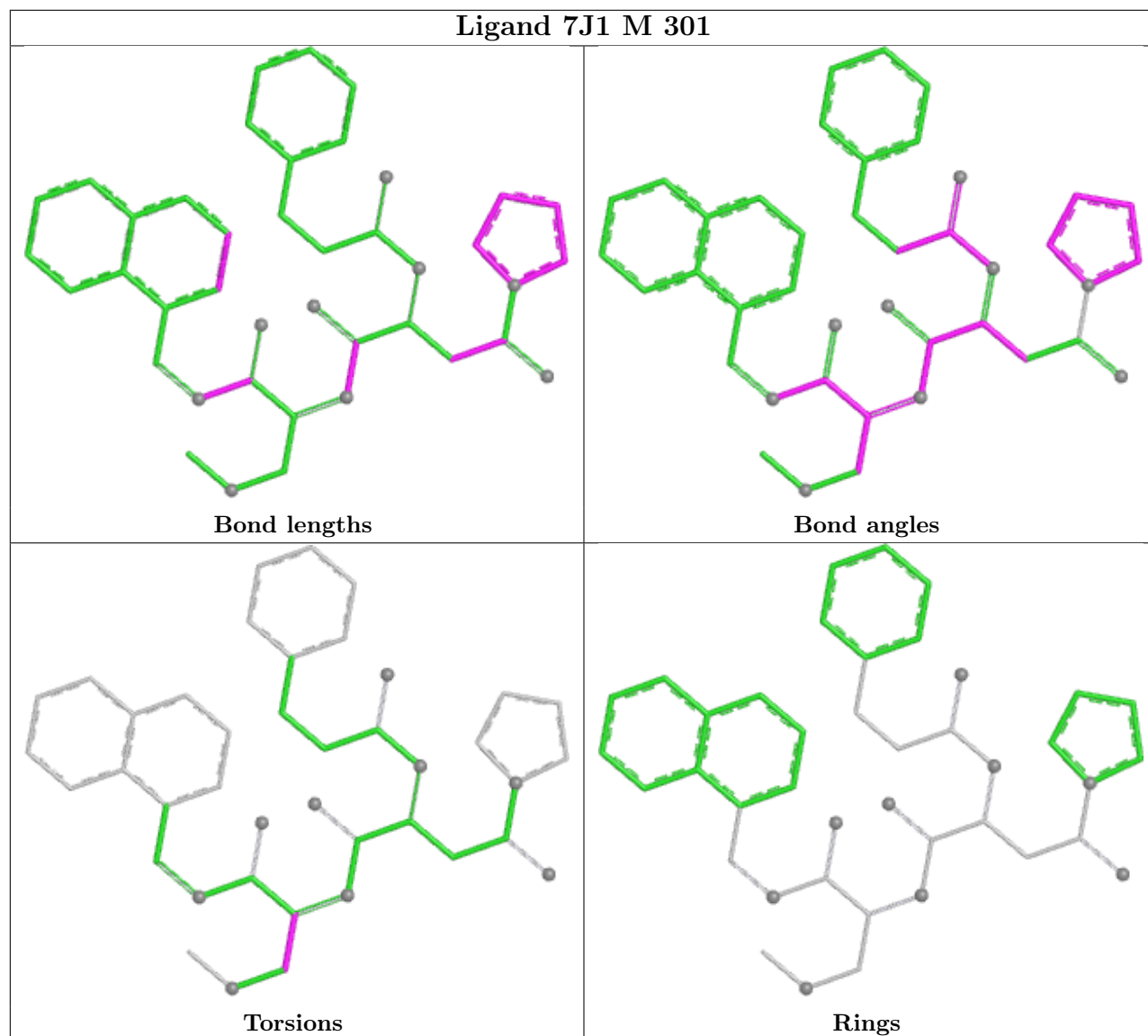
There are no ring outliers.

2 monomers are involved in 2 short contacts:

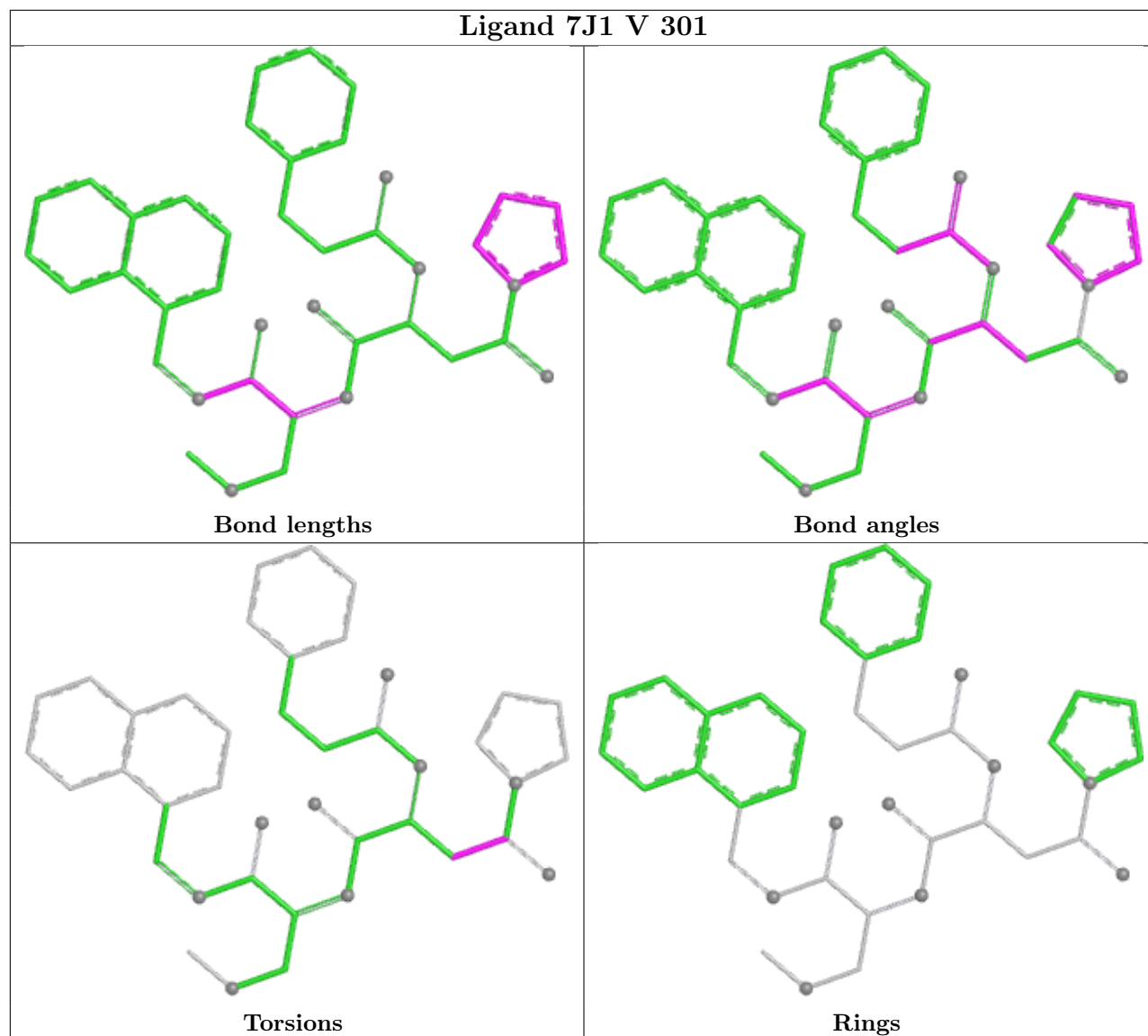
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | Y     | 301 | 7J1  | 1       | 0            |
| 3   | X     | 301 | 7J1  | 1       | 0            |

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.

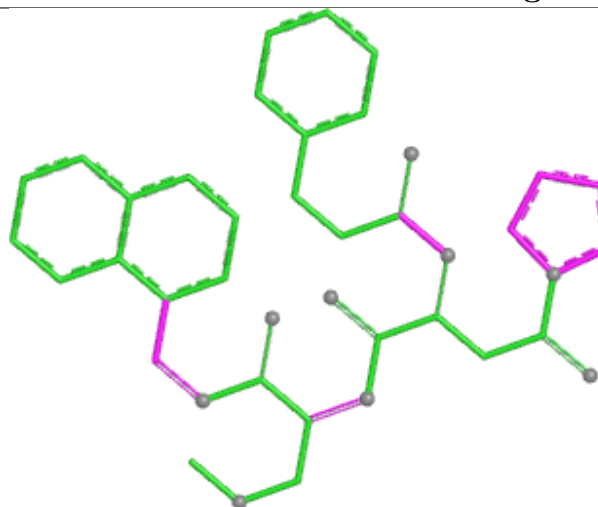
## Ligand 7J1 M 301



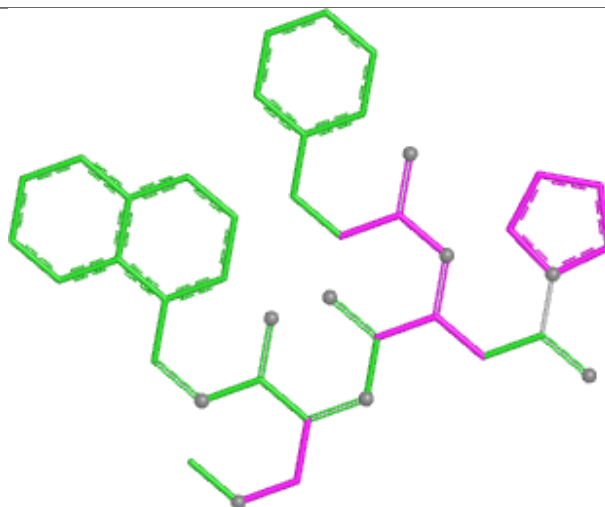
## Ligand 7J1 V 301



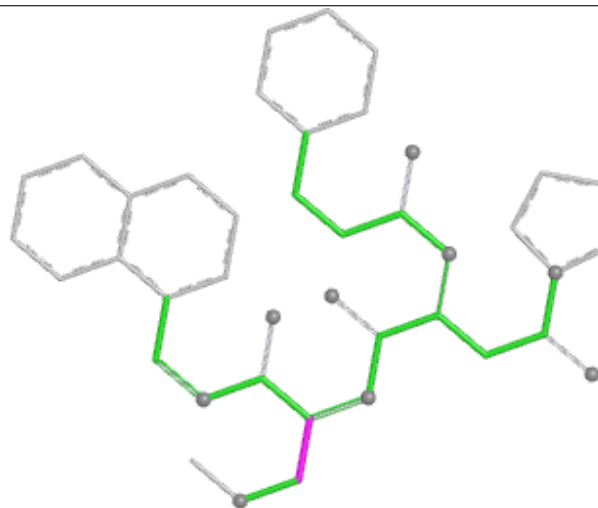
## Ligand 7J1 Y 301



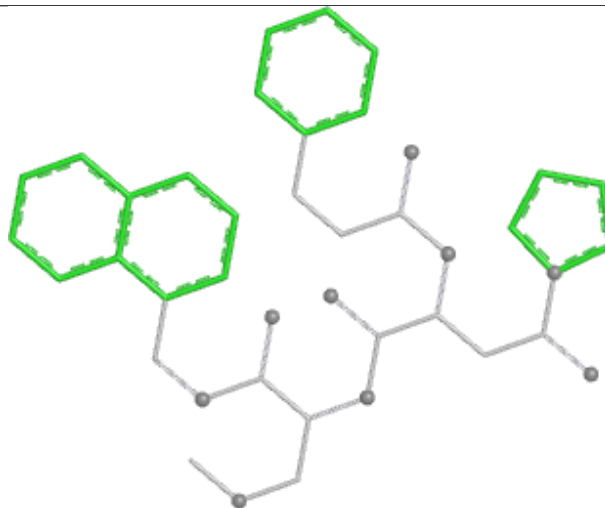
Bond lengths



Bond angles

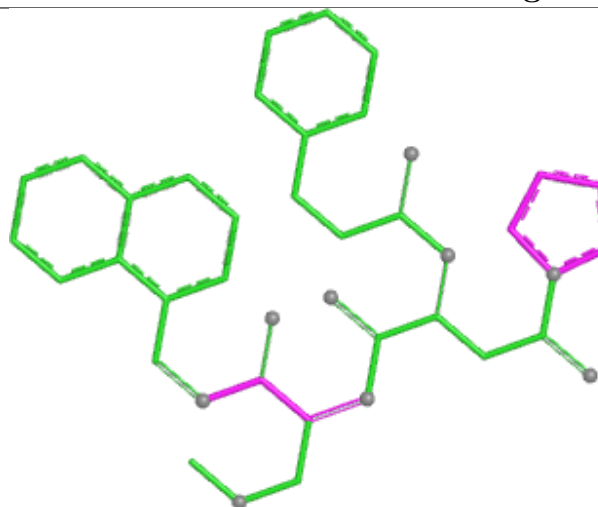


Torsions

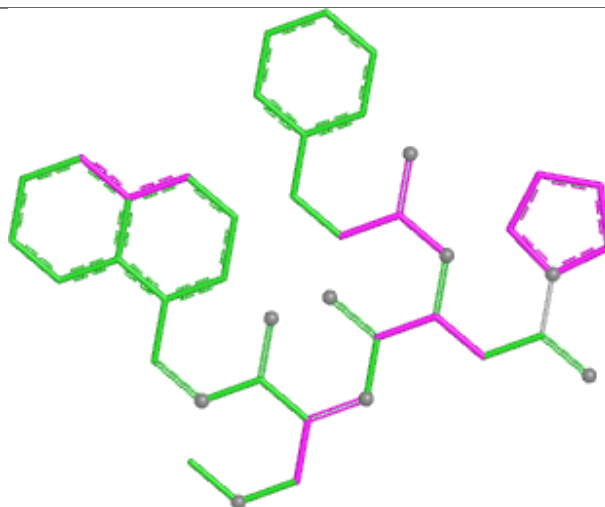


Rings

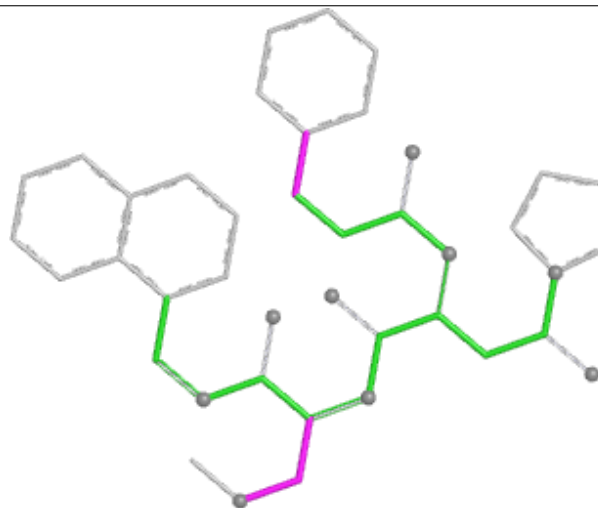
## Ligand 7J1 H 301



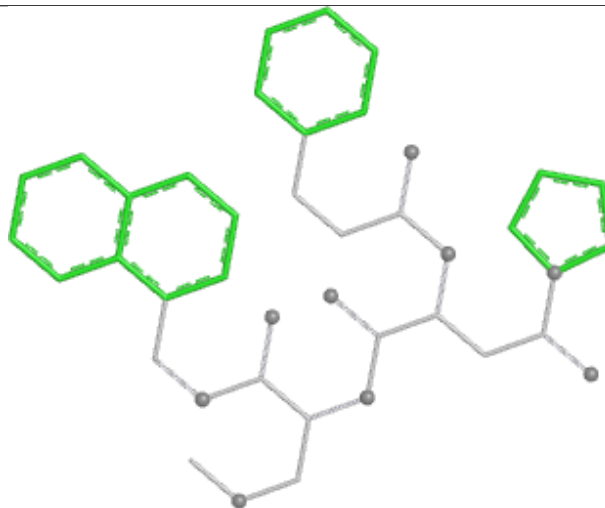
Bond lengths



Bond angles

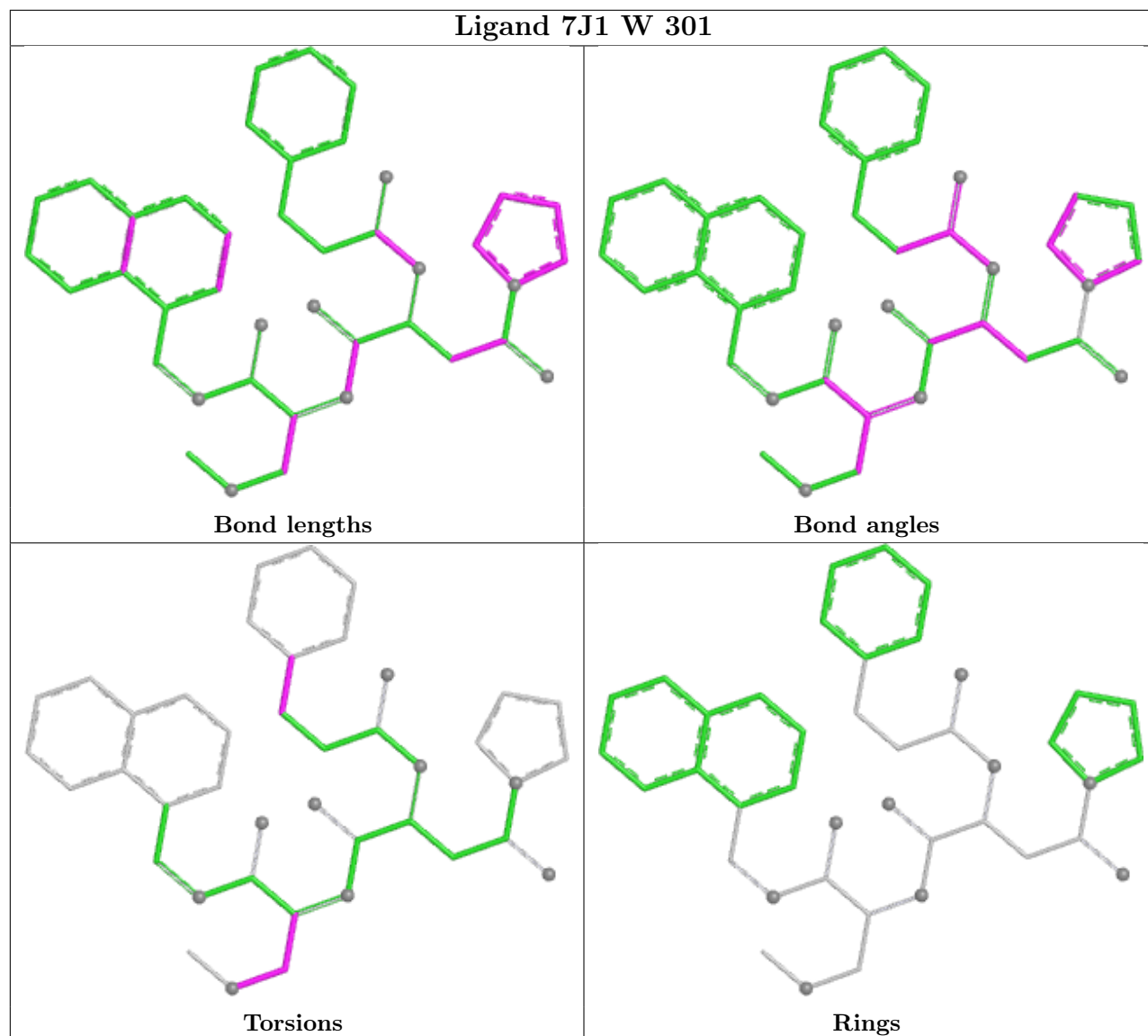


Torsions

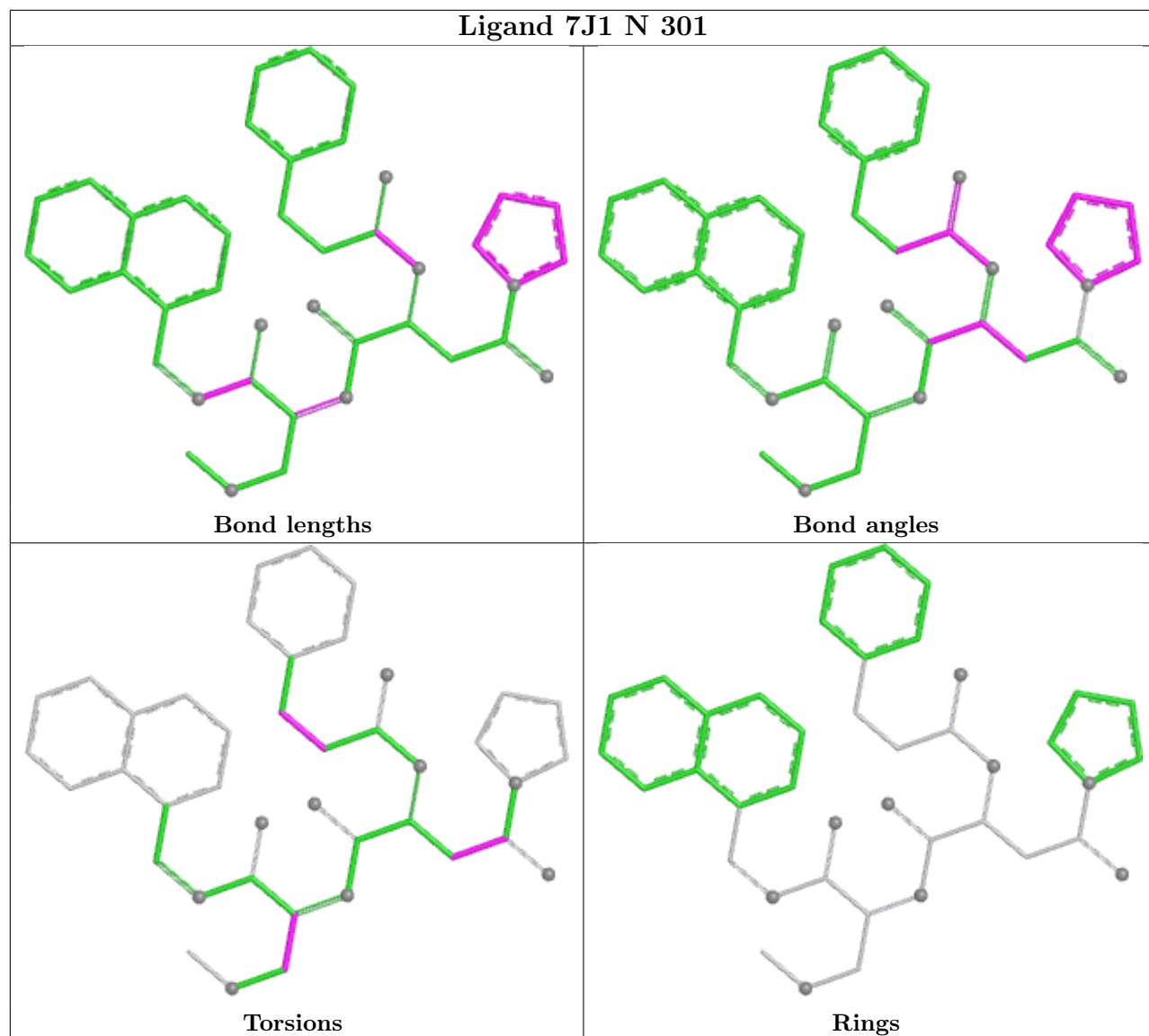


Rings

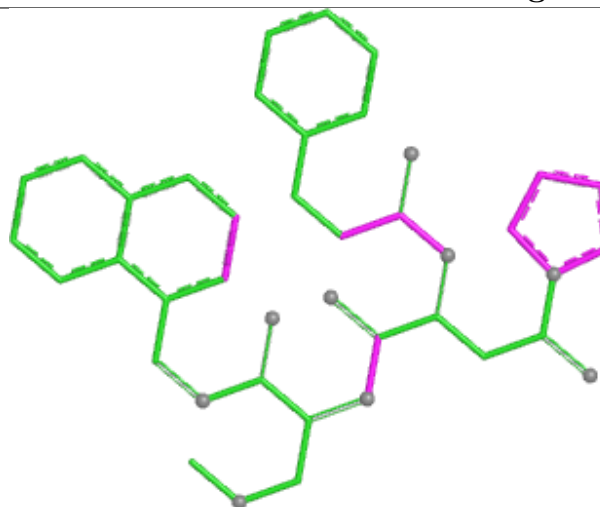
## Ligand 7J1 W 301



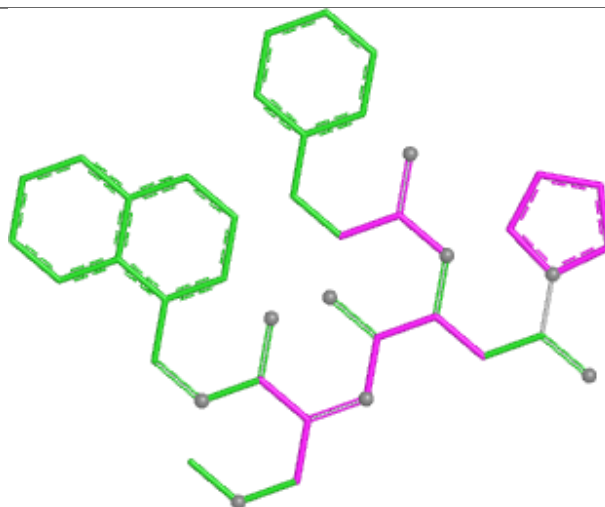
## Ligand 7J1 N 301



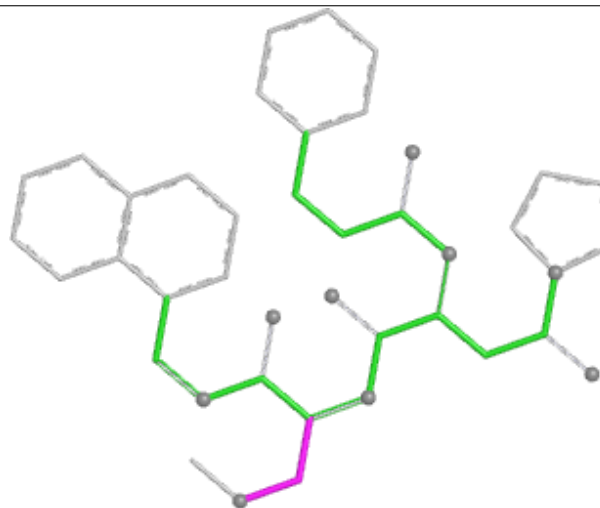
## Ligand 7J1 J 301



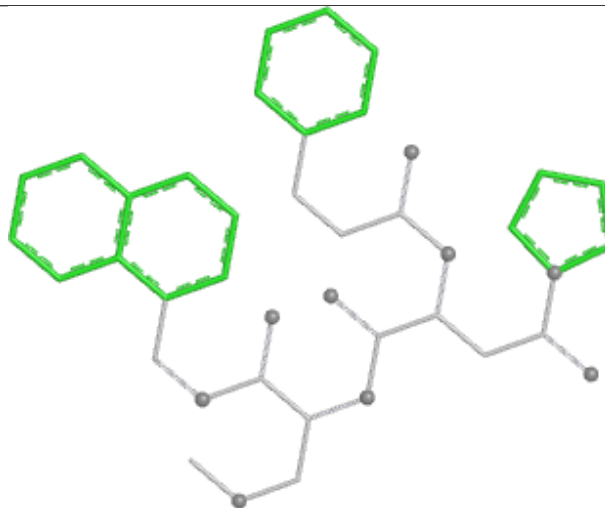
Bond lengths



Bond angles

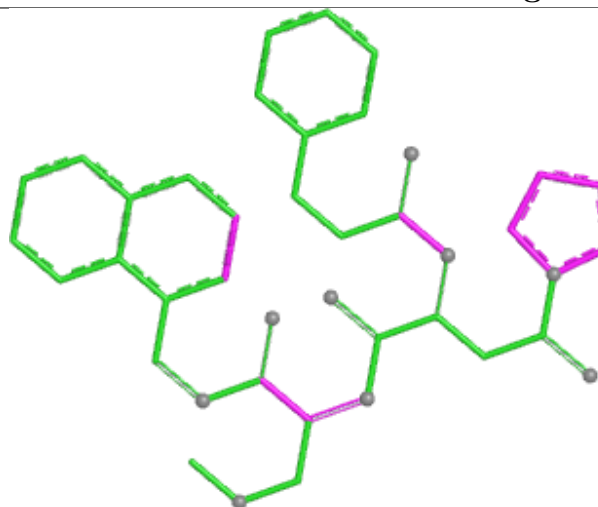


Torsions

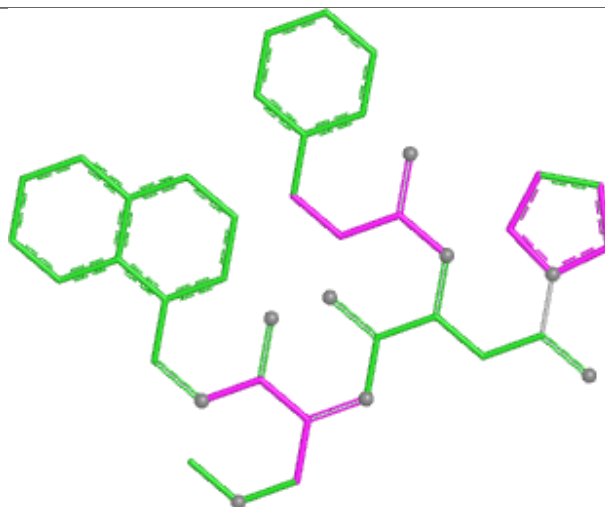


Rings

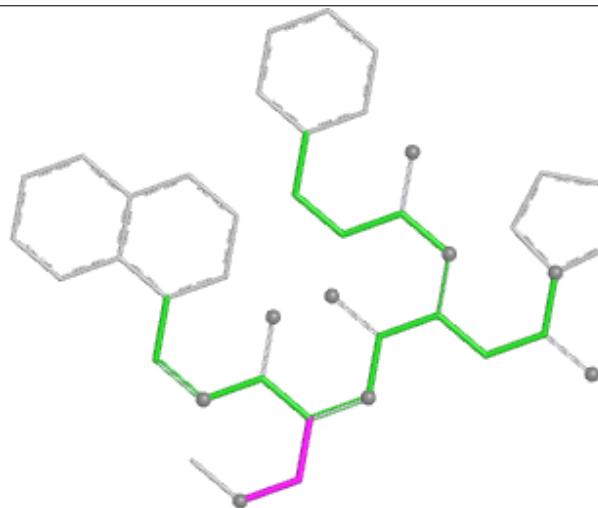
## Ligand 7J1 X 301



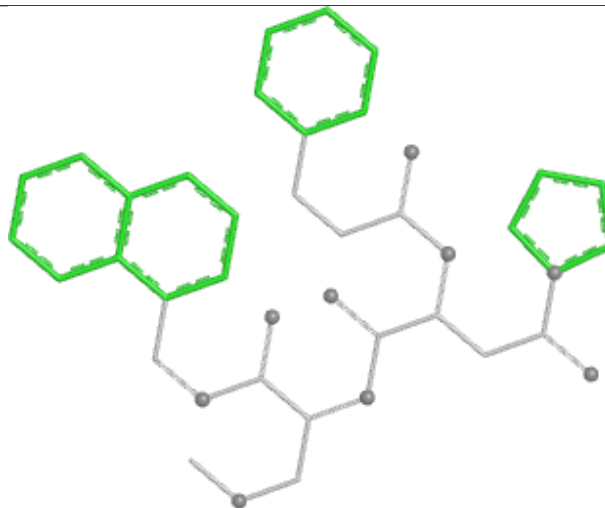
Bond lengths



Bond angles

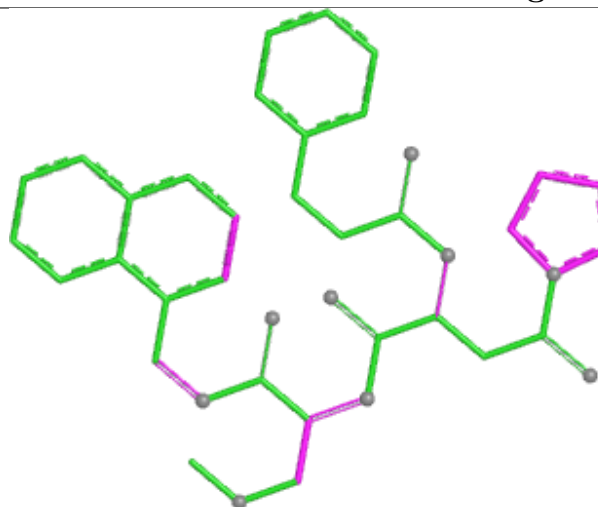


Torsions

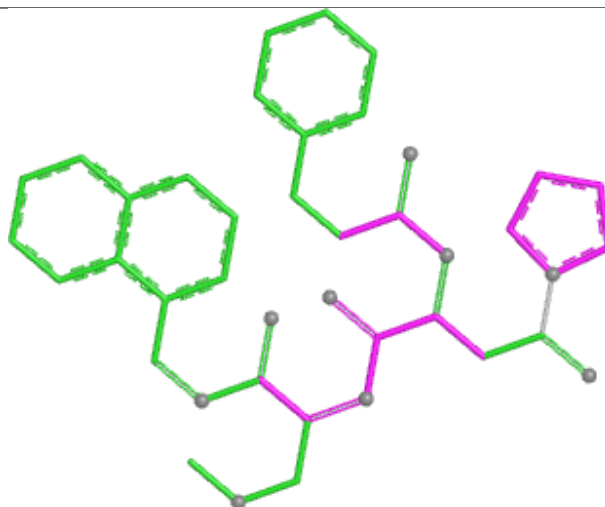


Rings

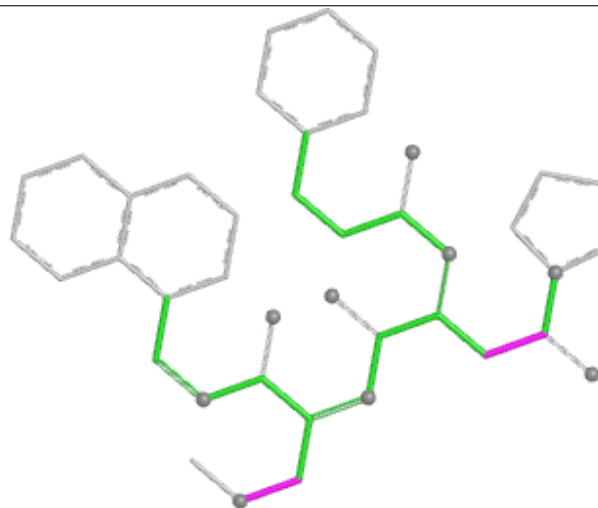
## Ligand 7J1 b 301



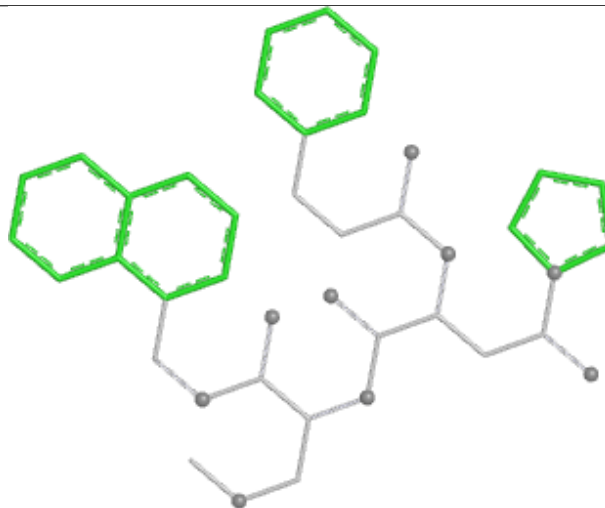
Bond lengths



Bond angles

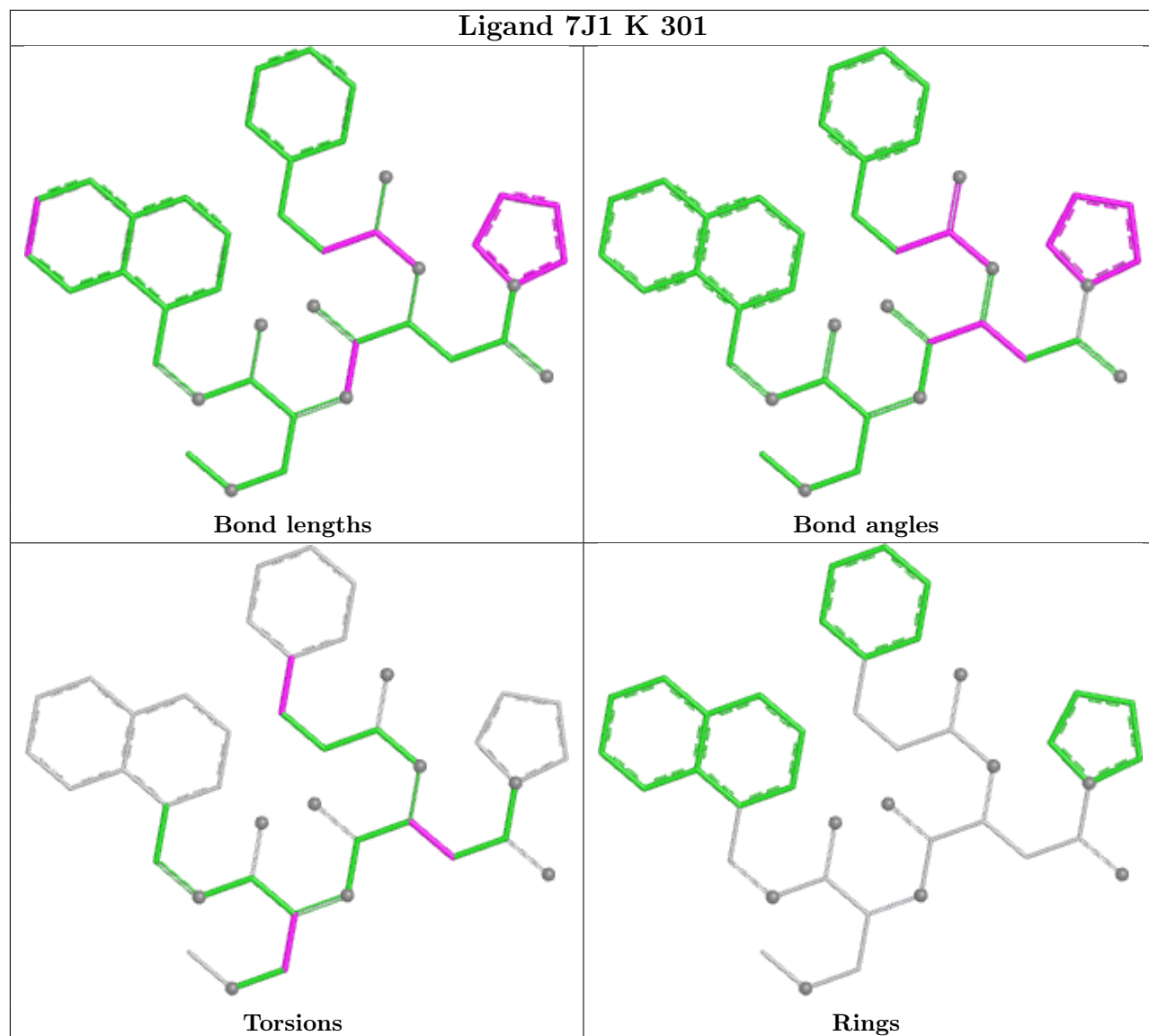


Torsions

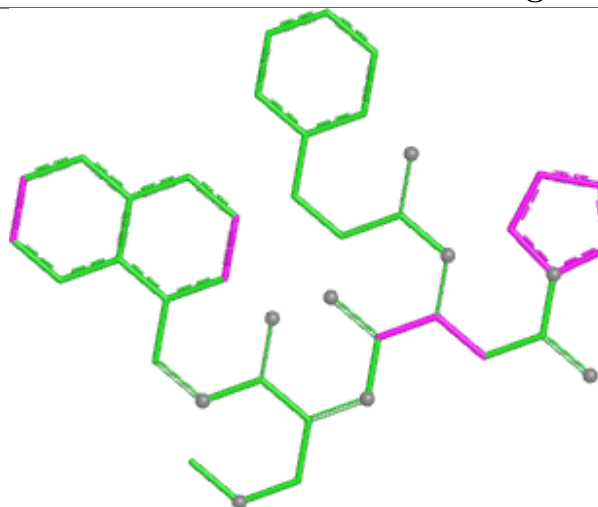


Rings

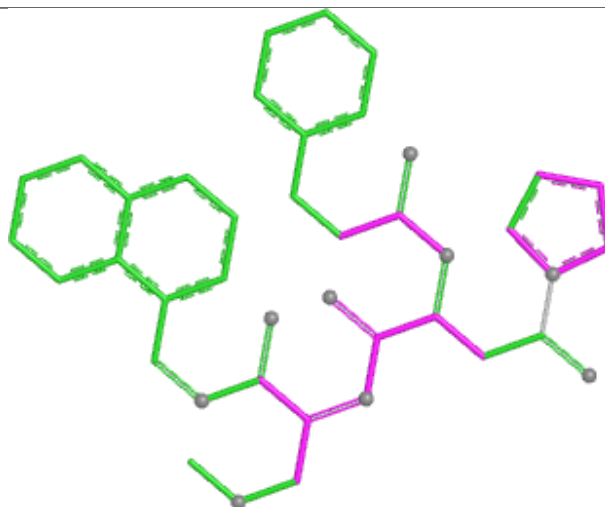
## Ligand 7J1 K 301



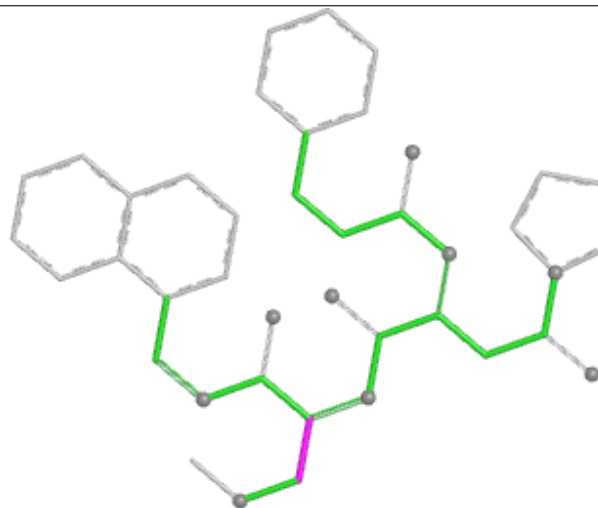
## Ligand 7J1 L 301



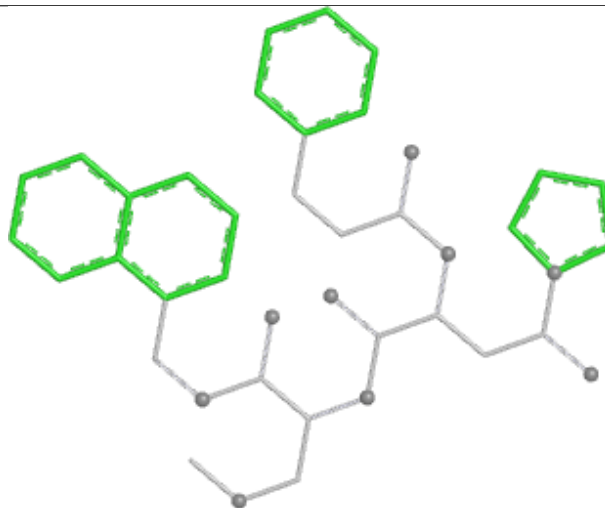
Bond lengths



Bond angles

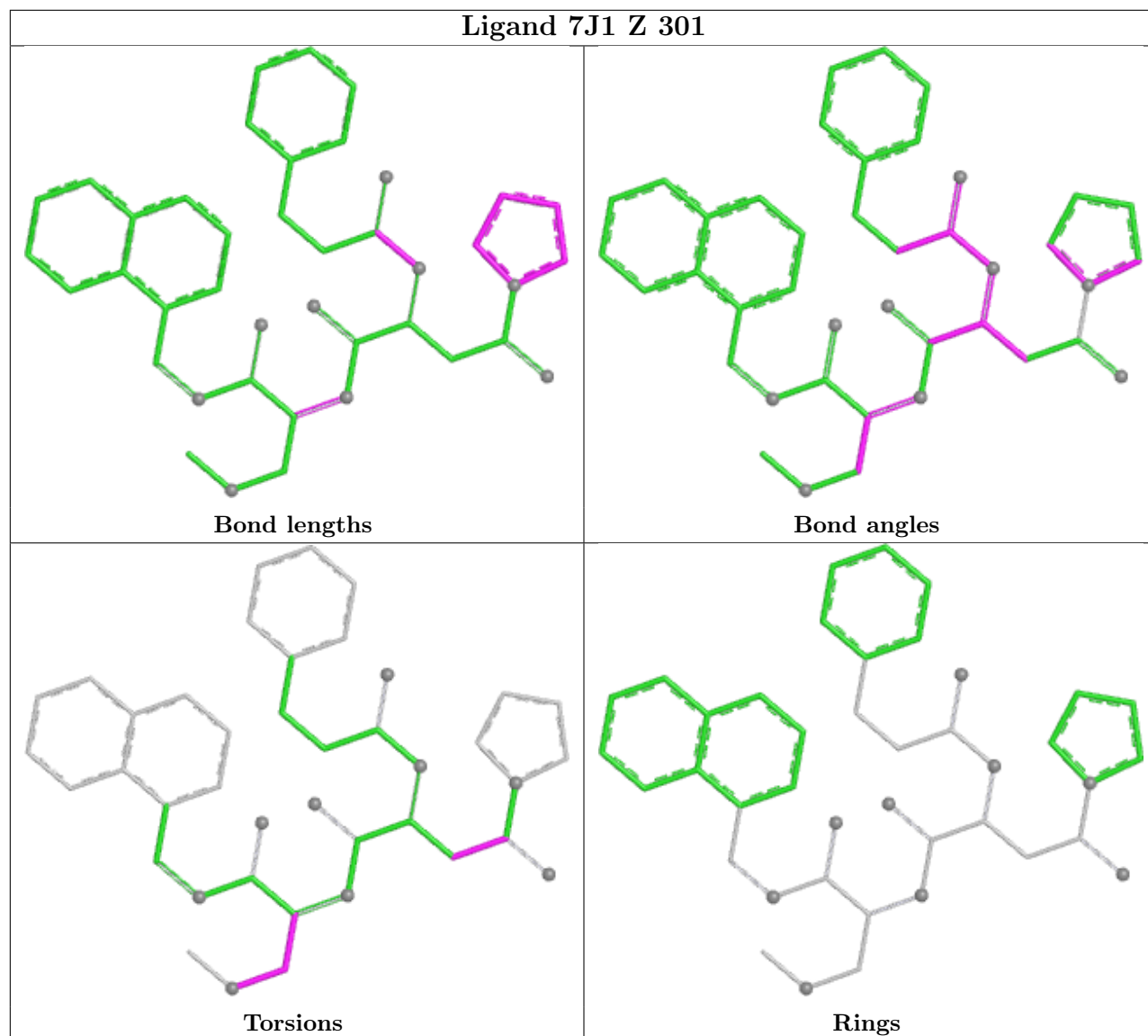


Torsions

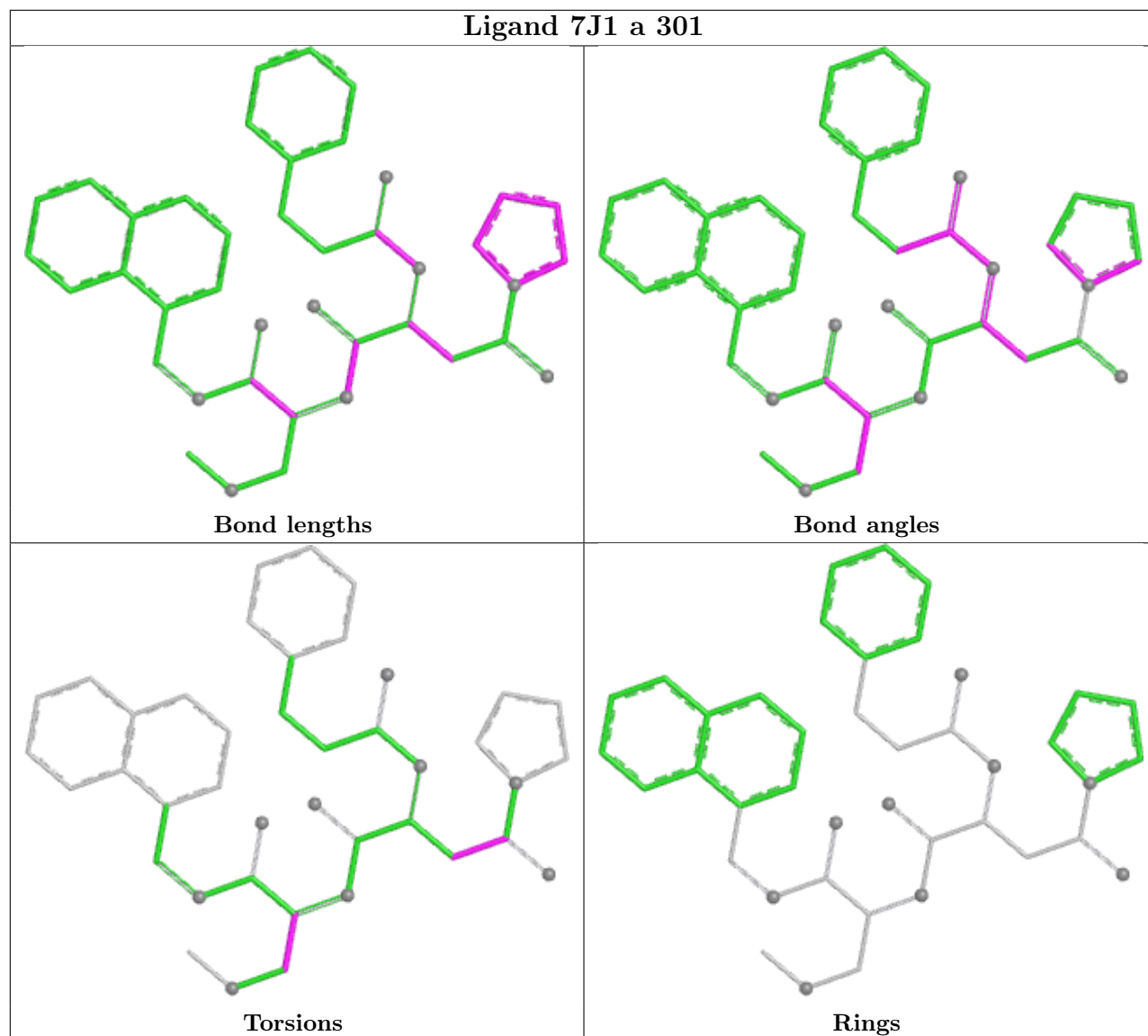


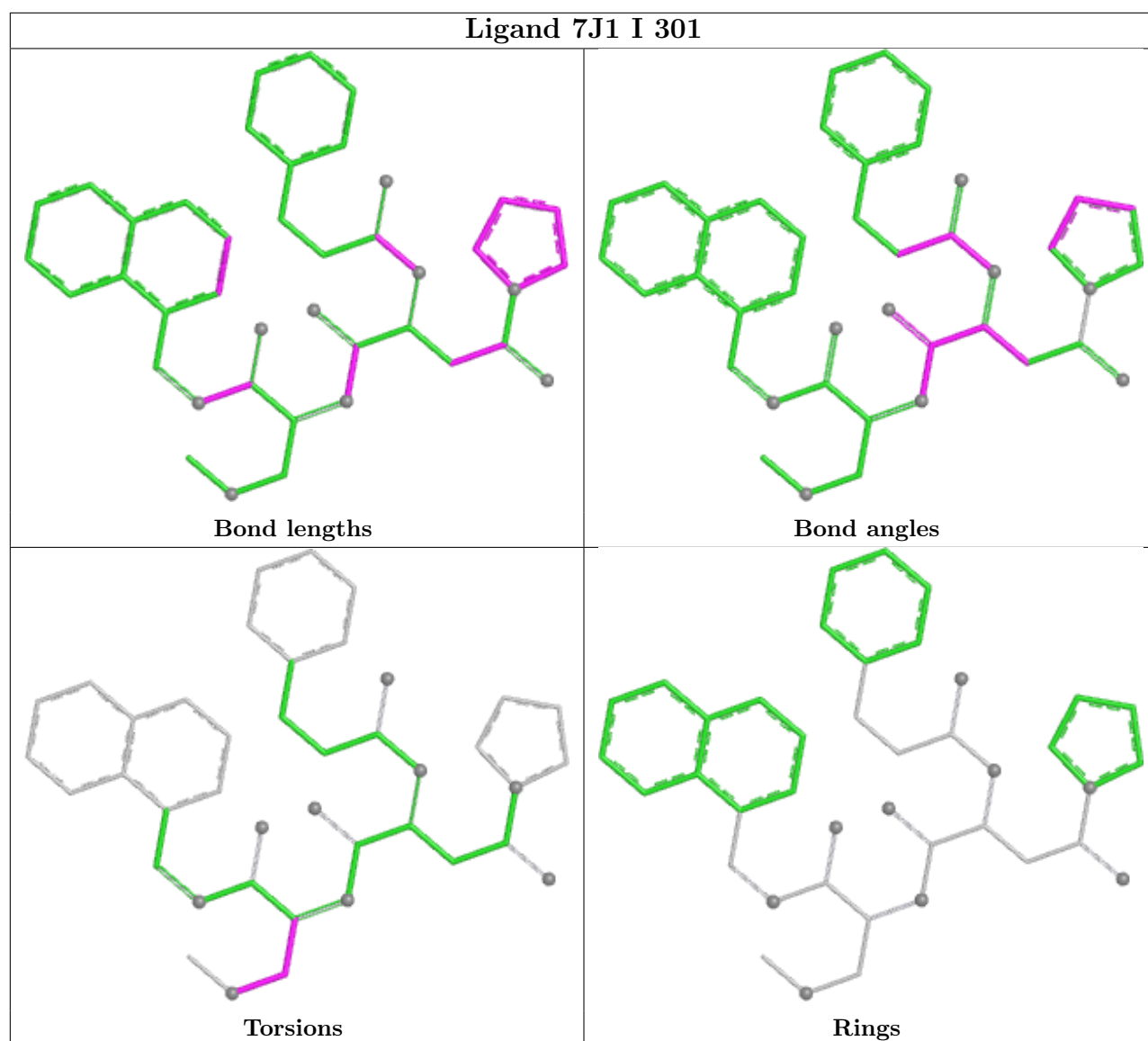
Rings

## Ligand 7J1 Z 301



## Ligand 7J1 a 301





## 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     | 218/240 (90%) | 0.19   | 5 (2%) 61 52  | 30, 50, 78, 104       | 0     |
| 1   | B     | 216/240 (90%) | 0.28   | 3 (1%) 73 67  | 34, 59, 93, 129       | 0     |
| 1   | C     | 217/240 (90%) | 0.42   | 5 (2%) 61 52  | 34, 63, 97, 118       | 0     |
| 1   | D     | 217/240 (90%) | 0.38   | 7 (3%) 50 40  | 34, 61, 91, 112       | 0     |
| 1   | E     | 218/240 (90%) | 0.26   | 5 (2%) 61 52  | 28, 59, 87, 129       | 0     |
| 1   | F     | 215/240 (89%) | 0.49   | 6 (2%) 55 45  | 34, 63, 93, 108       | 0     |
| 1   | G     | 220/240 (91%) | 0.13   | 4 (1%) 67 60  | 33, 53, 83, 103       | 0     |
| 1   | O     | 216/240 (90%) | 0.50   | 12 (5%) 30 23 | 30, 65, 99, 127       | 0     |
| 1   | P     | 218/240 (90%) | 0.30   | 5 (2%) 61 52  | 34, 58, 90, 117       | 0     |
| 1   | Q     | 218/240 (90%) | 0.09   | 3 (1%) 73 67  | 30, 53, 81, 124       | 0     |
| 1   | R     | 217/240 (90%) | 0.16   | 3 (1%) 73 67  | 30, 53, 81, 99        | 0     |
| 1   | S     | 218/240 (90%) | 0.07   | 3 (1%) 73 67  | 28, 50, 89, 104       | 0     |
| 1   | T     | 218/240 (90%) | 0.36   | 4 (1%) 67 60  | 33, 59, 91, 118       | 0     |
| 1   | U     | 217/240 (90%) | 0.10   | 3 (1%) 73 67  | 32, 52, 87, 105       | 0     |
| 2   | H     | 222/240 (92%) | -0.12  | 1 (0%) 87 85  | 30, 44, 67, 111       | 0     |
| 2   | I     | 222/240 (92%) | -0.19  | 2 (0%) 81 76  | 29, 40, 60, 77        | 0     |
| 2   | J     | 222/240 (92%) | -0.21  | 0 100 100     | 30, 42, 65, 103       | 0     |
| 2   | K     | 223/240 (92%) | 0.03   | 1 (0%) 88 87  | 28, 45, 66, 84        | 0     |
| 2   | L     | 223/240 (92%) | -0.01  | 2 (0%) 81 76  | 31, 43, 70, 95        | 0     |
| 2   | M     | 222/240 (92%) | -0.04  | 3 (1%) 73 67  | 30, 44, 68, 111       | 0     |
| 2   | N     | 223/240 (92%) | 0.13   | 3 (1%) 75 69  | 34, 49, 76, 115       | 0     |
| 2   | V     | 223/240 (92%) | -0.19  | 0 100 100     | 31, 41, 63, 79        | 0     |
| 2   | W     | 223/240 (92%) | -0.05  | 1 (0%) 88 87  | 30, 42, 67, 92        | 0     |
| 2   | X     | 222/240 (92%) | -0.22  | 0 100 100     | 29, 40, 64, 108       | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 2   | Y     | 223/240 (92%)   | 0.02   | 3 (1%) 75 69  | 28, 41, 63, 99        | 0     |
| 2   | Z     | 222/240 (92%)   | -0.09  | 1 (0%) 87 85  | 29, 42, 68, 95        | 0     |
| 2   | a     | 223/240 (92%)   | -0.06  | 1 (0%) 88 87  | 32, 46, 75, 99        | 0     |
| 2   | b     | 223/240 (92%)   | -0.16  | 2 (0%) 81 76  | 28, 42, 64, 97        | 0     |
| All | All   | 6159/6720 (91%) | 0.09   | 88 (1%) 73 67 | 28, 48, 86, 129       | 0     |

All (88) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | U     | 9   | MET  | 4.9  |
| 1   | A     | 183 | ILE  | 4.8  |
| 1   | O     | 235 | VAL  | 4.7  |
| 1   | P     | 235 | VAL  | 4.0  |
| 1   | F     | 204 | GLY  | 3.9  |
| 1   | U     | 235 | VAL  | 3.7  |
| 1   | D     | 203 | LEU  | 3.7  |
| 1   | F     | 234 | LEU  | 3.7  |
| 1   | E     | 153 | PHE  | 3.6  |
| 1   | G     | 193 | ALA  | 3.5  |
| 1   | O     | 162 | PRO  | 3.3  |
| 1   | E     | 202 | THR  | 3.3  |
| 1   | P     | 202 | THR  | 3.3  |
| 1   | C     | 235 | VAL  | 3.1  |
| 1   | A     | 202 | THR  | 3.1  |
| 1   | O     | 31  | VAL  | 3.0  |
| 1   | B     | 179 | ASP  | 3.0  |
| 1   | D     | 235 | VAL  | 3.0  |
| 2   | L     | 223 | GLY  | 2.9  |
| 1   | A     | 192 | SER  | 2.9  |
| 1   | C     | 11  | GLN  | 2.8  |
| 1   | D     | 175 | ALA  | 2.8  |
| 2   | N     | 223 | GLY  | 2.8  |
| 1   | Q     | 235 | VAL  | 2.7  |
| 1   | R     | 235 | VAL  | 2.7  |
| 2   | Y     | 106 | GLY  | 2.7  |
| 1   | D     | 44  | GLU  | 2.7  |
| 1   | Q     | 23  | GLY  | 2.6  |
| 2   | K     | 223 | GLY  | 2.6  |
| 2   | I     | 24  | ASN  | 2.6  |
| 1   | C     | 203 | LEU  | 2.6  |
| 1   | G     | 203 | LEU  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | N     | 115 | GLN  | 2.6  |
| 1   | G     | 202 | THR  | 2.6  |
| 1   | E     | 175 | ALA  | 2.6  |
| 1   | O     | 234 | LEU  | 2.6  |
| 1   | Q     | 44  | GLU  | 2.5  |
| 1   | F     | 205 | VAL  | 2.5  |
| 1   | P     | 165 | ASN  | 2.5  |
| 2   | N     | 163 | GLY  | 2.5  |
| 1   | A     | 30  | VAL  | 2.5  |
| 1   | T     | 202 | THR  | 2.4  |
| 1   | O     | 185 | VAL  | 2.4  |
| 1   | O     | 184 | ALA  | 2.4  |
| 1   | D     | 205 | VAL  | 2.3  |
| 1   | C     | 182 | ARG  | 2.3  |
| 2   | M     | 115 | GLN  | 2.3  |
| 2   | H     | 114 | PRO  | 2.3  |
| 1   | E     | 154 | VAL  | 2.3  |
| 2   | b     | 113 | ASP  | 2.3  |
| 1   | G     | 48  | ARG  | 2.3  |
| 1   | B     | 235 | VAL  | 2.3  |
| 2   | W     | 223 | GLY  | 2.3  |
| 2   | b     | 223 | GLY  | 2.3  |
| 1   | O     | 191 | GLY  | 2.2  |
| 1   | D     | 230 | LEU  | 2.2  |
| 1   | P     | 190 | ALA  | 2.2  |
| 1   | U     | 234 | LEU  | 2.2  |
| 1   | O     | 205 | VAL  | 2.2  |
| 1   | S     | 153 | PHE  | 2.2  |
| 1   | O     | 42  | VAL  | 2.2  |
| 2   | L     | 55  | PHE  | 2.2  |
| 1   | T     | 203 | LEU  | 2.1  |
| 1   | E     | 36  | ALA  | 2.1  |
| 1   | R     | 175 | ALA  | 2.1  |
| 2   | I     | 183 | GLY  | 2.1  |
| 2   | Y     | 158 | THR  | 2.1  |
| 1   | O     | 228 | SER  | 2.1  |
| 1   | S     | 192 | SER  | 2.1  |
| 1   | T     | 174 | ASN  | 2.1  |
| 1   | D     | 223 | ARG  | 2.1  |
| 1   | O     | 10  | GLU  | 2.1  |
| 1   | R     | 49  | SER  | 2.1  |
| 2   | M     | 206 | PRO  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | S     | 171 | TYR  | 2.1  |
| 1   | F     | 151 | PRO  | 2.0  |
| 1   | A     | 122 | LEU  | 2.0  |
| 1   | P     | 203 | LEU  | 2.0  |
| 1   | F     | 111 | PHE  | 2.0  |
| 1   | T     | 163 | ILE  | 2.0  |
| 2   | Y     | 112 | SER  | 2.0  |
| 1   | B     | 151 | PRO  | 2.0  |
| 1   | F     | 33  | LEU  | 2.0  |
| 1   | O     | 188 | LEU  | 2.0  |
| 1   | C     | 204 | GLY  | 2.0  |
| 2   | a     | 167 | ALA  | 2.0  |
| 2   | M     | 54  | GLU  | 2.0  |
| 2   | Z     | 161 | ASP  | 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | 7J1  | N     | 301 | 41/41 | 0.93 | 0.11 | 35,46,62,67                | 0     |
| 3   | 7J1  | b     | 301 | 41/41 | 0.93 | 0.11 | 27,36,53,66                | 0     |
| 3   | 7J1  | J     | 301 | 41/41 | 0.94 | 0.09 | 20,33,54,57                | 0     |
| 3   | 7J1  | X     | 301 | 41/41 | 0.94 | 0.10 | 29,36,57,63                | 0     |
| 3   | 7J1  | a     | 301 | 41/41 | 0.94 | 0.10 | 29,38,49,59                | 0     |
| 3   | 7J1  | K     | 301 | 41/41 | 0.94 | 0.10 | 39,50,63,72                | 0     |
| 3   | 7J1  | W     | 301 | 41/41 | 0.95 | 0.09 | 24,36,55,63                | 0     |
| 3   | 7J1  | M     | 301 | 41/41 | 0.95 | 0.10 | 30,37,53,58                | 0     |
| 3   | 7J1  | Y     | 301 | 41/41 | 0.95 | 0.09 | 21,38,57,63                | 0     |

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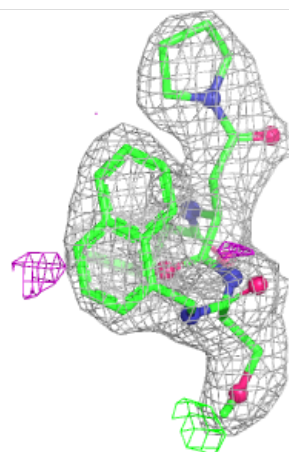
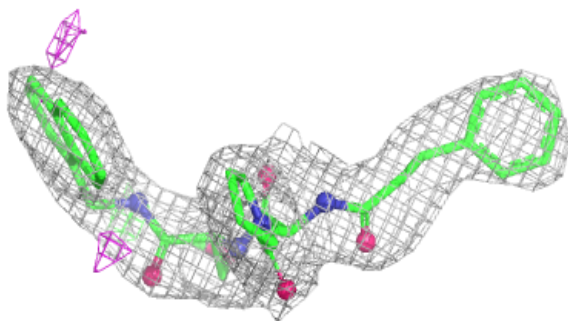
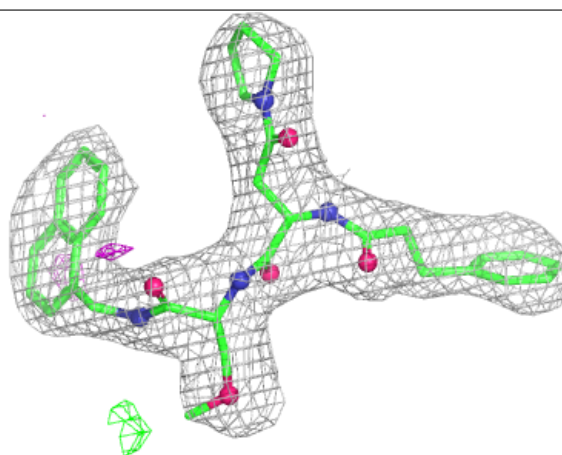
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | 7J1  | L     | 301 | 41/41 | 0.95 | 0.09 | 23,38,55,59                 | 0     |
| 3   | 7J1  | V     | 301 | 41/41 | 0.95 | 0.09 | 31,43,50,55                 | 0     |
| 3   | 7J1  | Z     | 301 | 41/41 | 0.96 | 0.09 | 29,38,53,60                 | 0     |
| 3   | 7J1  | I     | 301 | 41/41 | 0.96 | 0.09 | 25,38,47,54                 | 0     |
| 3   | 7J1  | H     | 301 | 41/41 | 0.96 | 0.08 | 24,36,51,63                 | 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.

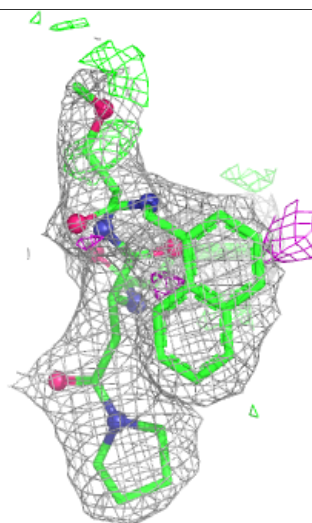
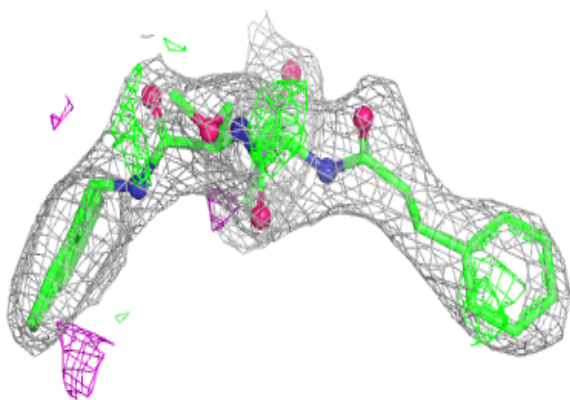
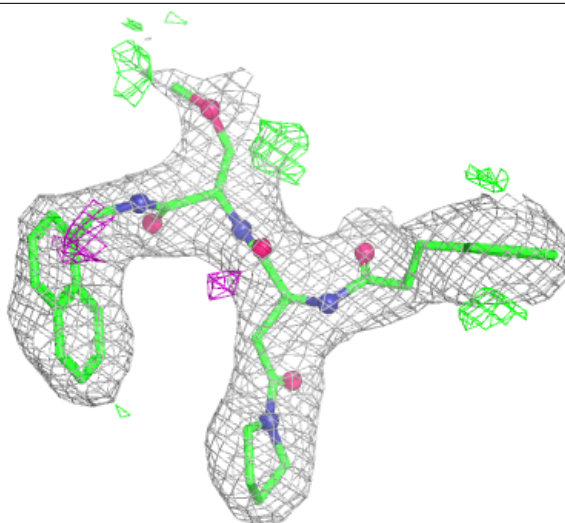
**Electron density around 7J1 N 301:**

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



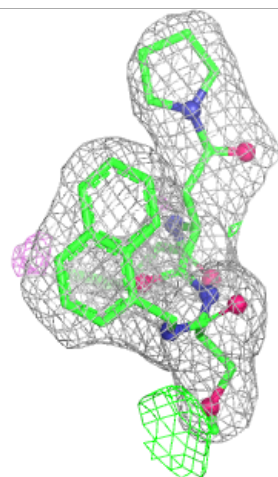
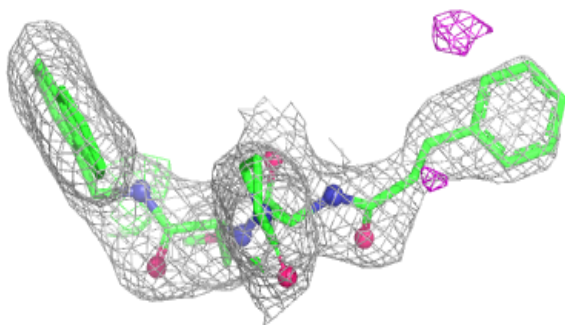
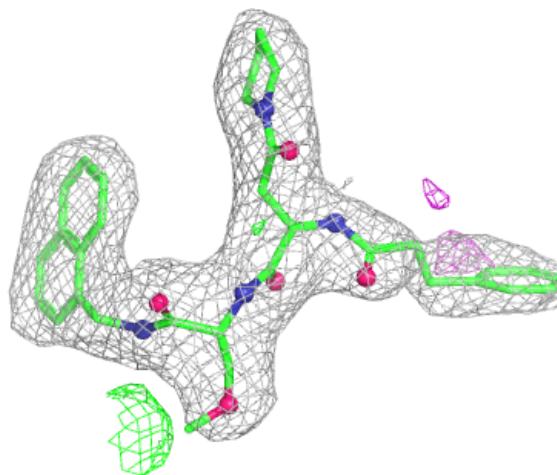
**Electron density around 7J1 b 301:**

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



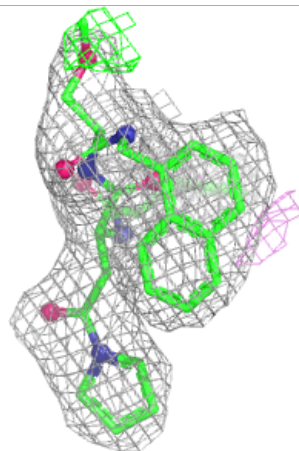
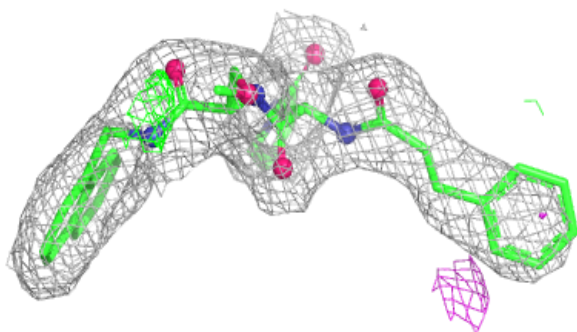
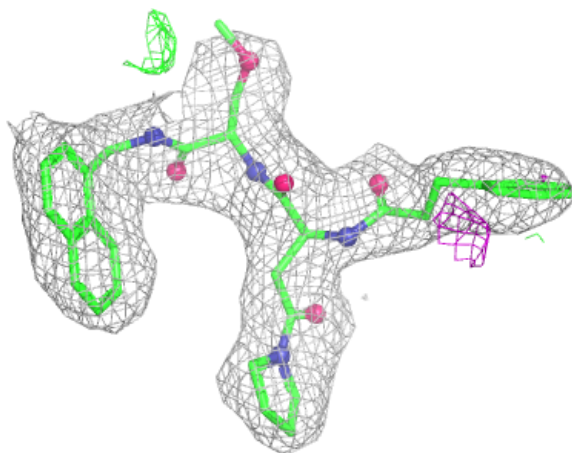
**Electron density around 7J1 J 301:**

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



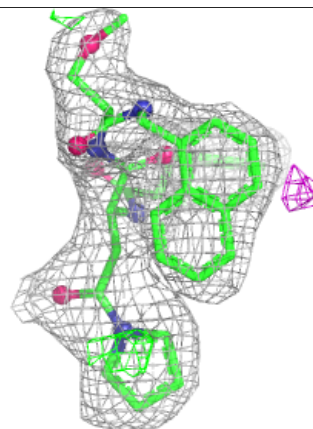
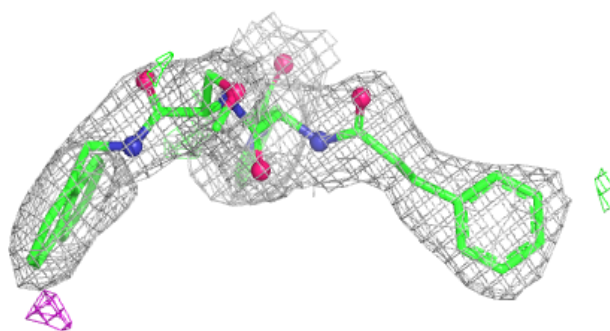
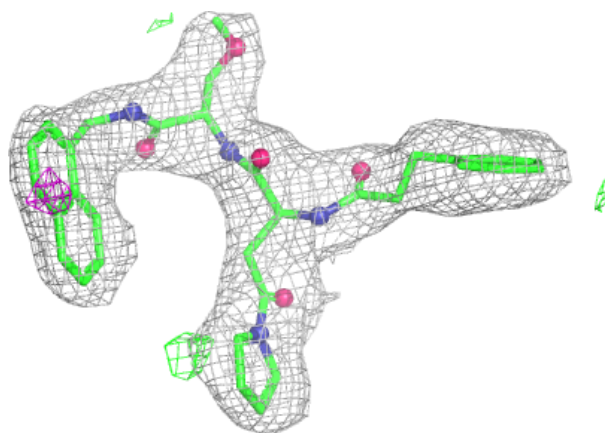
**Electron density around 7J1 X 301:**

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



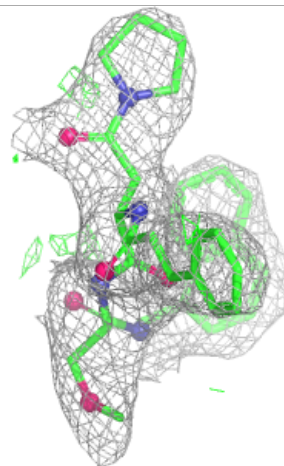
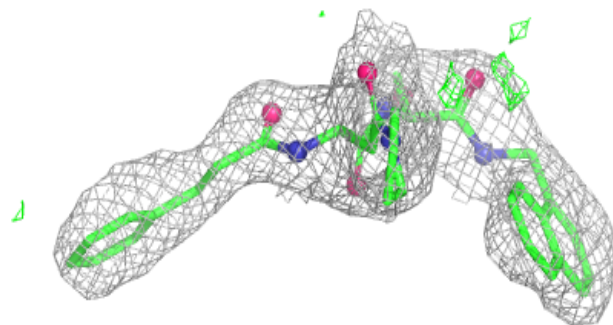
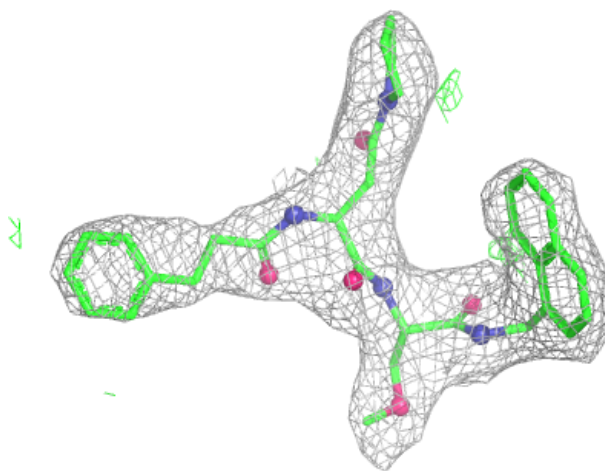
**Electron density around 7J1 a 301:**

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



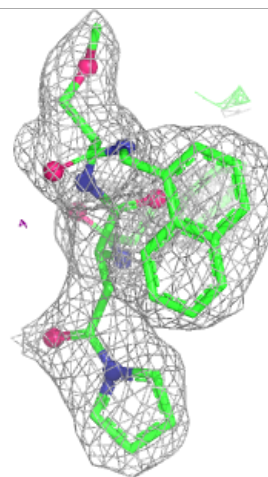
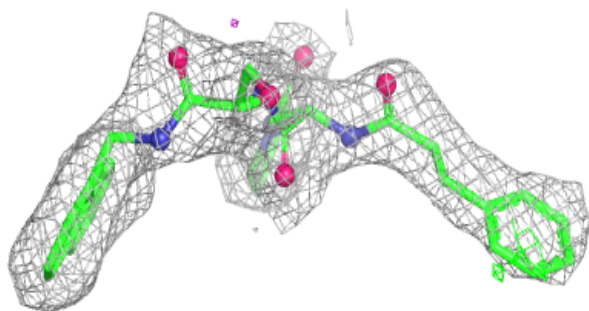
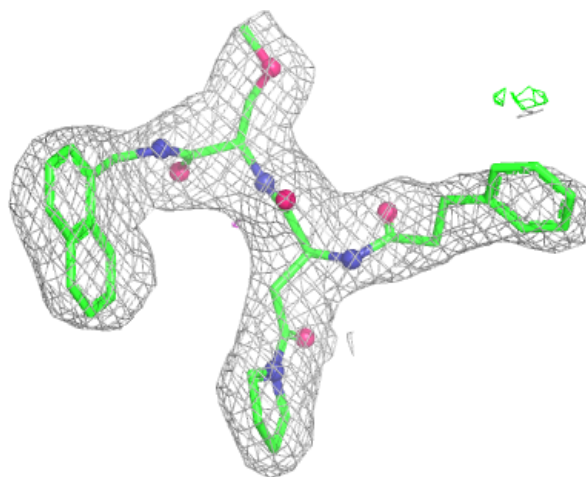
**Electron density around 7J1 K 301:**

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



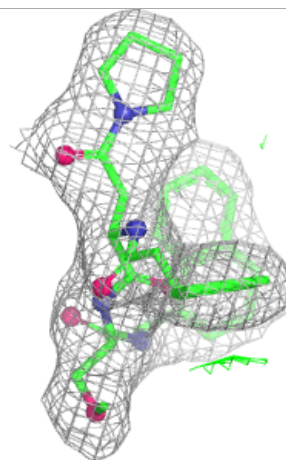
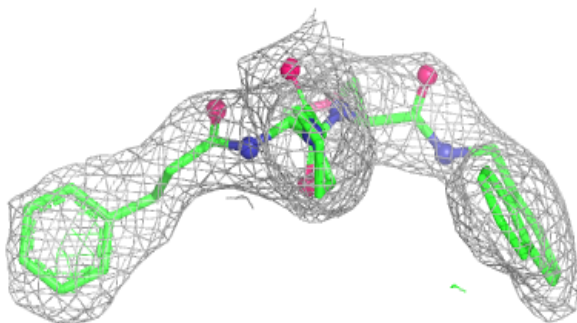
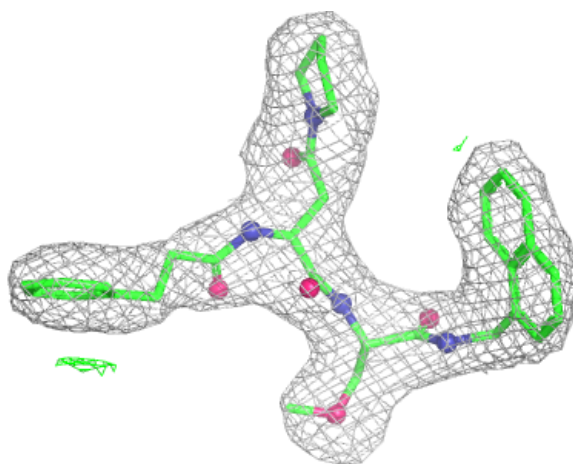
**Electron density around 7J1 W 301:**

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



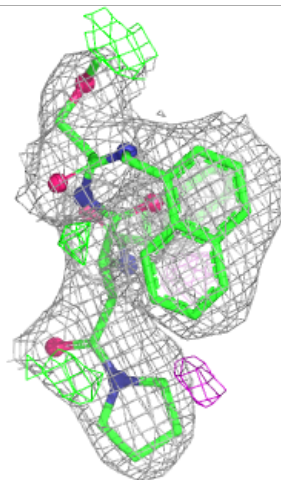
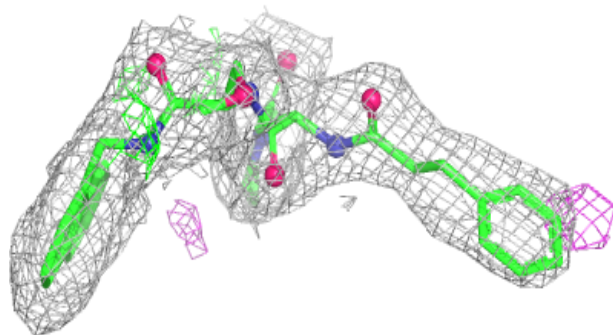
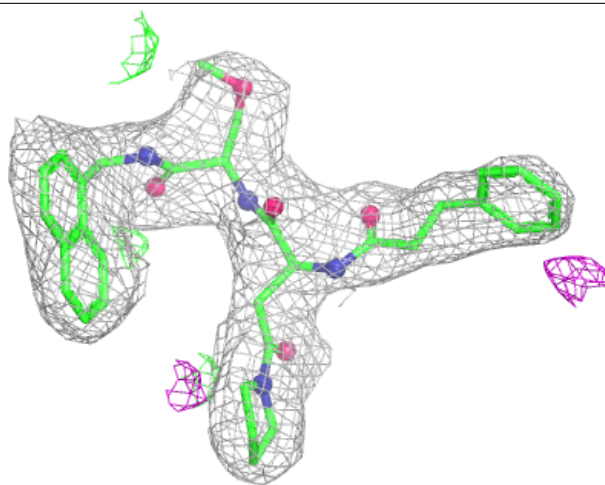
**Electron density around 7J1 M 301:**

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



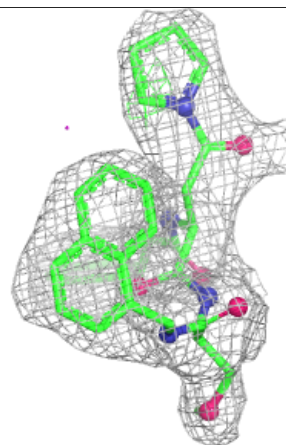
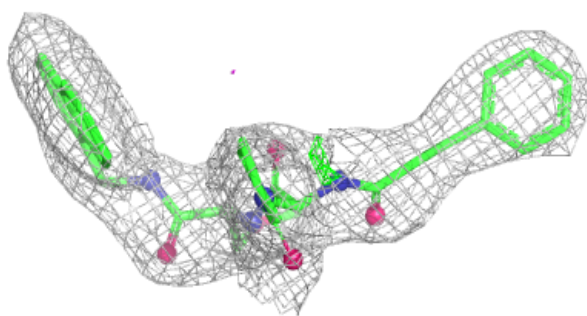
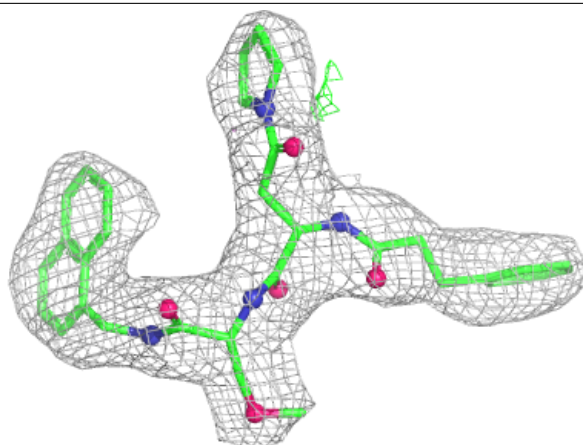
**Electron density around 7J1 Y 301:**

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



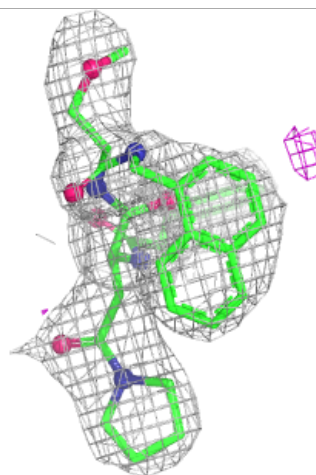
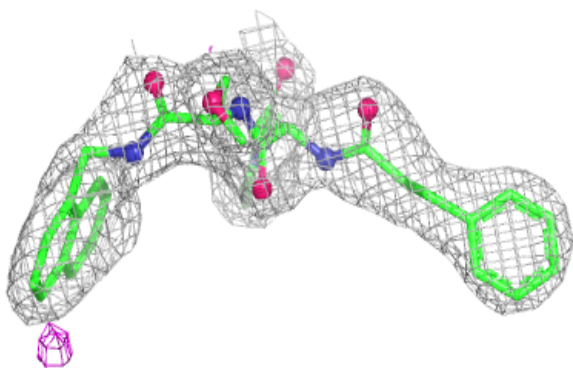
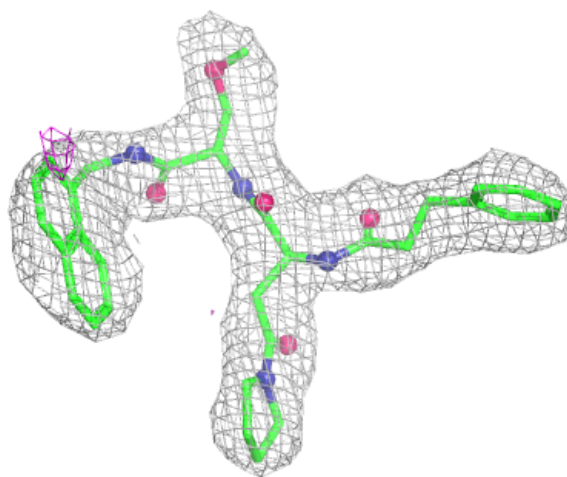
**Electron density around 7J1 L 301:**

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



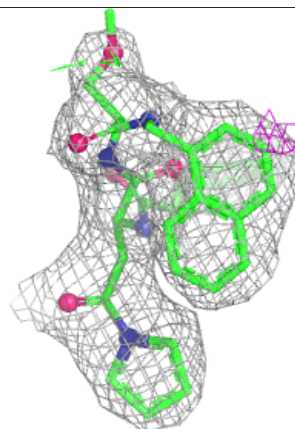
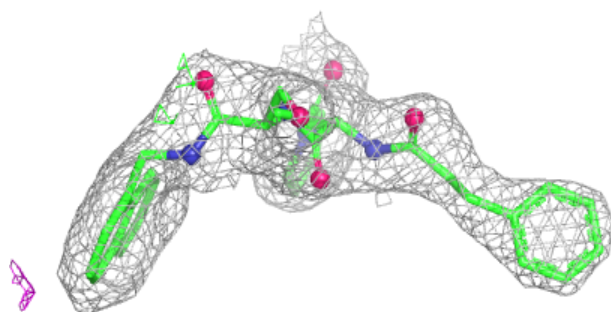
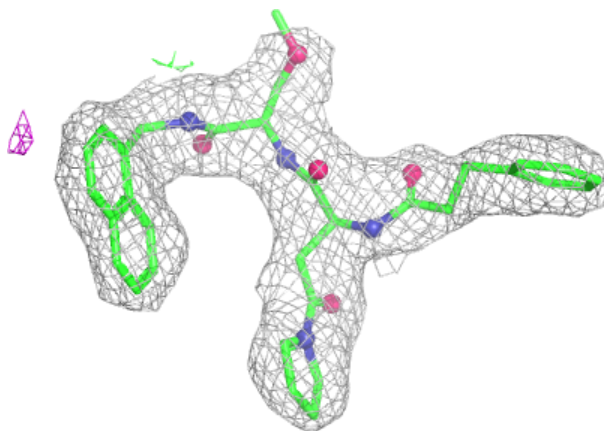
**Electron density around 7J1 V 301:**

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



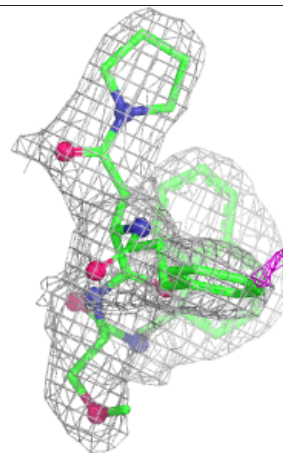
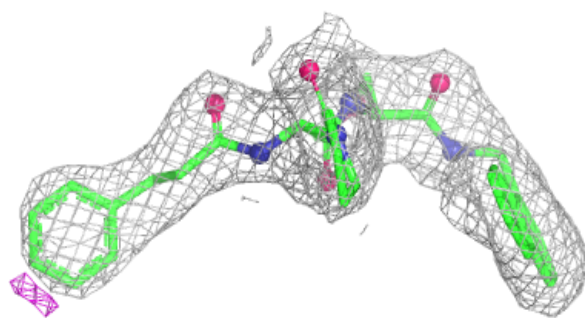
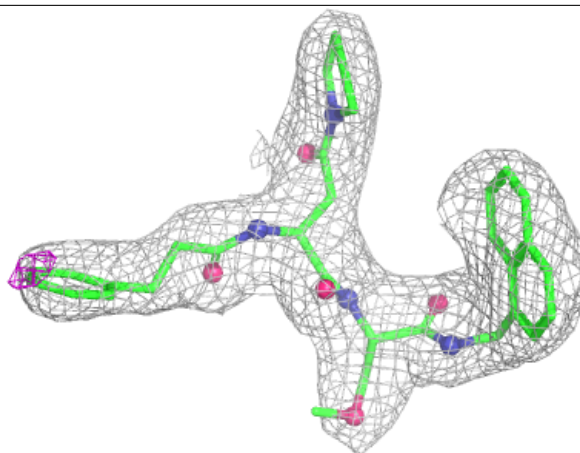
**Electron density around 7J1 Z 301:**

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



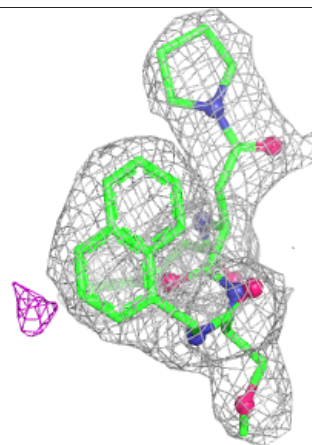
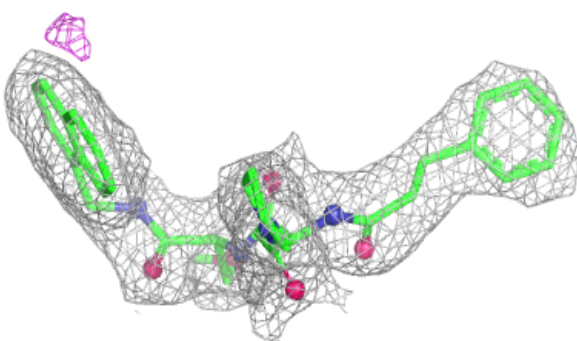
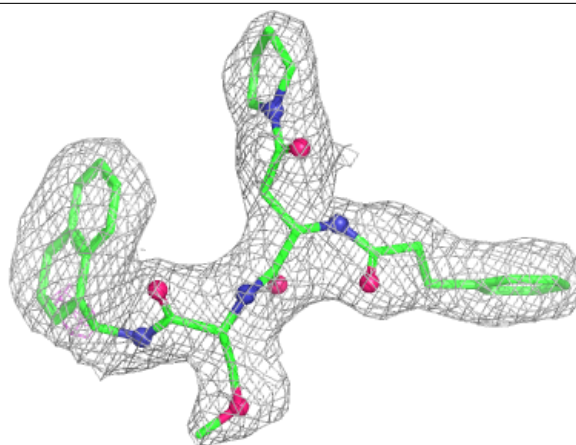
**Electron density around 7J1 I 301:**

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



**Electron density around 7J1 H 301:**

$2mF_o-DF_c$  (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.