



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:10 PM UTC

PDB ID : 6YFE / pdb\_00006yfe  
Title : Virus-like particle of Beihai levi-like virus 19  
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.  
Deposited on : 2020-03-26  
Resolution : 3.79 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                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

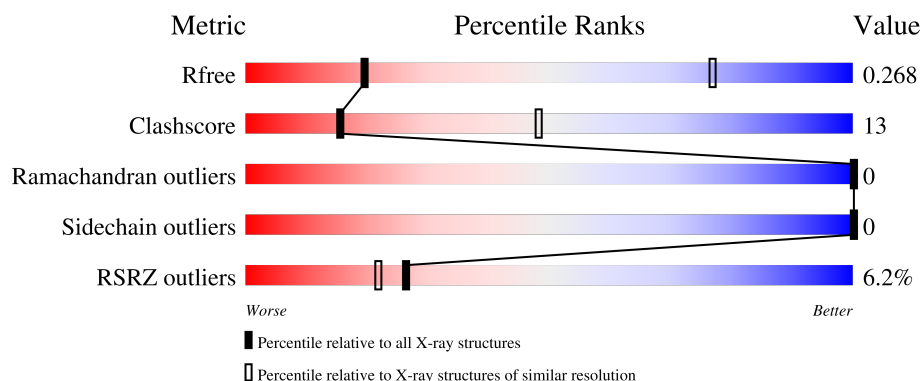
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.79 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1065 (3.96-3.64)                                      |
| Clashscore            | 190562                      | 1012 (3.94-3.66)                                      |
| Ramachandran outliers | 187476                      | 1048 (3.96-3.64)                                      |
| Sidechain outliers    | 187428                      | 1043 (3.96-3.64)                                      |
| RSRZ outliers         | 180081                      | 1064 (3.96-3.64)                                      |

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   | AA    | 134    | <div> <div>3%</div> <div>74%</div> <div>26%</div> </div>               |
| 1   | AB    | 134    | <div> <div>7%</div> <div>65%</div> <div>27%</div> <div>8%</div> </div> |
| 1   | AC    | 134    | <div> <div>7%</div> <div>71%</div> <div>29%</div> </div>               |
| 1   | AD    | 134    | <div> <div>9%</div> <div>81%</div> <div>19%</div> </div>               |
| 1   | AE    | 134    | <div> <div>6%</div> <div>63%</div> <div>29%</div> <div>8%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AF    | 134    |                  |
| 1   | AG    | 134    |                  |
| 1   | AH    | 134    |                  |
| 1   | AI    | 134    |                  |
| 1   | AJ    | 134    |                  |
| 1   | AK    | 134    |                  |
| 1   | AL    | 134    |                  |
| 1   | AM    | 134    |                  |
| 1   | AN    | 134    |                  |
| 1   | AO    | 134    |                  |
| 1   | AP    | 134    |                  |
| 1   | AQ    | 134    |                  |
| 1   | AR    | 134    |                  |
| 1   | AS    | 134    |                  |
| 1   | AT    | 134    |                  |
| 1   | AU    | 134    |                  |
| 1   | AV    | 134    |                  |
| 1   | AW    | 134    |                  |
| 1   | AX    | 134    |                  |
| 1   | AY    | 134    |                  |
| 1   | AZ    | 134    |                  |
| 1   | BA    | 134    |                  |
| 1   | BB    | 134    |                  |
| 1   | BC    | 134    |                  |
| 1   | BD    | 134    |                  |

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| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | BE    | 134    | <div> <div>4%</div> <div>74%</div> <div>26%</div> </div>               |
| 1   | BF    | 134    | <div> <div>7%</div> <div>66%</div> <div>25%</div> <div>8%</div> </div> |
| 1   | BG    | 134    | <div> <div>11%</div> <div>68%</div> <div>32%</div> </div>              |
| 1   | BH    | 134    | <div> <div>8%</div> <div>72%</div> <div>28%</div> </div>               |
| 1   | BI    | 134    | <div> <div>4%</div> <div>66%</div> <div>25%</div> <div>8%</div> </div> |
| 1   | BJ    | 134    | <div> <div>4%</div> <div>70%</div> <div>30%</div> </div>               |
| 1   | BK    | 134    | <div> <div>9%</div> <div>75%</div> <div>25%</div> </div>               |
| 1   | BL    | 134    | <div> <div>3%</div> <div>72%</div> <div>20%</div> <div>8%</div> </div> |
| 1   | BM    | 134    | <div> <div>3%</div> <div>78%</div> <div>22%</div> </div>               |
| 1   | BN    | 134    | <div> <div>2%</div> <div>75%</div> <div>25%</div> </div>               |
| 1   | BO    | 134    | <div> <div>4%</div> <div>66%</div> <div>26%</div> <div>8%</div> </div> |
| 1   | BP    | 134    | <div> <div>6%</div> <div>68%</div> <div>32%</div> </div>               |
| 1   | BQ    | 134    | <div> <div>4%</div> <div>74%</div> <div>26%</div> </div>               |
| 1   | BR    | 134    | <div> <div>6%</div> <div>66%</div> <div>26%</div> <div>8%</div> </div> |
| 1   | BS    | 134    | <div> <div>6%</div> <div>69%</div> <div>31%</div> </div>               |
| 1   | BT    | 134    | <div> <div>7%</div> <div>73%</div> <div>27%</div> </div>               |
| 1   | BU    | 134    | <div> <div>6%</div> <div>66%</div> <div>25%</div> <div>8%</div> </div> |
| 1   | BV    | 134    | <div> <div>10%</div> <div>69%</div> <div>31%</div> </div>              |
| 1   | BW    | 134    | <div> <div>7%</div> <div>74%</div> <div>26%</div> </div>               |
| 1   | BX    | 134    | <div> <div>4%</div> <div>63%</div> <div>29%</div> <div>8%</div> </div> |
| 1   | BY    | 134    | <div> <div>4%</div> <div>63%</div> <div>37%</div> </div>               |
| 1   | BZ    | 134    | <div> <div>4%</div> <div>80%</div> <div>20%</div> </div>               |
| 1   | CA    | 134    | <div> <div>7%</div> <div>66%</div> <div>25%</div> <div>8%</div> </div> |
| 1   | CB    | 134    | <div> <div>7%</div> <div>69%</div> <div>31%</div> </div>               |
| 1   | CC    | 134    | <div> <div>%</div> <div>72%</div> <div>28%</div> </div>                |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | CD    | 134    |                  |
| 1   | CE    | 134    |                  |
| 1   | CF    | 134    |                  |
| 1   | CG    | 134    |                  |
| 1   | CH    | 134    |                  |
| 1   | CI    | 134    |                  |
| 1   | CJ    | 134    |                  |
| 1   | CK    | 134    |                  |
| 1   | CL    | 134    |                  |
| 1   | CM    | 134    |                  |
| 1   | CN    | 134    |                  |
| 1   | CO    | 134    |                  |
| 1   | CP    | 134    |                  |
| 1   | CQ    | 134    |                  |
| 1   | CR    | 134    |                  |
| 1   | CS    | 134    |                  |
| 1   | CT    | 134    |                  |
| 1   | CU    | 134    |                  |
| 1   | CV    | 134    |                  |
| 1   | CW    | 134    |                  |
| 1   | CX    | 134    |                  |
| 1   | CY    | 134    |                  |
| 1   | CZ    | 134    |                  |
| 1   | DA    | 134    |                  |
| 1   | DB    | 134    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | DC    | 134    |                  |
| 1   | DD    | 134    |                  |
| 1   | DE    | 134    |                  |
| 1   | DF    | 134    |                  |
| 1   | DG    | 134    |                  |
| 1   | DH    | 134    |                  |
| 1   | DI    | 134    |                  |
| 1   | DJ    | 134    |                  |
| 1   | DK    | 134    |                  |
| 1   | DL    | 134    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 89070 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 coat protein.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 1   | AA    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AB    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | AC    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AD    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AE    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | AF    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AG    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AH    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | AI    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AJ    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AK    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | AL    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AM    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AN    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | AO    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AP    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 1   | AQ    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | AR    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AS    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AT    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | AU    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AV    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AW    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | AX    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AY    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | AZ    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BA    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BB    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BC    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BD    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BE    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BF    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BG    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BH    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BI    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BJ    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BK    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 1   | BL    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BM    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BN    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BO    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BP    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BQ    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BR    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BS    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BT    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BU    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BV    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BW    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BX    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | BY    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | BZ    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CA    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CB    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CC    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CD    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CE    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CF    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 1   | CG    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CH    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CI    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CJ    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CK    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CL    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CM    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CN    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CO    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CP    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CQ    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CR    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CS    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CT    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CU    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CV    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CW    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CX    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | CY    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | CZ    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | DA    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 1   | DB    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | DC    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | DD    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | DE    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | DF    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | DG    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | DH    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | DI    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | DJ    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |
| 1   | DK    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 599 | 162 | 179 |         |         |       |
| 1   | DL    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 642 | 174 | 198 |         |         |       |

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | AA    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | AB    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | AC    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | AE    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | AF    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | AG    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | AH    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | AK    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | AM    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AN    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AQ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AW    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BB    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BC    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BH    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BI    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BL    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BR    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BT    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BX    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CC    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CD    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CJ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CS    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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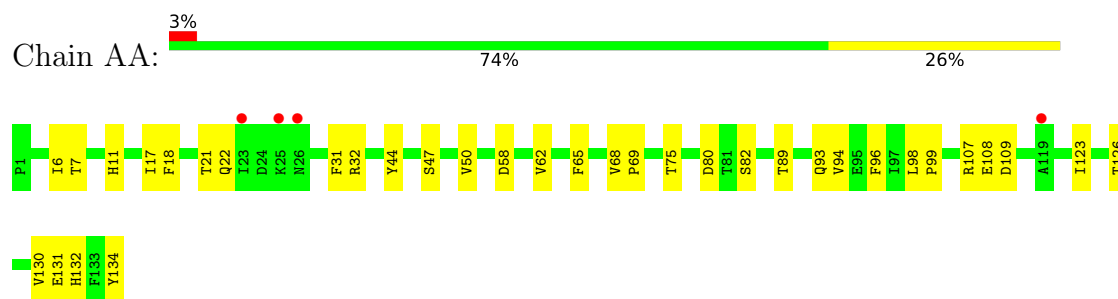
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | CV    | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

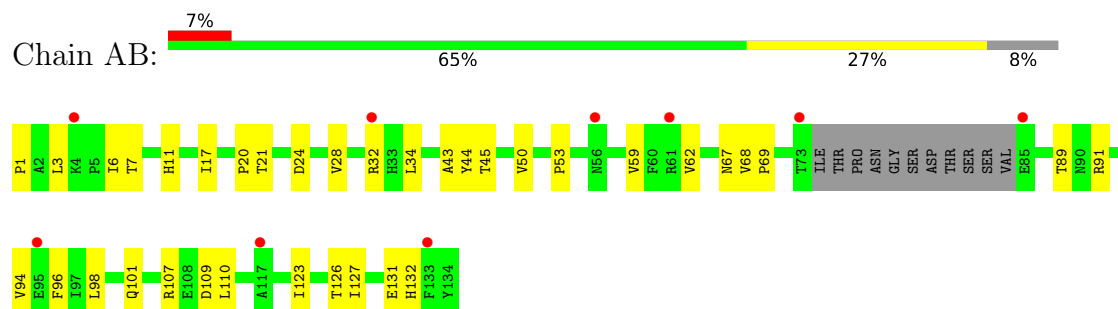
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

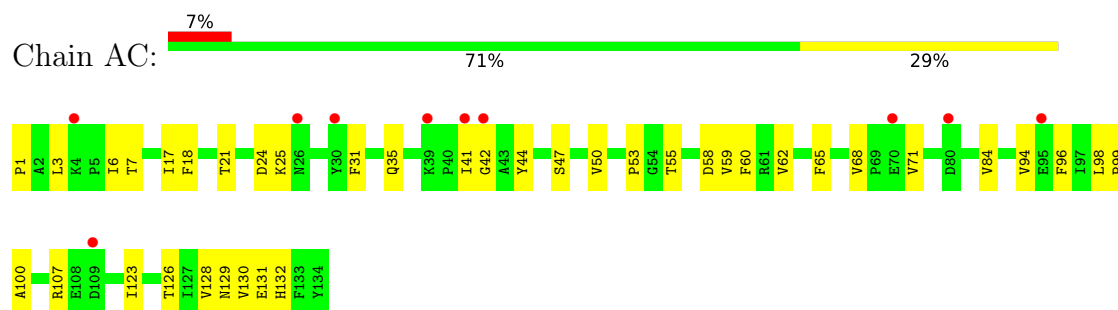
- Molecule 1: coat protein



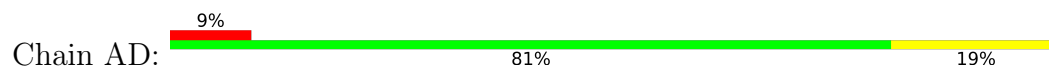
- Molecule 1: coat protein

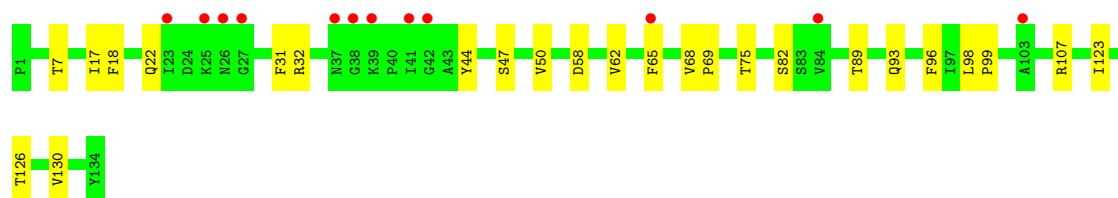


- Molecule 1: coat protein

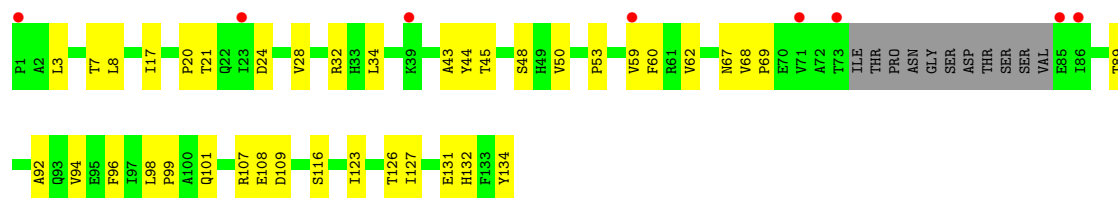


- Molecule 1: coat protein

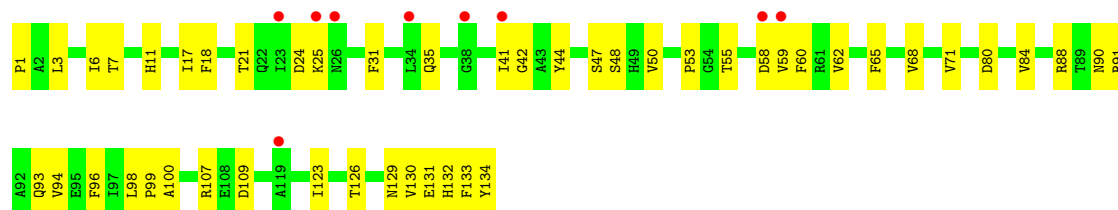




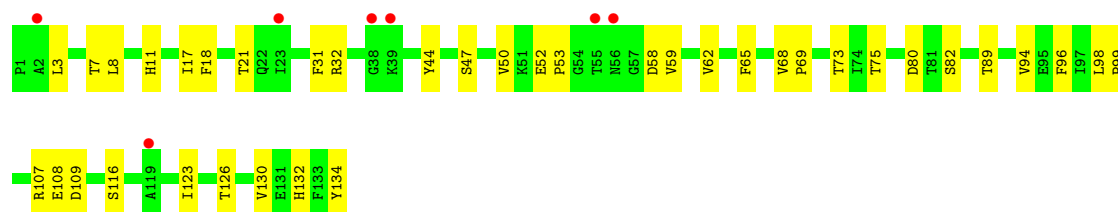
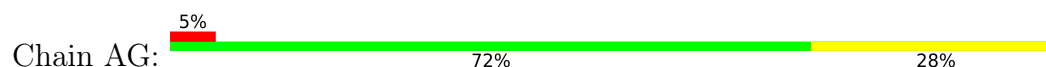
- Molecule 1: coat protein



- Molecule 1: coat protein



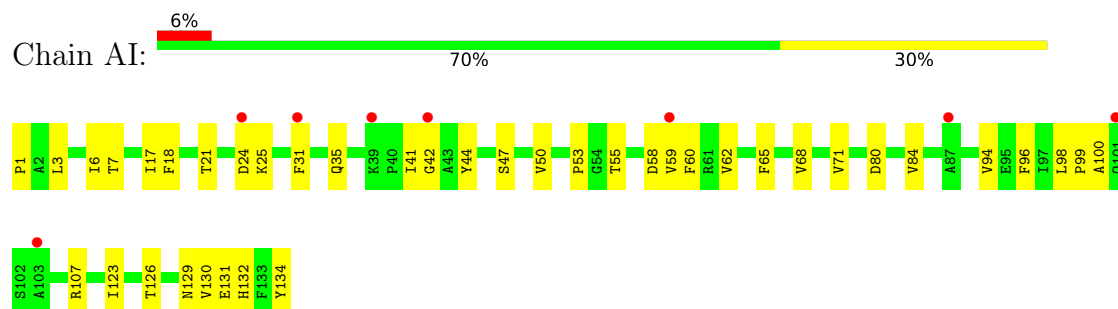
- Molecule 1: coat protein



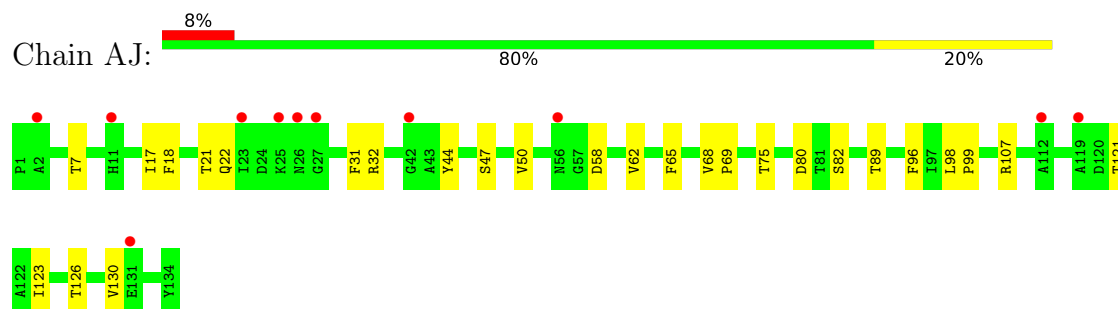
- Molecule 1: coat protein



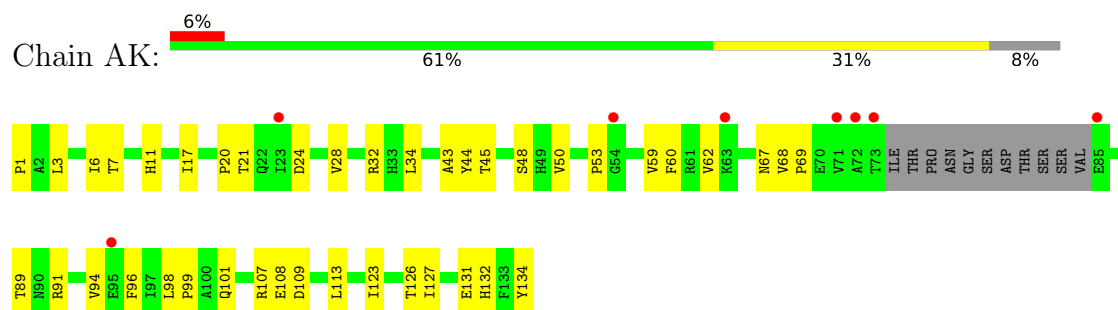
- Molecule 1: coat protein



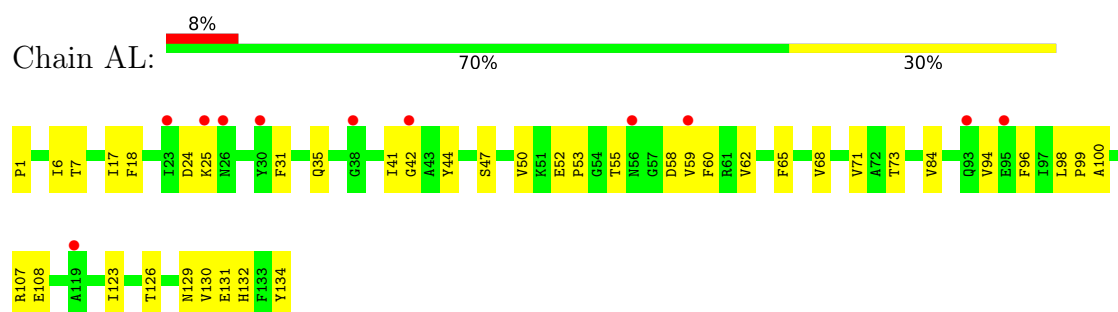
- Molecule 1: coat protein



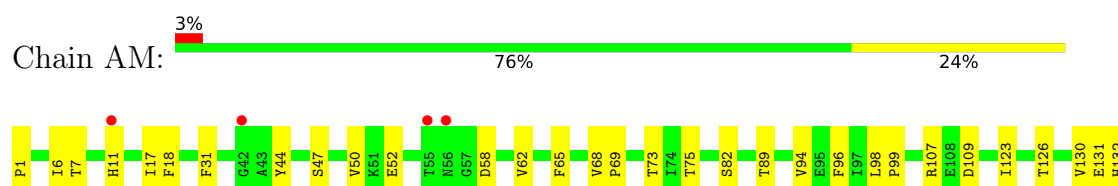
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



F133  
Y134

- Molecule 1: coat protein

Chain AN: 

P1 A2 L3 I6 T7 I17 P20 T21 T24 V28 R32 R33 L34 A43 Y44 T45 V50 P53 N56 V59 F60 R61 V62 N67 V68 P69 T73 ILE THR PRO ASN GLY ASP THR SER SER SER VAL E85 I86 A87 R88 T89 V94 E95 F96

I97 L98 Q101 R107 E108 D109 I123 T126 I127 E131 F133 Y134

- Molecule 1: coat protein

Chain AO: 

P1 A2 L3 T7 I17 F18 Q21 Q22 I23 D24 K25 F31 Q35 I41 Q42 A43 Y44 S47 V50 P53 G54 T55 N56 G57 D58 V59 F60 R61 V62 F65 V68 V71 D80 V84 F96 I97 L98 P99 A100 R107 A119 I123

T126 V130 Y134

- Molecule 1: coat protein

Chain AP: 

P1 A2 L3 K4 T7 L8 H11 I17 F18 T21 Q22 I23 D24 K25 N26 Y30 F31 R32 I41 Y44 S47 V50 G54 E52 N56 G57 D58 V62 F65 V68 P69 T73 I74 T75 P76 N77 G78 S79 D80 T81 S82 T89 V94 E95

F96 I97 L98 P99 R107 E108 S116 A119 I123 T126 V130 E131 H132 F133 Y134

- Molecule 1: coat protein

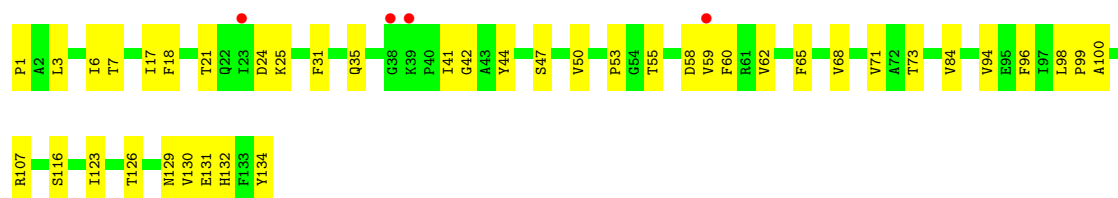
Chain AQ: 

P1 A2 L3 I6 T7 H11 I17 P20 T21 Q22 I23 D24 V28 R32 R33 L34 A43 Y44 T45 V50 R51 E52 P53 G54 T55 N56 V59 F60 R61 V62 N67 V68 P69 E70 A72 T73 ILE THR PRO ASN GLY SER ASP THR SER SER VAL E85

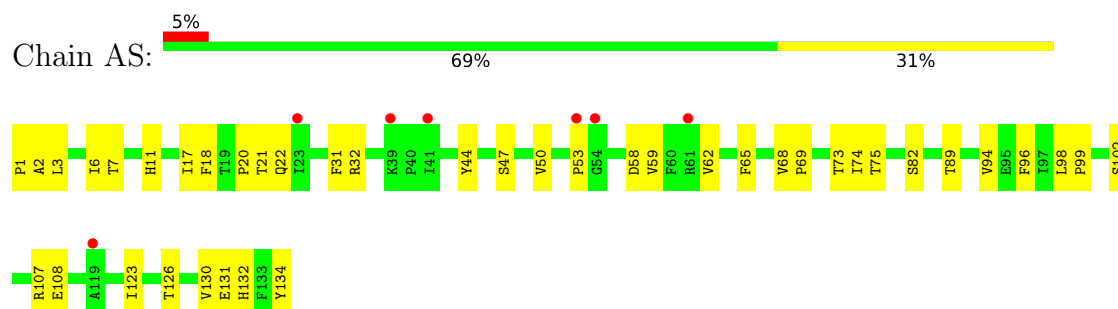
T89 N90 R91 V94 E95 F96 I97 L98 Q101 T105 V106 R107 E108 D109 I123 T126 I127 H132 F133 Y134

- Molecule 1: coat protein

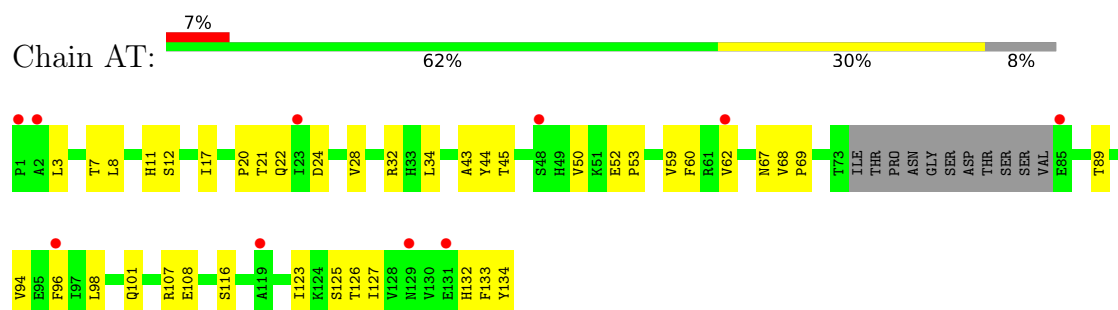
Chain AR: 



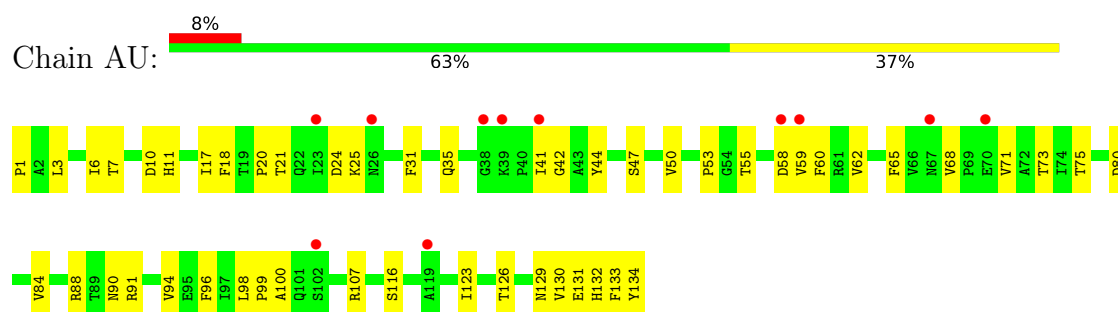
- Molecule 1: coat protein



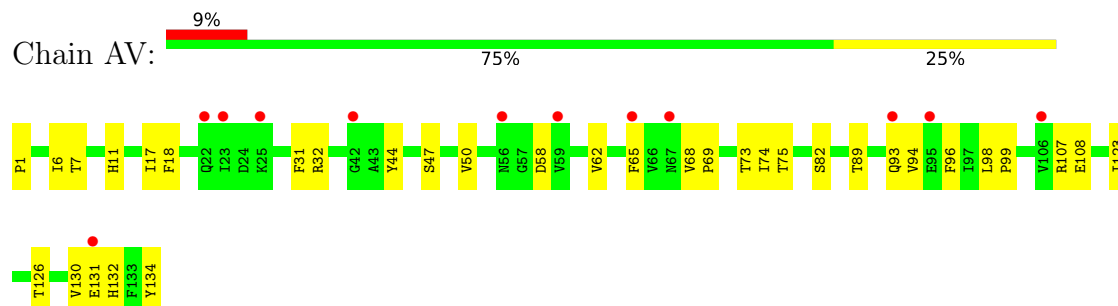
- Molecule 1: coat protein



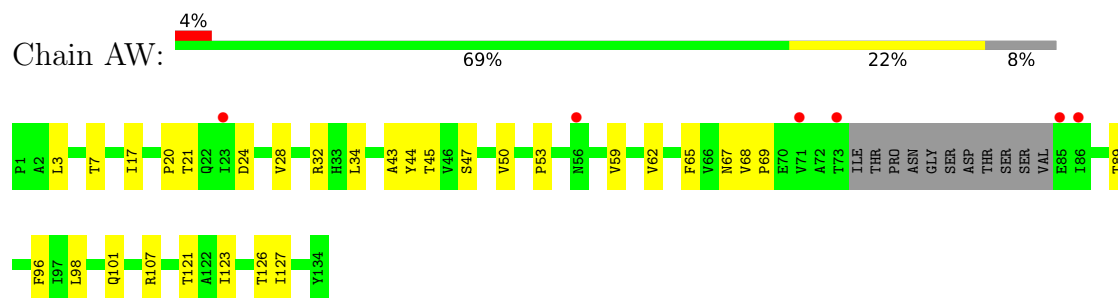
- Molecule 1: coat protein



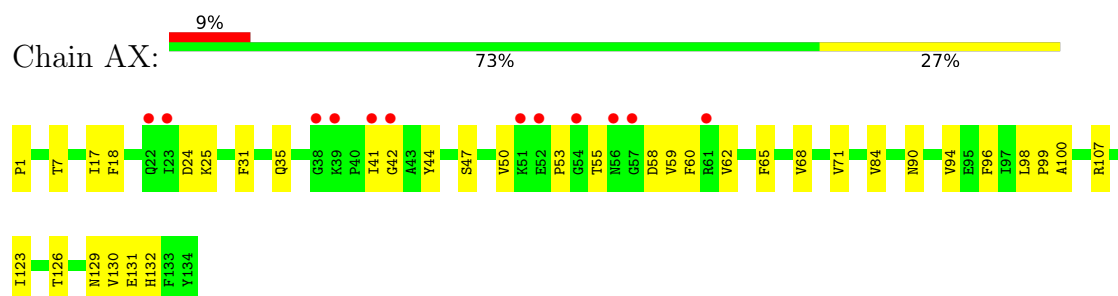
- Molecule 1: coat protein



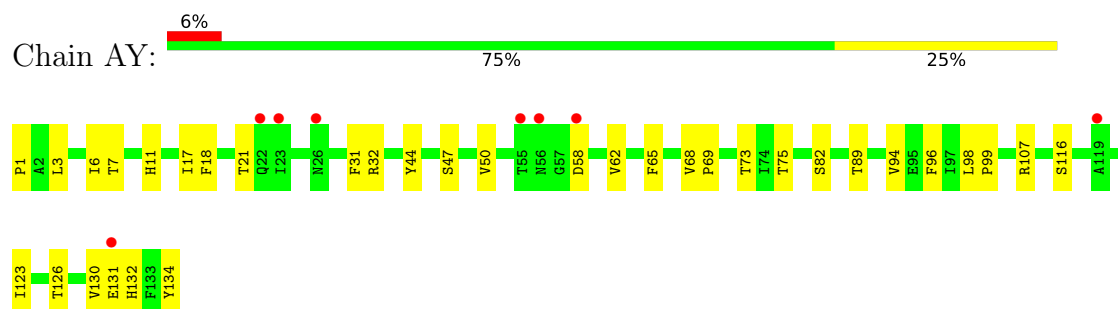
## • Molecule 1: coat protein



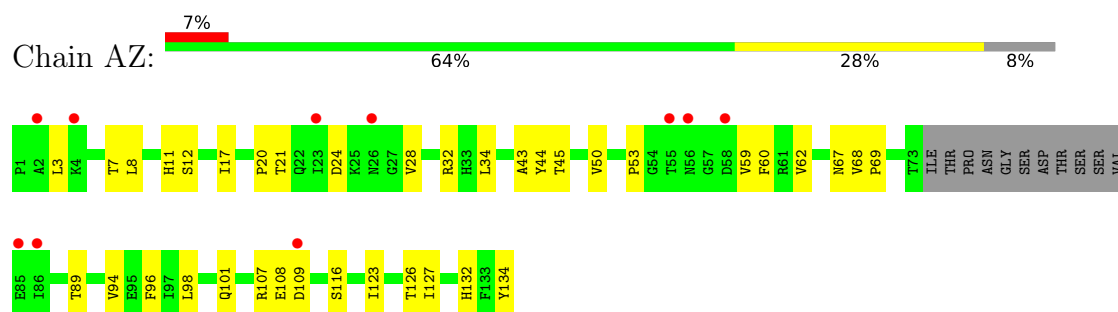
## • Molecule 1: coat protein



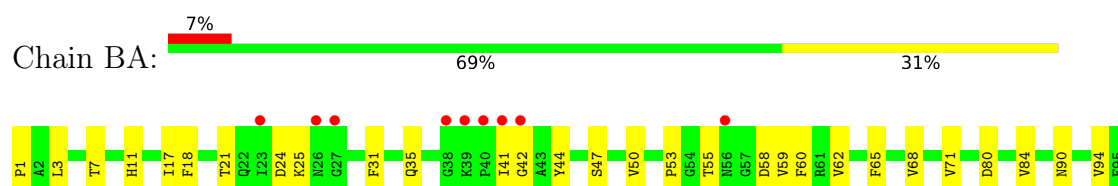
## • Molecule 1: coat protein



## • Molecule 1: coat protein

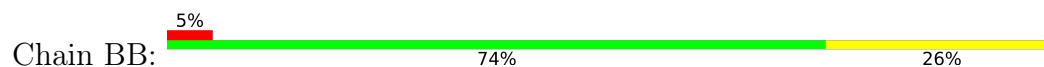


## • Molecule 1: coat protein





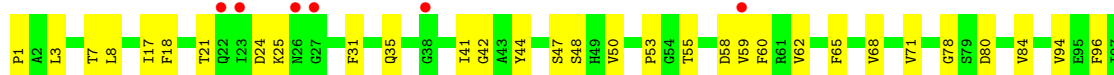
- Molecule 1: coat protein



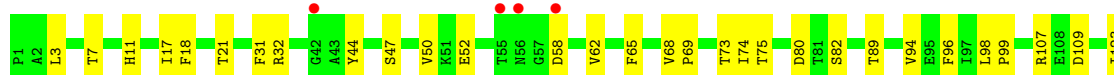
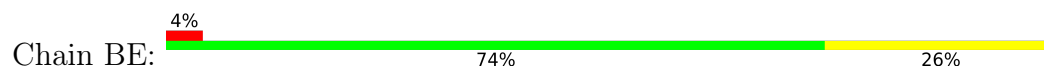
- Molecule 1: coat protein



- Molecule 1: coat protein

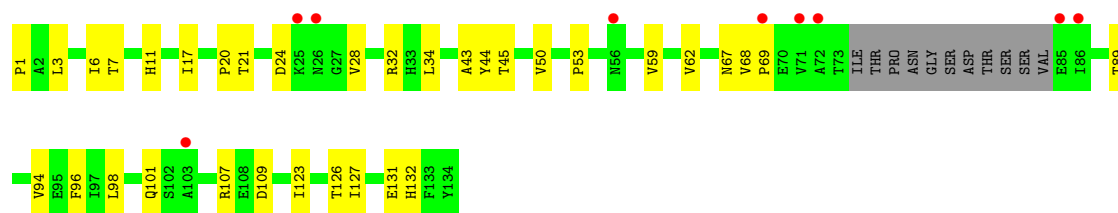


- Molecule 1: coat protein

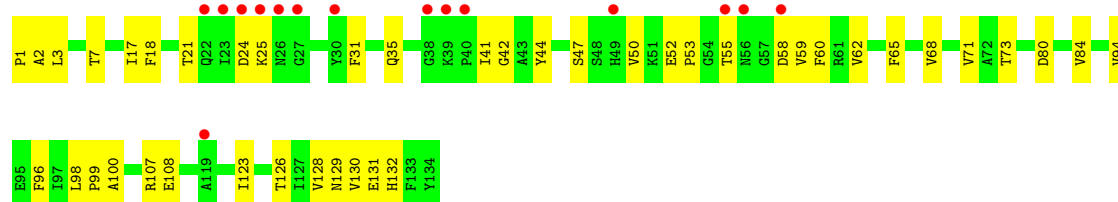


- Molecule 1: coat protein

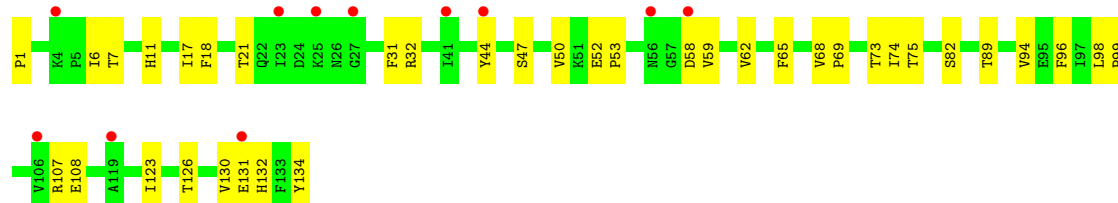
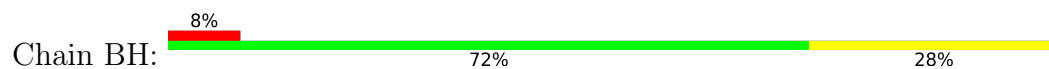




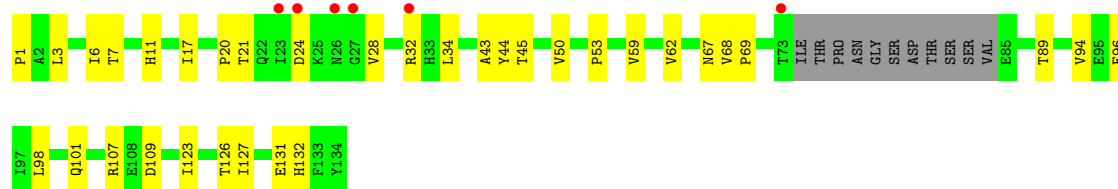
• Molecule 1: coat protein



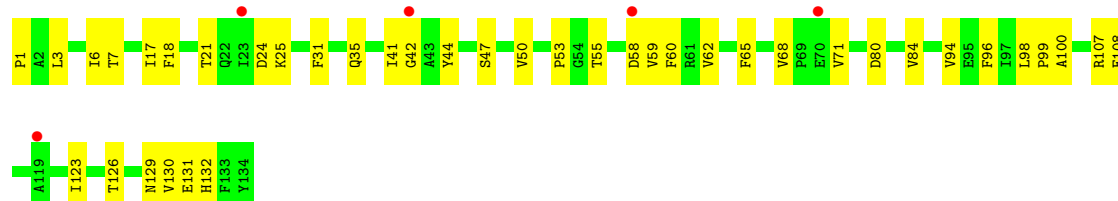
• Molecule 1: coat protein



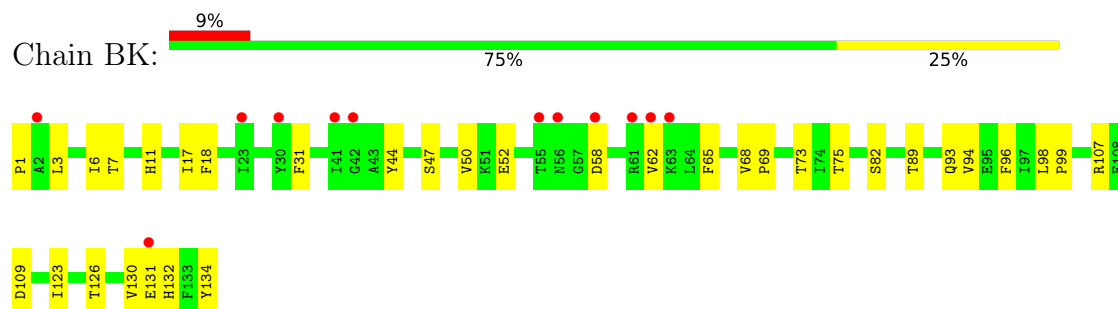
• Molecule 1: coat protein



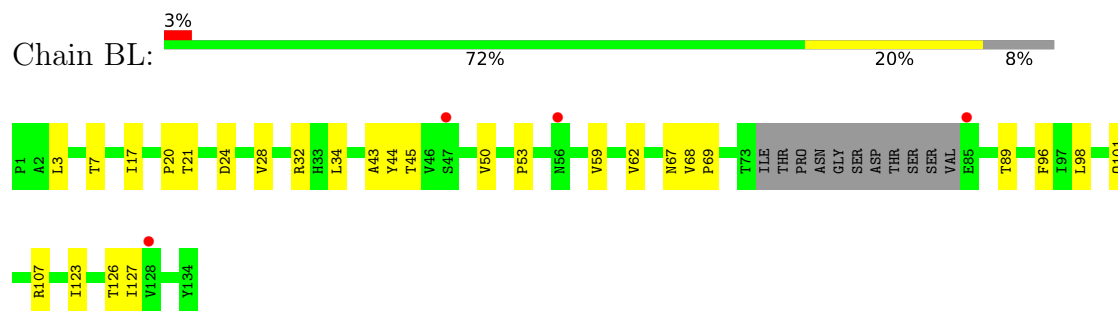
• Molecule 1: coat protein



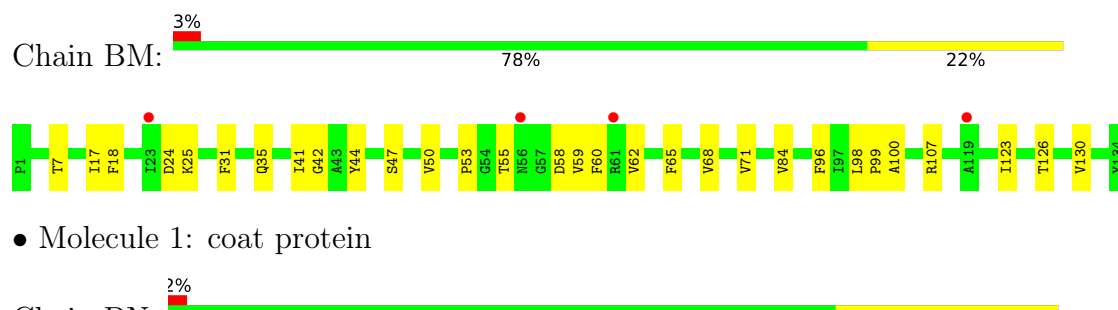
- Molecule 1: coat protein



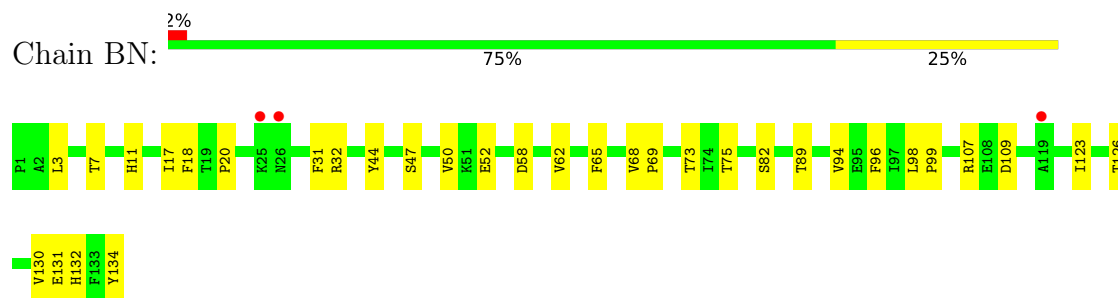
- Molecule 1: coat protein



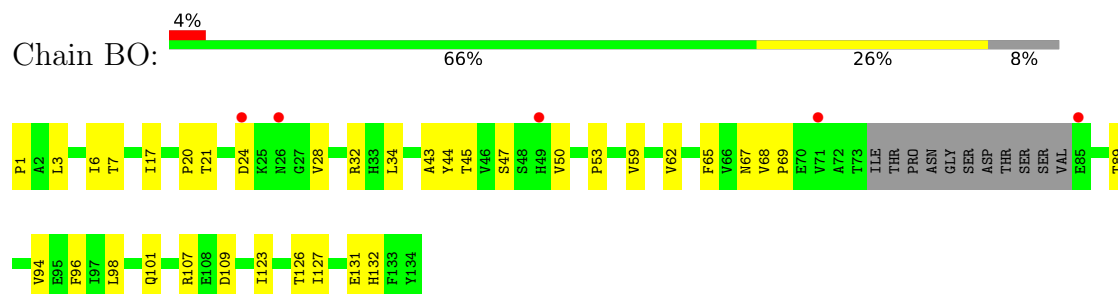
- Molecule 1: coat protein



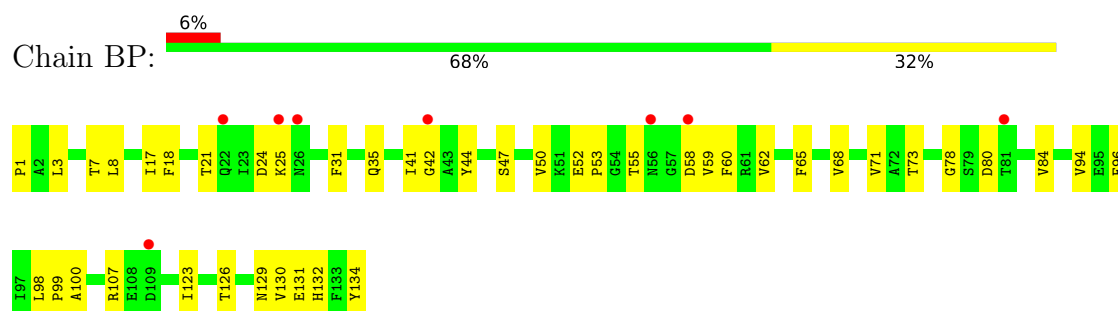
- Molecule 1: coat protein



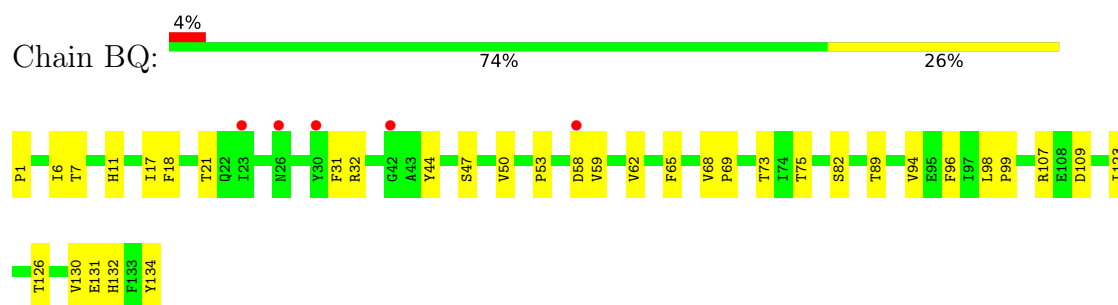
- Molecule 1: coat protein



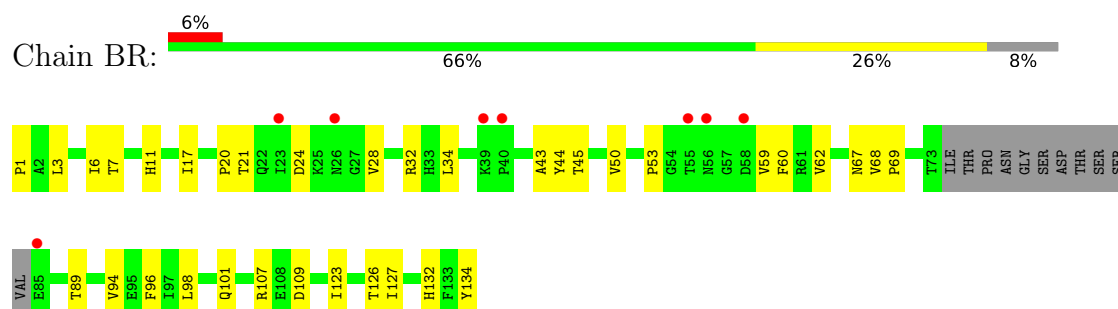
- Molecule 1: coat protein



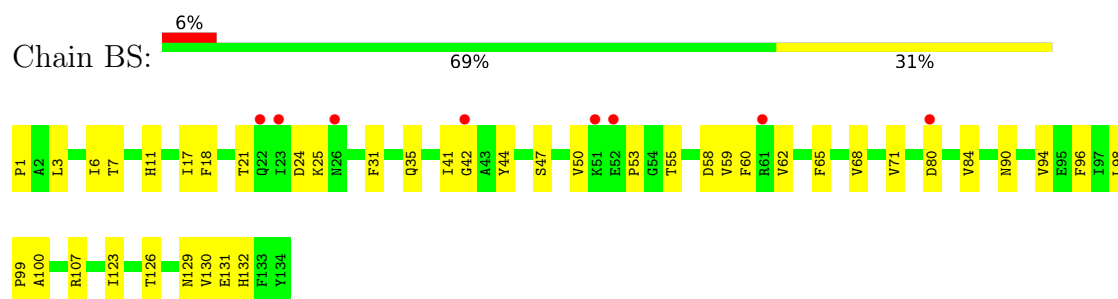
- Molecule 1: coat protein



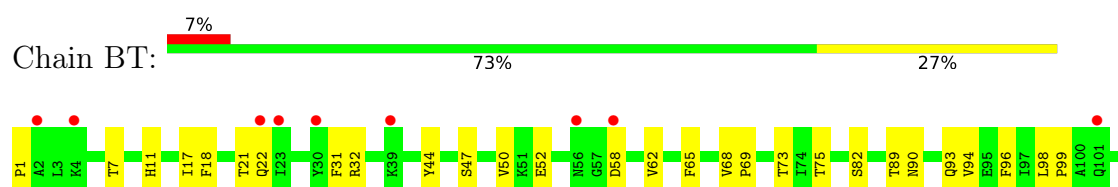
- Molecule 1: coat protein



- Molecule 1: coat protein

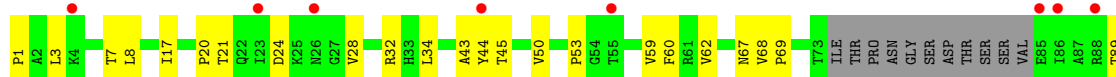


- Molecule 1: coat protein

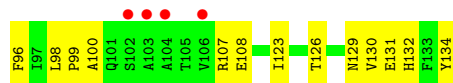




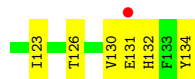
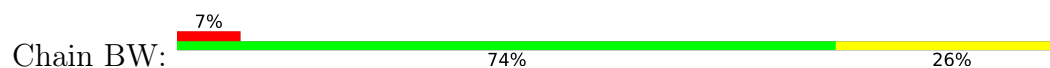
- Molecule 1: coat protein



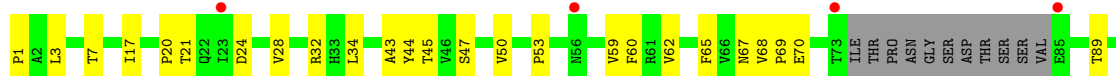
- Molecule 1: coat protein



- Molecule 1: coat protein

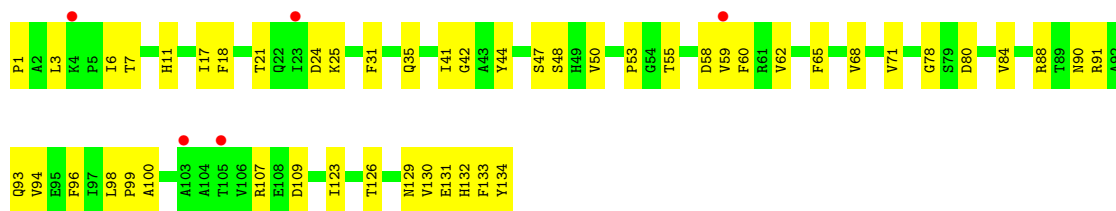


- Molecule 1: coat protein

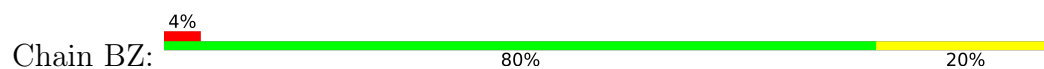


- Molecule 1: coat protein





• Molecule 1: coat protein



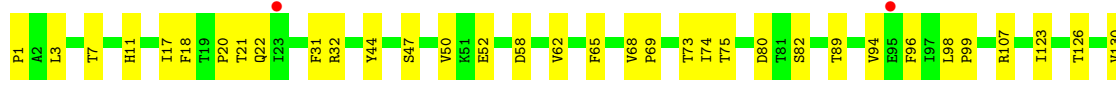
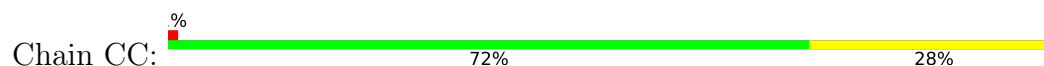
• Molecule 1: coat protein



• Molecule 1: coat protein

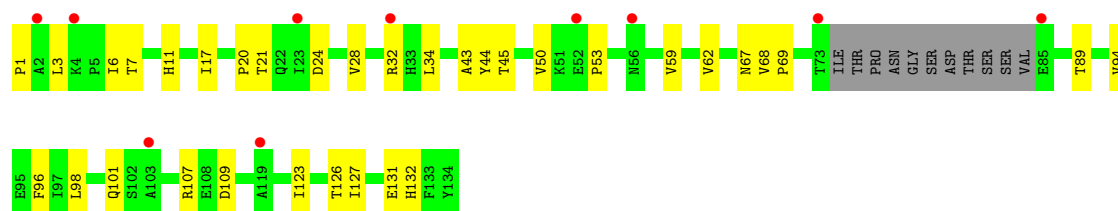


• Molecule 1: coat protein

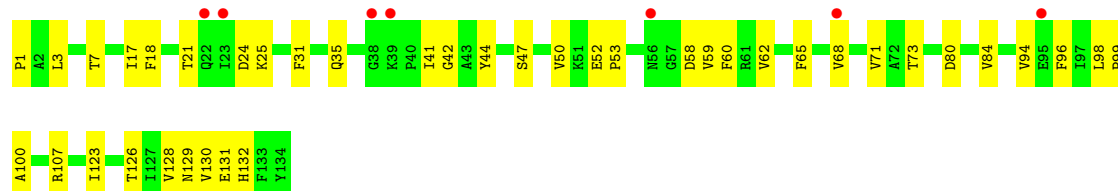
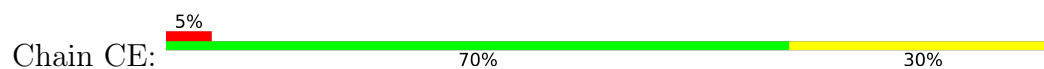


• Molecule 1: coat protein

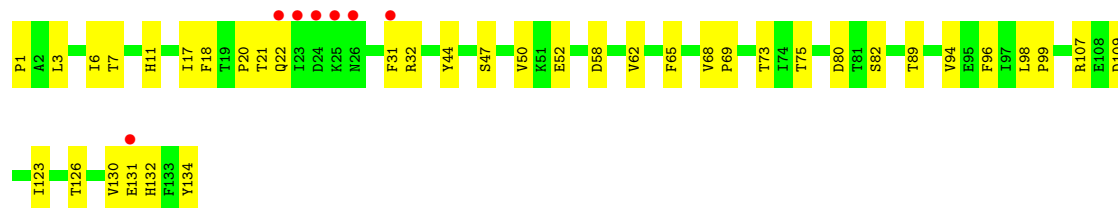
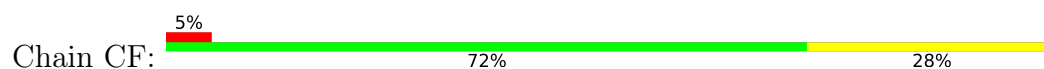




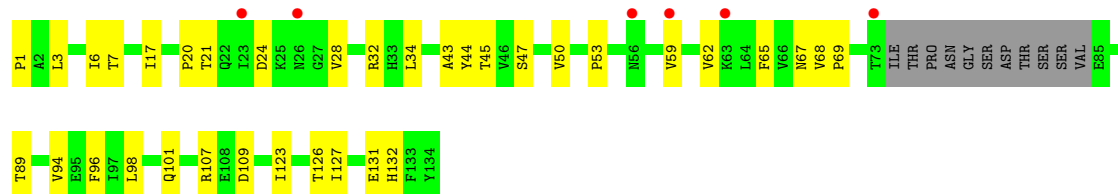
• Molecule 1: coat protein



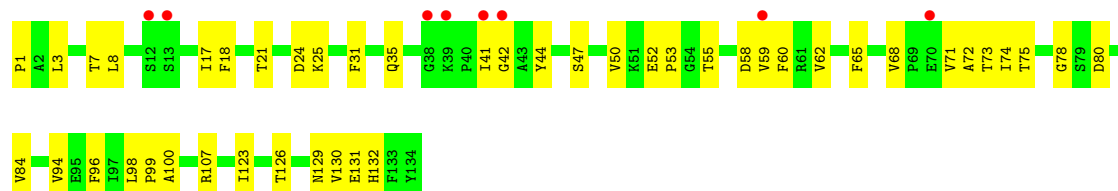
• Molecule 1: coat protein



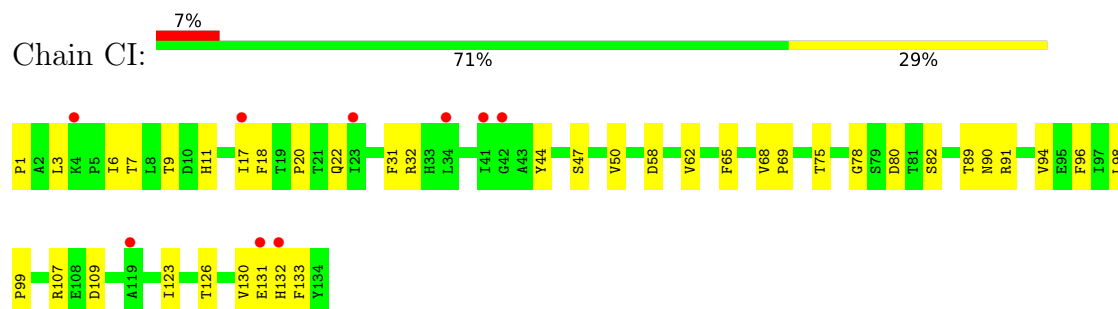
• Molecule 1: coat protein



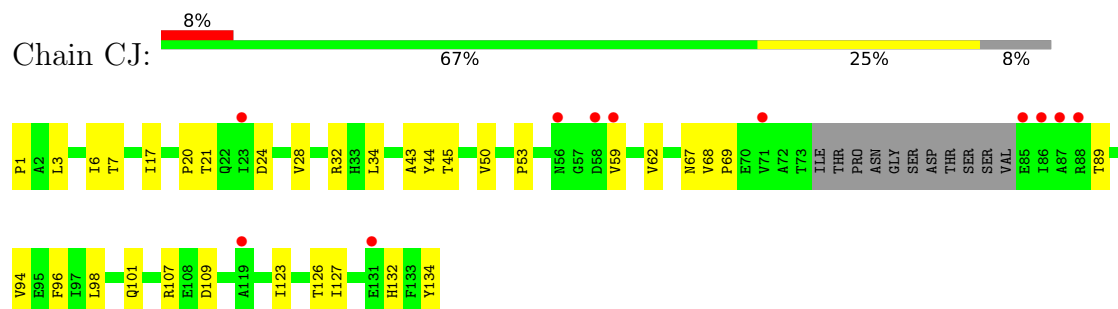
• Molecule 1: coat protein



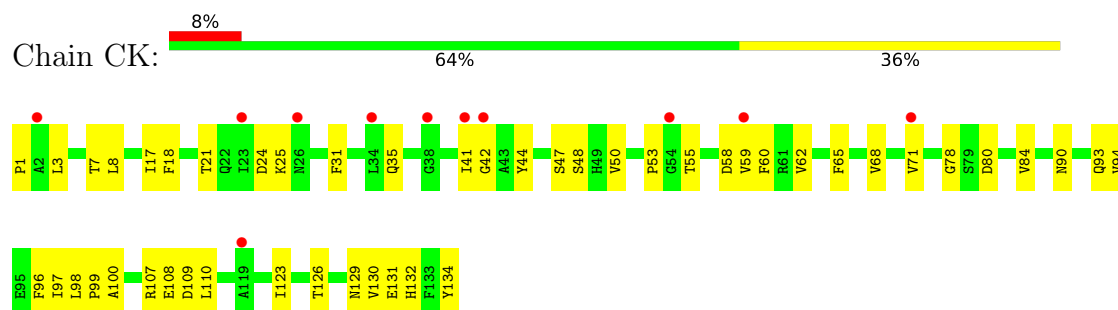
- Molecule 1: coat protein



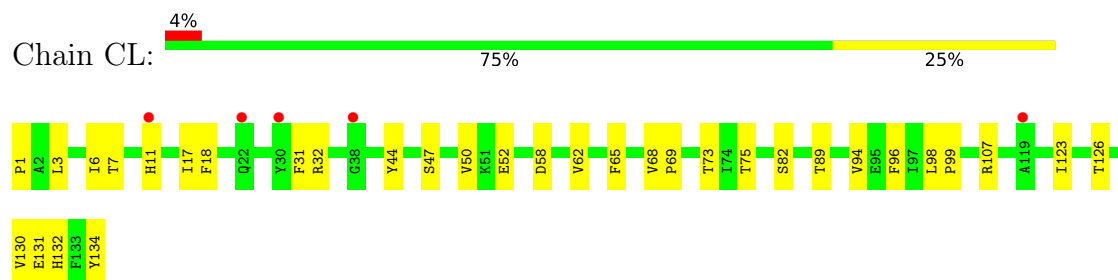
- Molecule 1: coat protein



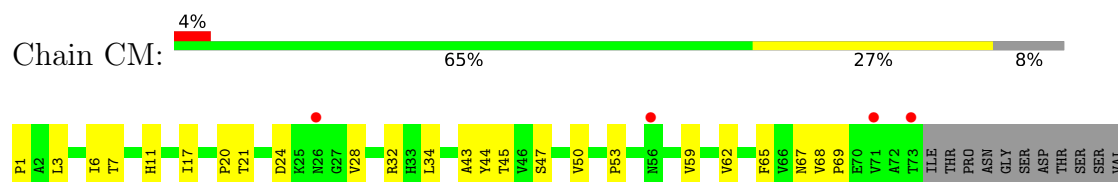
- Molecule 1: coat protein

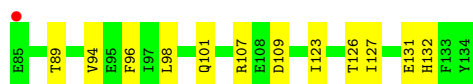


- Molecule 1: coat protein

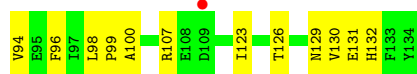
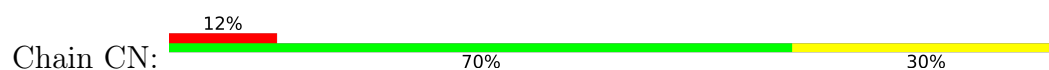


- Molecule 1: coat protein

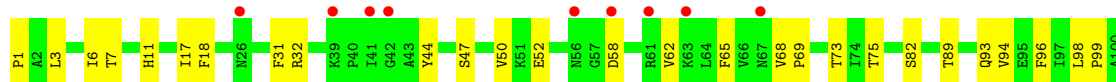
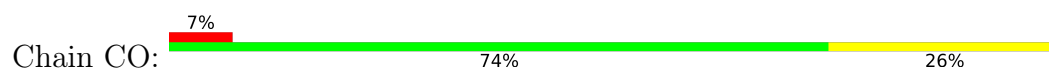




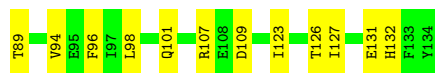
- Molecule 1: coat protein



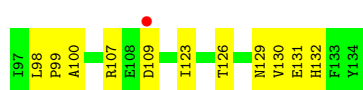
- Molecule 1: coat protein



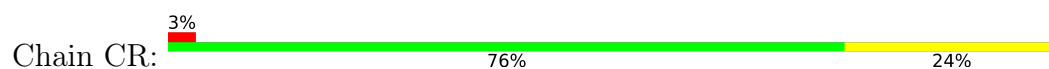
- Molecule 1: coat protein

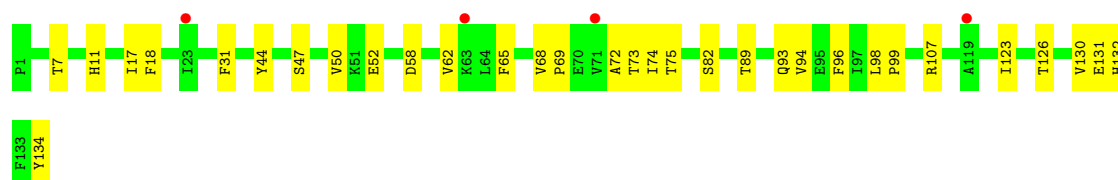


- Molecule 1: coat protein

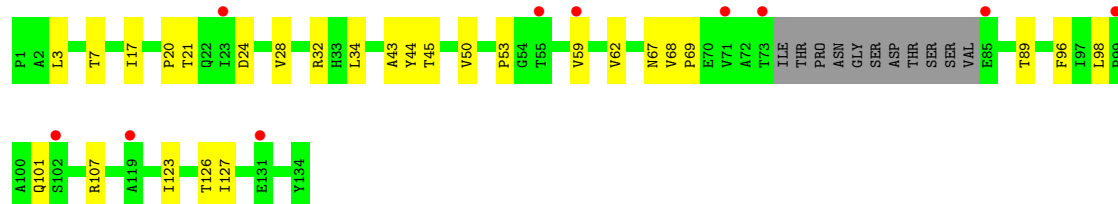
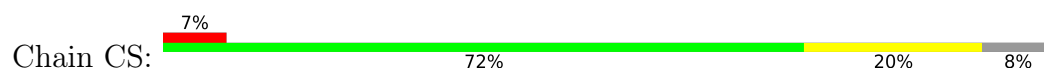


- Molecule 1: coat protein

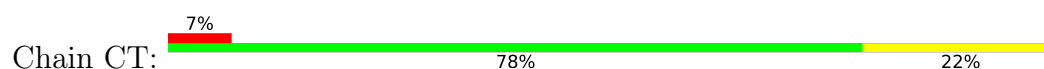




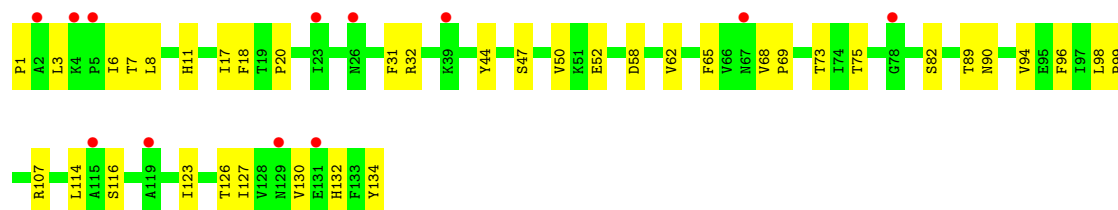
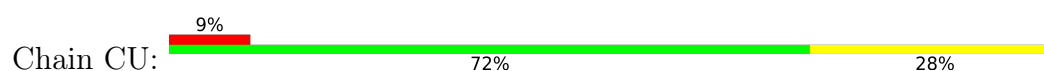
- Molecule 1: coat protein



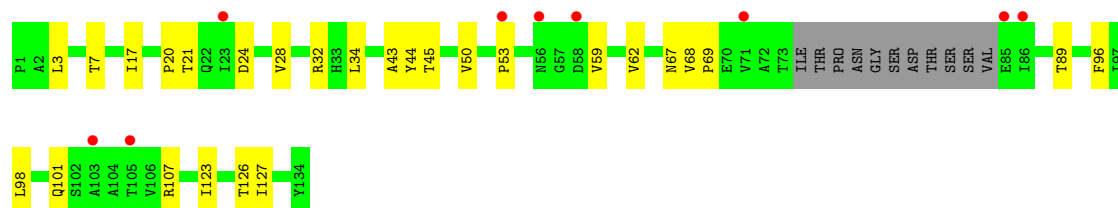
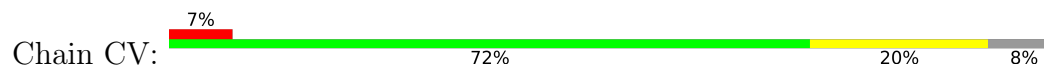
- Molecule 1: coat protein



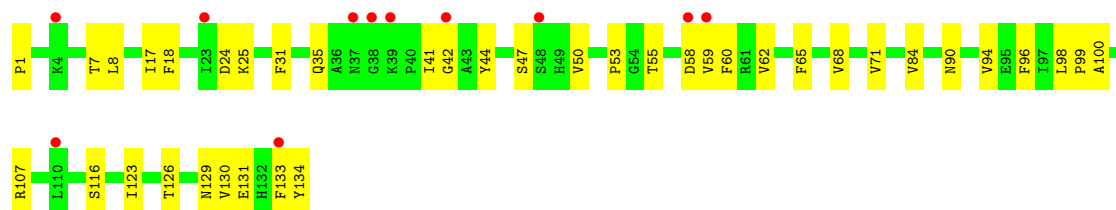
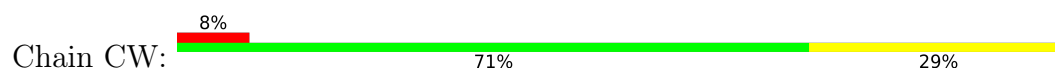
- Molecule 1: coat protein



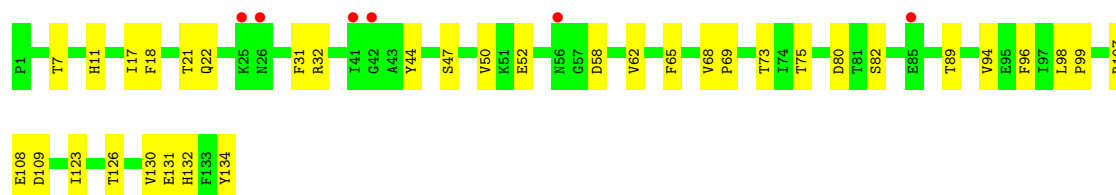
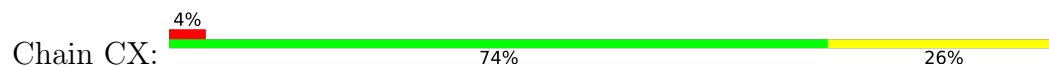
- Molecule 1: coat protein



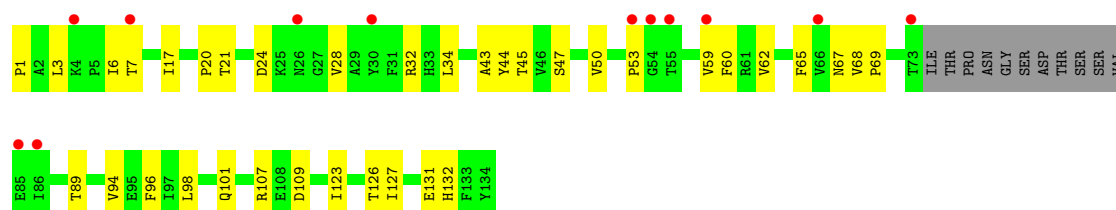
- Molecule 1: coat protein



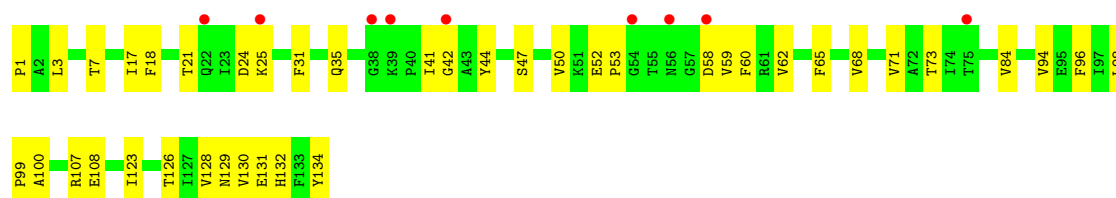
- Molecule 1: coat protein



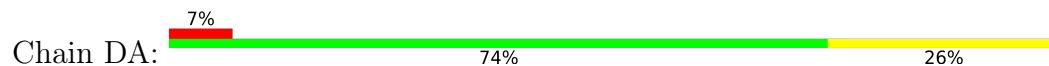
- Molecule 1: coat protein

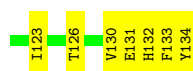


- Molecule 1: coat protein

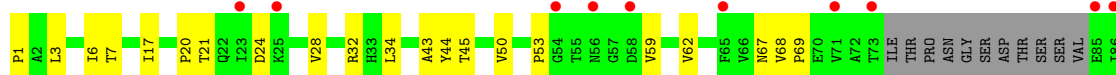


- Molecule 1: coat protein





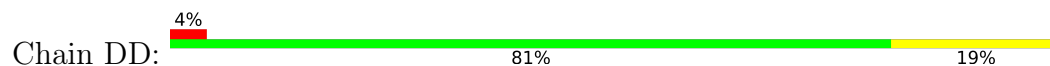
- Molecule 1: coat protein



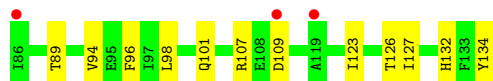
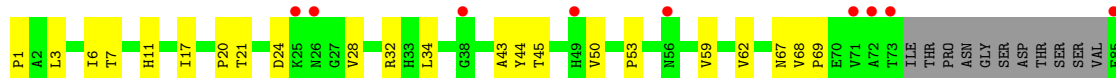
- Molecule 1: coat protein



- Molecule 1: coat protein

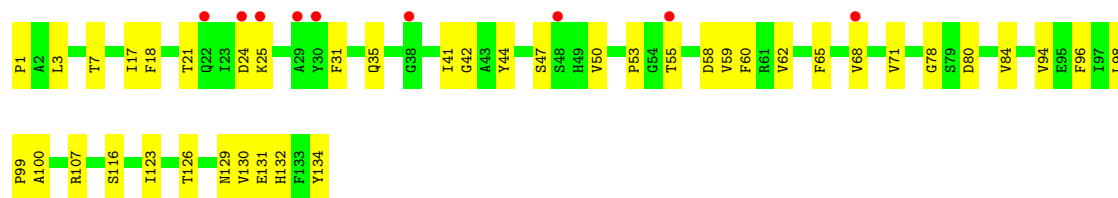


- Molecule 1: coat protein

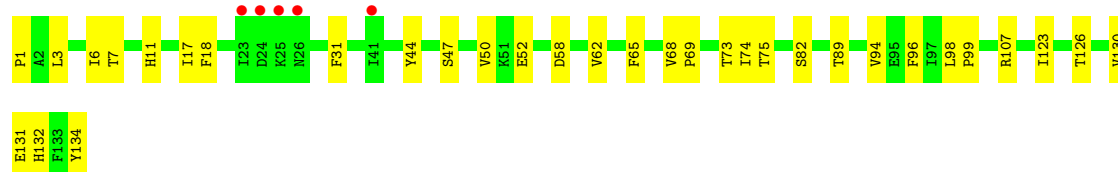
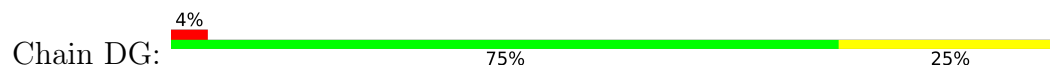


- Molecule 1: coat protein

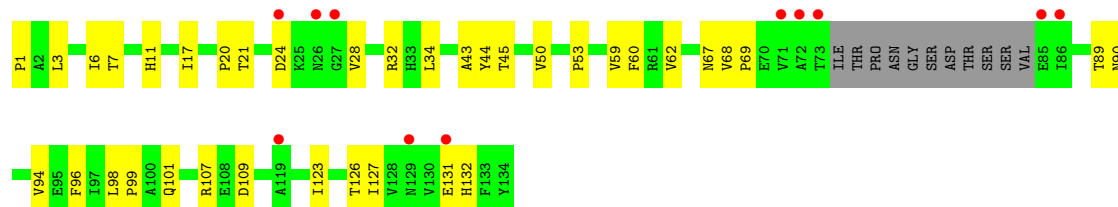




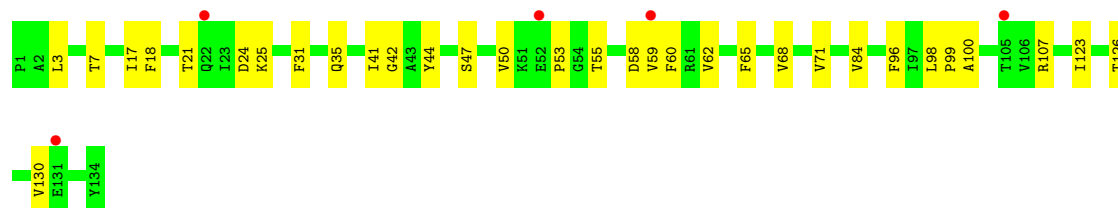
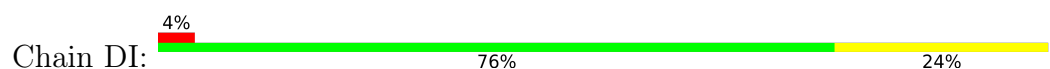
- Molecule 1: coat protein



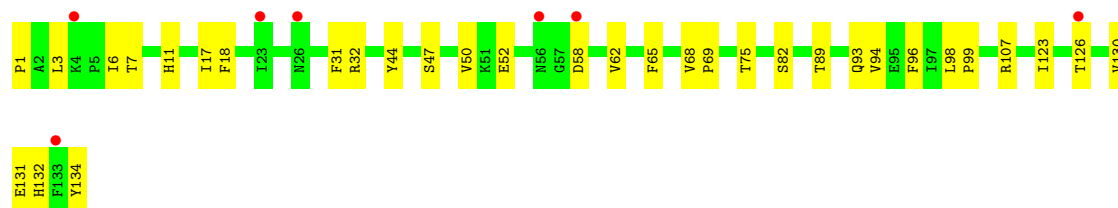
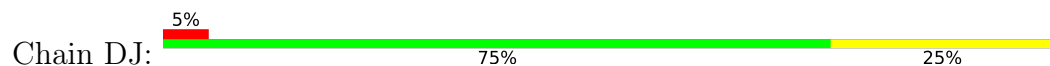
- Molecule 1: coat protein



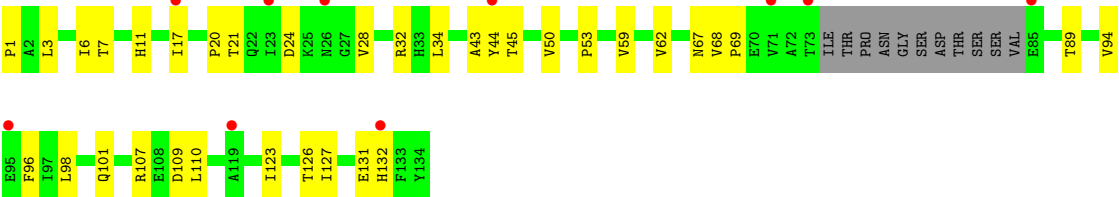
- Molecule 1: coat protein



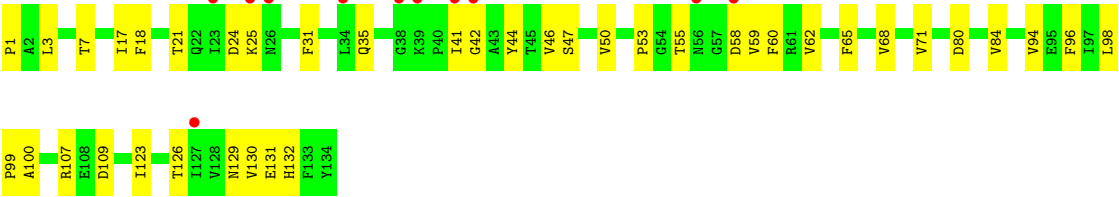
- Molecule 1: coat protein



- Molecule 1: coat protein



• Molecule 1: coat protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 298.11Å 325.05Å 346.02Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 41.39 – 3.79<br>41.39 – 3.79                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (41.39-3.79)<br>97.9 (41.39-3.79)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.37                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.10 (at 3.77Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.14_3260                                            | Depositor        |
| R, $R_{free}$                                                           | 0.261 , 0.267<br>0.263 , 0.268                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 9977 reflections (3.09%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 102.6                                                       | Xtriage          |
| Anisotropy                                                              | 0.195                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 81.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 89070                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 107.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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   | AA    | 0.20         | 0/1034  | 0.47        | 0/1412  |
| 1   | AB    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | AC    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | AD    | 0.21         | 0/1034  | 0.48        | 0/1412  |
| 1   | AE    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | AF    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | AG    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | AH    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | AI    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | AJ    | 0.21         | 0/1034  | 0.48        | 0/1412  |
| 1   | AK    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | AL    | 0.24         | 0/1034  | 0.47        | 0/1412  |
| 1   | AM    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | AN    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | AO    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | AP    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | AQ    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | AR    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | AS    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | AT    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | AU    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | AV    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | AW    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | AX    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | AY    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | AZ    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | BA    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BB    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | BC    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | BD    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BE    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | BF    | 0.23         | 0/958   | 0.50        | 0/1305  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | BG    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BH    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | BI    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | BJ    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BK    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | BL    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | BM    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BN    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | BO    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | BP    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BQ    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | BR    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | BS    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BT    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | BU    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | BV    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BW    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | BX    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | BY    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | BZ    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | CA    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | CB    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | CC    | 0.21         | 0/1034  | 0.48        | 0/1412  |
| 1   | CD    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | CE    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | CF    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | CG    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | CH    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | CI    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | CJ    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | CK    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | CL    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | CM    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | CN    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | CO    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | CP    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | CQ    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | CR    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | CS    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | CT    | 0.24         | 0/1034  | 0.48        | 0/1412  |
| 1   | CU    | 0.21         | 0/1034  | 0.47        | 0/1412  |
| 1   | CV    | 0.23         | 0/958   | 0.50        | 0/1305  |
| 1   | CW    | 0.24         | 0/1034  | 0.48        | 0/1412  |

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 1   | CX    | 0.21         | 0/1034  | 0.47        | 0/1412   |
| 1   | CY    | 0.23         | 0/958   | 0.50        | 0/1305   |
| 1   | CZ    | 0.24         | 0/1034  | 0.48        | 0/1412   |
| 1   | DA    | 0.21         | 0/1034  | 0.47        | 0/1412   |
| 1   | DB    | 0.23         | 0/958   | 0.50        | 0/1305   |
| 1   | DC    | 0.24         | 0/1034  | 0.47        | 0/1412   |
| 1   | DD    | 0.21         | 0/1034  | 0.47        | 0/1412   |
| 1   | DE    | 0.23         | 0/958   | 0.50        | 0/1305   |
| 1   | DF    | 0.24         | 0/1034  | 0.48        | 0/1412   |
| 1   | DG    | 0.21         | 0/1034  | 0.47        | 0/1412   |
| 1   | DH    | 0.23         | 0/958   | 0.50        | 0/1305   |
| 1   | DI    | 0.24         | 0/1034  | 0.48        | 0/1412   |
| 1   | DJ    | 0.21         | 0/1034  | 0.47        | 0/1412   |
| 1   | DK    | 0.23         | 0/958   | 0.50        | 0/1305   |
| 1   | DL    | 0.24         | 0/1034  | 0.48        | 0/1412   |
| All | All   | 0.23         | 0/90780 | 0.48        | 0/123870 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 1014  | 0        | 1020     | 44      | 0            |
| 1   | AB    | 940   | 0        | 950      | 38      | 0            |
| 1   | AC    | 1014  | 0        | 1020     | 41      | 0            |
| 1   | AD    | 1014  | 0        | 1020     | 17      | 0            |
| 1   | AE    | 940   | 0        | 950      | 47      | 0            |
| 1   | AF    | 1014  | 0        | 1020     | 65      | 0            |
| 1   | AG    | 1014  | 0        | 1020     | 38      | 0            |
| 1   | AH    | 940   | 0        | 950      | 36      | 0            |
| 1   | AI    | 1014  | 0        | 1020     | 39      | 0            |
| 1   | AJ    | 1014  | 0        | 1020     | 19      | 1            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AK    | 940   | 0        | 950      | 46      | 0            |
| 1   | AL    | 1014  | 0        | 1020     | 39      | 0            |
| 1   | AM    | 1014  | 0        | 1020     | 28      | 0            |
| 1   | AN    | 940   | 0        | 950      | 33      | 0            |
| 1   | AO    | 1014  | 0        | 1020     | 24      | 0            |
| 1   | AP    | 1014  | 0        | 1020     | 63      | 0            |
| 1   | AQ    | 940   | 0        | 950      | 42      | 0            |
| 1   | AR    | 1014  | 0        | 1020     | 40      | 0            |
| 1   | AS    | 1014  | 0        | 1020     | 43      | 0            |
| 1   | AT    | 940   | 0        | 950      | 47      | 1            |
| 1   | AU    | 1014  | 0        | 1020     | 70      | 0            |
| 1   | AV    | 1014  | 0        | 1020     | 34      | 0            |
| 1   | AW    | 940   | 0        | 950      | 19      | 1            |
| 1   | AX    | 1014  | 0        | 1020     | 35      | 0            |
| 1   | AY    | 1014  | 0        | 1020     | 33      | 0            |
| 1   | AZ    | 940   | 0        | 950      | 33      | 1            |
| 1   | BA    | 1014  | 0        | 1020     | 42      | 0            |
| 1   | BB    | 1014  | 0        | 1020     | 38      | 0            |
| 1   | BC    | 940   | 0        | 950      | 32      | 0            |
| 1   | BD    | 1014  | 0        | 1020     | 45      | 0            |
| 1   | BE    | 1014  | 0        | 1020     | 32      | 0            |
| 1   | BF    | 940   | 0        | 950      | 34      | 0            |
| 1   | BG    | 1014  | 0        | 1020     | 42      | 0            |
| 1   | BH    | 1014  | 0        | 1020     | 36      | 0            |
| 1   | BI    | 940   | 0        | 950      | 32      | 0            |
| 1   | BJ    | 1014  | 0        | 1020     | 38      | 0            |
| 1   | BK    | 1014  | 0        | 1020     | 34      | 0            |
| 1   | BL    | 940   | 0        | 950      | 17      | 0            |
| 1   | BM    | 1014  | 0        | 1020     | 21      | 0            |
| 1   | BN    | 1014  | 0        | 1020     | 34      | 0            |
| 1   | BO    | 940   | 0        | 950      | 33      | 0            |
| 1   | BP    | 1014  | 0        | 1020     | 39      | 0            |
| 1   | BQ    | 1014  | 0        | 1020     | 35      | 0            |
| 1   | BR    | 940   | 0        | 950      | 33      | 0            |
| 1   | BS    | 1014  | 0        | 1020     | 38      | 0            |
| 1   | BT    | 1014  | 0        | 1020     | 39      | 0            |
| 1   | BU    | 940   | 0        | 950      | 29      | 0            |
| 1   | BV    | 1014  | 0        | 1020     | 45      | 0            |
| 1   | BW    | 1014  | 0        | 1020     | 34      | 0            |
| 1   | BX    | 940   | 0        | 950      | 38      | 0            |
| 1   | BY    | 1014  | 0        | 1020     | 67      | 0            |
| 1   | BZ    | 1014  | 0        | 1020     | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | CA    | 940   | 0        | 950      | 31      | 0            |
| 1   | CB    | 1014  | 0        | 1020     | 40      | 0            |
| 1   | CC    | 1014  | 0        | 1020     | 35      | 0            |
| 1   | CD    | 940   | 0        | 950      | 28      | 0            |
| 1   | CE    | 1014  | 0        | 1020     | 41      | 0            |
| 1   | CF    | 1014  | 0        | 1020     | 37      | 0            |
| 1   | CG    | 940   | 0        | 950      | 29      | 0            |
| 1   | CH    | 1014  | 0        | 1020     | 53      | 0            |
| 1   | CI    | 1014  | 0        | 1020     | 50      | 0            |
| 1   | CJ    | 940   | 0        | 950      | 29      | 0            |
| 1   | CK    | 1014  | 0        | 1020     | 69      | 0            |
| 1   | CL    | 1014  | 0        | 1020     | 35      | 0            |
| 1   | CM    | 940   | 0        | 950      | 31      | 0            |
| 1   | CN    | 1014  | 0        | 1020     | 38      | 0            |
| 1   | CO    | 1014  | 0        | 1020     | 33      | 0            |
| 1   | CP    | 940   | 0        | 950      | 32      | 0            |
| 1   | CQ    | 1014  | 0        | 1020     | 41      | 0            |
| 1   | CR    | 1014  | 0        | 1020     | 30      | 0            |
| 1   | CS    | 940   | 0        | 950      | 21      | 0            |
| 1   | CT    | 1014  | 0        | 1020     | 21      | 0            |
| 1   | CU    | 1014  | 0        | 1020     | 50      | 0            |
| 1   | CV    | 940   | 0        | 950      | 18      | 0            |
| 1   | CW    | 1014  | 0        | 1020     | 39      | 0            |
| 1   | CX    | 1014  | 0        | 1020     | 37      | 0            |
| 1   | CY    | 940   | 0        | 950      | 36      | 0            |
| 1   | CZ    | 1014  | 0        | 1020     | 39      | 0            |
| 1   | DA    | 1014  | 0        | 1020     | 40      | 0            |
| 1   | DB    | 940   | 0        | 950      | 31      | 0            |
| 1   | DC    | 1014  | 0        | 1020     | 38      | 0            |
| 1   | DD    | 1014  | 0        | 1020     | 19      | 0            |
| 1   | DE    | 940   | 0        | 950      | 27      | 0            |
| 1   | DF    | 1014  | 0        | 1020     | 39      | 0            |
| 1   | DG    | 1014  | 0        | 1020     | 32      | 0            |
| 1   | DH    | 940   | 0        | 950      | 36      | 0            |
| 1   | DI    | 1014  | 0        | 1020     | 23      | 0            |
| 1   | DJ    | 1014  | 0        | 1020     | 35      | 0            |
| 1   | DK    | 940   | 0        | 950      | 34      | 0            |
| 1   | DL    | 1014  | 0        | 1020     | 41      | 0            |
| 2   | AA    | 1     | 0        | 0        | 0       | 0            |
| 2   | AB    | 1     | 0        | 0        | 0       | 0            |
| 2   | AC    | 1     | 0        | 0        | 0       | 0            |
| 2   | AE    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | AF    | 1     | 0        | 0        | 0       | 0            |
| 2   | AG    | 1     | 0        | 0        | 0       | 0            |
| 2   | AH    | 1     | 0        | 0        | 0       | 0            |
| 2   | AK    | 1     | 0        | 0        | 0       | 0            |
| 2   | AM    | 1     | 0        | 0        | 0       | 0            |
| 2   | AN    | 1     | 0        | 0        | 0       | 0            |
| 2   | AQ    | 1     | 0        | 0        | 0       | 0            |
| 2   | AW    | 1     | 0        | 0        | 0       | 0            |
| 2   | AZ    | 1     | 0        | 0        | 0       | 0            |
| 2   | BB    | 1     | 0        | 0        | 0       | 0            |
| 2   | BC    | 1     | 0        | 0        | 0       | 0            |
| 2   | BF    | 1     | 0        | 0        | 0       | 0            |
| 2   | BH    | 1     | 0        | 0        | 0       | 0            |
| 2   | BI    | 1     | 0        | 0        | 0       | 0            |
| 2   | BK    | 1     | 0        | 0        | 0       | 0            |
| 2   | BL    | 1     | 0        | 0        | 0       | 0            |
| 2   | BR    | 1     | 0        | 0        | 0       | 0            |
| 2   | BT    | 1     | 0        | 0        | 0       | 0            |
| 2   | BX    | 1     | 0        | 0        | 0       | 0            |
| 2   | CA    | 1     | 0        | 0        | 0       | 0            |
| 2   | CC    | 1     | 0        | 0        | 0       | 0            |
| 2   | CD    | 1     | 0        | 0        | 0       | 0            |
| 2   | CF    | 1     | 0        | 0        | 0       | 0            |
| 2   | CJ    | 1     | 0        | 0        | 0       | 0            |
| 2   | CS    | 1     | 0        | 0        | 0       | 0            |
| 2   | CV    | 1     | 0        | 0        | 0       | 0            |
| All | All   | 89070 | 0        | 89700    | 2402    | 2            |

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 13.

All (2402) 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:AR:1:PRO:HD3   | 1:CH:131:GLU:HB3 | 1.39                     | 1.03              |
| 1:AU:129:ASN:O   | 1:CI:32:ARG:NH1  | 1.91                     | 1.02              |
| 1:AP:134:TYR:CD1 | 1:AU:3:LEU:HD23  | 1.96                     | 1.01              |
| 1:AC:1:PRO:HD3   | 1:BV:131:GLU:HB3 | 1.46                     | 0.97              |
| 1:AF:1:PRO:HD3   | 1:BY:131:GLU:HB3 | 1.47                     | 0.97              |
| 1:AU:90:ASN:CG   | 1:CK:99:PRO:HD2  | 1.93                     | 0.93              |
| 1:AF:131:GLU:HB3 | 1:BY:1:PRO:HD3   | 1.52                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AS:32:ARG:NH1   | 1:CK:129:ASN:O    | 2.03                     | 0.91              |
| 1:BJ:1:PRO:HD3    | 1:DC:131:GLU:HB3  | 1.51                     | 0.91              |
| 1:CK:80:ASP:HB2   | 1:CR:73:THR:H     | 1.33                     | 0.91              |
| 1:AS:132:HIS:HB2  | 1:BY:21:THR:O     | 1.73                     | 0.89              |
| 1:AT:21:THR:O     | 1:BX:132:HIS:HB2  | 1.72                     | 0.88              |
| 1:AL:1:PRO:HD3    | 1:CE:131:GLU:HB3  | 1.55                     | 0.88              |
| 1:AE:60:PHE:CE1   | 1:CU:130:VAL:HG11 | 2.09                     | 0.87              |
| 1:AQ:3:LEU:HD23   | 1:AT:134:TYR:CD1  | 2.09                     | 0.87              |
| 1:AC:131:GLU:HB3  | 1:BV:1:PRO:HD3    | 1.55                     | 0.87              |
| 1:AI:1:PRO:HD3    | 1:CB:131:GLU:HB3  | 1.58                     | 0.86              |
| 1:AP:130:VAL:HG11 | 1:AT:60:PHE:CE1   | 2.11                     | 0.86              |
| 1:AX:131:GLU:HB3  | 1:CN:1:PRO:HD3    | 1.58                     | 0.86              |
| 1:BD:80:ASP:HB2   | 1:BH:73:THR:H     | 1.40                     | 0.84              |
| 1:AR:129:ASN:O    | 1:CF:32:ARG:NH1   | 2.09                     | 0.84              |
| 1:BB:32:ARG:NH1   | 1:CW:129:ASN:O    | 2.10                     | 0.84              |
| 1:AK:109:ASP:HB3  | 1:CI:11:HIS:HB2   | 1.60                     | 0.83              |
| 1:BS:1:PRO:HD3    | 1:DL:131:GLU:HB3  | 1.60                     | 0.83              |
| 1:BG:1:PRO:HD3    | 1:CZ:131:GLU:HB3  | 1.62                     | 0.81              |
| 1:AS:134:TYR:HB2  | 1:BY:3:LEU:HD23   | 1.62                     | 0.81              |
| 1:AU:11:HIS:H     | 1:CK:109:ASP:HB3  | 1.43                     | 0.81              |
| 1:AP:130:VAL:HG11 | 1:AT:60:PHE:CD1   | 2.17                     | 0.80              |
| 1:BD:129:ASN:O    | 1:CU:32:ARG:NH1   | 2.14                     | 0.80              |
| 1:AU:90:ASN:ND2   | 1:CK:99:PRO:HD2   | 1.97                     | 0.80              |
| 1:BA:131:GLU:HB3  | 1:CQ:1:PRO:HD3    | 1.64                     | 0.79              |
| 1:BP:129:ASN:O    | 1:DD:32:ARG:NH1   | 2.15                     | 0.79              |
| 1:AG:32:ARG:NH1   | 1:CB:129:ASN:O    | 2.15                     | 0.79              |
| 1:AP:32:ARG:NH1   | 1:CH:129:ASN:O    | 2.16                     | 0.79              |
| 1:AL:129:ASN:O    | 1:CC:32:ARG:NH1   | 2.16                     | 0.79              |
| 1:AF:3:LEU:HD23   | 1:CU:134:TYR:CD1  | 2.17                     | 0.79              |
| 1:BG:129:ASN:O    | 1:CX:32:ARG:NH1   | 2.17                     | 0.78              |
| 1:AK:109:ASP:HB3  | 1:CI:11:HIS:CB    | 2.14                     | 0.78              |
| 1:BN:32:ARG:NH1   | 1:DF:129:ASN:O    | 2.16                     | 0.78              |
| 1:AE:60:PHE:CD1   | 1:CU:130:VAL:HG11 | 2.19                     | 0.78              |
| 1:AI:129:ASN:O    | 1:BZ:32:ARG:NH1   | 2.16                     | 0.78              |
| 1:AE:108:GLU:OE1  | 1:CU:11:HIS:NE2   | 2.16                     | 0.78              |
| 1:BS:129:ASN:O    | 1:DJ:32:ARG:NH1   | 2.17                     | 0.78              |
| 1:AP:116:SER:OG   | 1:AT:8:LEU:HB3    | 1.84                     | 0.77              |
| 1:AV:32:ARG:NH1   | 1:CN:129:ASN:O    | 2.17                     | 0.77              |
| 1:CC:73:THR:H     | 1:CH:80:ASP:HB2   | 1.50                     | 0.77              |
| 1:BA:129:ASN:O    | 1:CO:32:ARG:NH1   | 2.16                     | 0.77              |
| 1:BO:1:PRO:HD3    | 1:DG:131:GLU:HB3  | 1.66                     | 0.77              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AX:129:ASN:O    | 1:CL:32:ARG:NH1  | 2.17                     | 0.76              |
| 1:BB:11:HIS:HB2   | 1:DH:109:ASP:HB3 | 1.65                     | 0.76              |
| 1:AX:1:PRO:HD3    | 1:CN:131:GLU:HB3 | 1.68                     | 0.76              |
| 1:BT:131:GLU:HB3  | 1:DK:1:PRO:HD3   | 1.68                     | 0.76              |
| 1:BP:80:ASP:HB2   | 1:DG:73:THR:H    | 1.49                     | 0.76              |
| 1:AH:3:LEU:HD23   | 1:AZ:134:TYR:CD1 | 2.21                     | 0.75              |
| 1:AP:80:ASP:CB    | 1:CH:73:THR:H    | 1.99                     | 0.75              |
| 1:BP:131:GLU:HB3  | 1:DF:1:PRO:HD3   | 1.69                     | 0.75              |
| 1:AS:94:VAL:HG13  | 1:BX:94:VAL:HG22 | 1.68                     | 0.75              |
| 1:BJ:131:GLU:HB3  | 1:DC:1:PRO:HD3   | 1.67                     | 0.75              |
| 1:BS:131:GLU:HB3  | 1:DL:1:PRO:HD3   | 1.67                     | 0.75              |
| 1:AA:109:ASP:HB3  | 1:AQ:11:HIS:H    | 1.51                     | 0.75              |
| 1:AY:32:ARG:NH1   | 1:CQ:129:ASN:O   | 2.20                     | 0.75              |
| 1:AU:1:PRO:HD3    | 1:CK:131:GLU:HB3 | 1.68                     | 0.74              |
| 1:BQ:32:ARG:NH1   | 1:DL:129:ASN:O   | 2.20                     | 0.74              |
| 1:AF:129:ASN:O    | 1:BW:32:ARG:NH1  | 2.19                     | 0.74              |
| 1:BG:131:GLU:HB3  | 1:CZ:1:PRO:HD3   | 1.69                     | 0.74              |
| 1:AS:73:THR:H     | 1:BY:80:ASP:HB2  | 1.52                     | 0.74              |
| 1:CF:131:GLU:HB3  | 1:CP:1:PRO:HD3   | 1.70                     | 0.74              |
| 1:BE:131:GLU:HB3  | 1:DE:1:PRO:HD3   | 1.69                     | 0.74              |
| 1:AA:32:ARG:NH1   | 1:BV:129:ASN:O   | 2.20                     | 0.74              |
| 1:AK:123:ILE:HD11 | 1:CI:6:ILE:HD13  | 1.70                     | 0.74              |
| 1:AJ:32:ARG:NH1   | 1:CE:129:ASN:O   | 2.21                     | 0.73              |
| 1:AD:32:ARG:NH1   | 1:BY:129:ASN:O   | 2.21                     | 0.73              |
| 1:BA:1:PRO:HD3    | 1:CQ:131:GLU:HB3 | 1.70                     | 0.73              |
| 1:CJ:94:VAL:HG22  | 1:CR:94:VAL:HG13 | 1.71                     | 0.72              |
| 1:CK:80:ASP:CB    | 1:CR:73:THR:H    | 2.01                     | 0.72              |
| 1:AC:129:ASN:O    | 1:BT:32:ARG:NH1  | 2.23                     | 0.72              |
| 1:AH:1:PRO:HD3    | 1:CX:131:GLU:HB3 | 1.72                     | 0.72              |
| 1:BI:1:PRO:HD3    | 1:BQ:131:GLU:HB3 | 1.72                     | 0.72              |
| 1:AV:73:THR:H     | 1:CB:80:ASP:HB2  | 1.54                     | 0.72              |
| 1:AU:130:VAL:HG11 | 1:CK:60:PHE:CE1  | 2.25                     | 0.72              |
| 1:CC:131:GLU:HB3  | 1:CG:1:PRO:HD3   | 1.71                     | 0.72              |
| 1:AK:131:GLU:HB3  | 1:CI:1:PRO:HD3   | 1.72                     | 0.71              |
| 1:AY:132:HIS:HB2  | 1:BV:21:THR:O    | 1.90                     | 0.71              |
| 1:BE:32:ARG:NH1   | 1:CZ:129:ASN:O   | 2.22                     | 0.71              |
| 1:AH:11:HIS:H     | 1:CX:109:ASP:HB3 | 1.54                     | 0.71              |
| 1:BE:73:THR:H     | 1:DF:80:ASP:HB2  | 1.57                     | 0.70              |
| 1:AG:130:VAL:HG11 | 1:AZ:60:PHE:CE1  | 2.27                     | 0.70              |
| 1:BO:94:VAL:HG22  | 1:DG:94:VAL:HG13 | 1.74                     | 0.69              |
| 1:AA:11:HIS:HB2   | 1:AQ:109:ASP:HB3 | 1.73                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AP:11:HIS:NE2  | 1:AT:108:GLU:OE1 | 2.25                     | 0.69              |
| 1:BD:80:ASP:CB   | 1:BH:73:THR:H    | 2.04                     | 0.69              |
| 1:CJ:1:PRO:HD3   | 1:CR:131:GLU:HB3 | 1.73                     | 0.69              |
| 1:BJ:129:ASN:O   | 1:DA:32:ARG:NH1  | 2.25                     | 0.69              |
| 1:AR:131:GLU:HB3 | 1:CH:1:PRO:HD3   | 1.74                     | 0.69              |
| 1:AC:53:PRO:HD3  | 1:AC:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:AG:132:HIS:HB2 | 1:BA:21:THR:O    | 1.94                     | 0.68              |
| 1:CW:53:PRO:HD3  | 1:CW:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:AB:109:ASP:HB3 | 1:DA:11:HIS:HB2  | 1.74                     | 0.68              |
| 1:AL:53:PRO:HD3  | 1:AL:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:AN:109:ASP:HB3 | 1:CL:11:HIS:HB2  | 1.74                     | 0.68              |
| 1:AR:53:PRO:HD3  | 1:AR:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:CQ:53:PRO:HD3  | 1:CQ:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:DF:53:PRO:HD3  | 1:DF:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:DL:53:PRO:HD3  | 1:DL:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:AI:53:PRO:HD3  | 1:AI:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:BR:7:THR:HG22  | 1:BR:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:CA:7:THR:HG22  | 1:CA:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:CT:53:PRO:HD3  | 1:CT:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:AL:131:GLU:HB3 | 1:CE:1:PRO:HD3   | 1.76                     | 0.68              |
| 1:AW:7:THR:HG22  | 1:AW:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:BD:53:PRO:HD3  | 1:BD:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:CE:53:PRO:HD3  | 1:CE:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:CJ:7:THR:HG22  | 1:CJ:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:CP:7:THR:HG22  | 1:CP:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:DB:7:THR:HG22  | 1:DB:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:DI:53:PRO:HD3  | 1:DI:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:AV:132:HIS:HB2 | 1:CB:21:THR:O    | 1.94                     | 0.68              |
| 1:AZ:7:THR:HG22  | 1:AZ:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:BC:7:THR:HG22  | 1:BC:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:BP:53:PRO:HD3  | 1:BP:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:BT:134:TYR:O   | 1:DK:3:LEU:N     | 2.18                     | 0.68              |
| 1:CD:7:THR:HG22  | 1:CD:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:CS:7:THR:HG22  | 1:CS:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:CV:7:THR:HG22  | 1:CV:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:AE:7:THR:HG22  | 1:AE:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:AO:53:PRO:HD3  | 1:AO:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:BO:7:THR:HG22  | 1:BO:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:BS:53:PRO:HD3  | 1:BS:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:BV:53:PRO:HD3  | 1:BV:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:AK:7:THR:HG22  | 1:AK:17:ILE:HG12 | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:CB:53:PRO:HD3  | 1:CB:60:PHE:CE1  | 2.29                     | 0.68              |
| 1:CM:7:THR:HG22  | 1:CM:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:CY:7:THR:HG22  | 1:CY:17:ILE:HG12 | 1.76                     | 0.68              |
| 1:AB:7:THR:HG22  | 1:AB:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:AX:53:PRO:HD3  | 1:AX:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:BI:7:THR:HG22  | 1:BI:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:BJ:53:PRO:HD3  | 1:BJ:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:CK:21:THR:O    | 1:CR:132:HIS:HB2 | 1.93                     | 0.67              |
| 1:CM:109:ASP:HB3 | 1:CO:11:HIS:HB2  | 1.77                     | 0.67              |
| 1:BA:53:PRO:HD3  | 1:BA:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:BG:53:PRO:HD3  | 1:BG:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:BL:7:THR:HG22  | 1:BL:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:AU:53:PRO:HD3  | 1:AU:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:AU:131:GLU:OE1 | 1:CK:1:PRO:HD3   | 1.94                     | 0.67              |
| 1:BF:7:THR:HG22  | 1:BF:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:BU:7:THR:HG22  | 1:BU:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:CG:7:THR:HG22  | 1:CG:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:CK:53:PRO:HD3  | 1:CK:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:CK:78:GLY:O    | 1:CR:74:ILE:HA   | 1.94                     | 0.67              |
| 1:CY:109:ASP:HB3 | 1:DJ:11:HIS:HB2  | 1.75                     | 0.67              |
| 1:DC:53:PRO:HD3  | 1:DC:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:DK:7:THR:HG22  | 1:DK:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:AF:53:PRO:HD3  | 1:AF:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:AT:7:THR:HG22  | 1:AT:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:BY:53:PRO:HD3  | 1:BY:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:AH:7:THR:HG22  | 1:AH:17:ILE:HG12 | 1.76                     | 0.67              |
| 1:CH:53:PRO:HD3  | 1:CH:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:CN:53:PRO:HD3  | 1:CN:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:CZ:53:PRO:HD3  | 1:CZ:60:PHE:CE1  | 2.29                     | 0.67              |
| 1:AP:8:LEU:HB3   | 1:AT:116:SER:OG  | 1.95                     | 0.67              |
| 1:AP:52:GLU:HG3  | 1:AT:132:HIS:HE1 | 1.58                     | 0.67              |
| 1:BD:7:THR:HG22  | 1:BD:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:DL:7:THR:HG22  | 1:DL:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:AO:7:THR:HG22  | 1:AO:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:AR:7:THR:HG22  | 1:AR:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:BP:7:THR:HG22  | 1:BP:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:BS:7:THR:HG22  | 1:BS:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:CH:7:THR:HG22  | 1:CH:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:CW:7:THR:HG22  | 1:CW:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:AL:7:THR:HG22  | 1:AL:17:ILE:HG12 | 1.77                     | 0.67              |
| 1:BI:109:ASP:HB3 | 1:BQ:11:HIS:HB2  | 1.77                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CE:7:THR:HG22  | 1:CE:17:ILE:HG12  | 1.77                     | 0.67              |
| 1:DE:7:THR:HG22  | 1:DE:17:ILE:HG12  | 1.76                     | 0.67              |
| 1:BM:53:PRO:HD3  | 1:BM:60:PHE:CE1   | 2.29                     | 0.66              |
| 1:DF:7:THR:HG22  | 1:DF:17:ILE:HG12  | 1.77                     | 0.66              |
| 1:AN:7:THR:HG22  | 1:AN:17:ILE:HG12  | 1.76                     | 0.66              |
| 1:AP:50:VAL:O    | 1:AT:132:HIS:NE2  | 2.29                     | 0.66              |
| 1:CN:7:THR:HG22  | 1:CN:17:ILE:HG12  | 1.77                     | 0.66              |
| 1:BX:7:THR:HG22  | 1:BX:17:ILE:HG12  | 1.76                     | 0.66              |
| 1:DC:7:THR:HG22  | 1:DC:17:ILE:HG12  | 1.77                     | 0.66              |
| 1:BJ:7:THR:HG22  | 1:BJ:17:ILE:HG12  | 1.77                     | 0.66              |
| 1:AX:7:THR:HG22  | 1:AX:17:ILE:HG12  | 1.77                     | 0.66              |
| 1:BE:131:GLU:HB3 | 1:DE:1:PRO:CD     | 2.26                     | 0.66              |
| 1:BP:3:LEU:HD23  | 1:DG:134:TYR:HB2  | 1.77                     | 0.66              |
| 1:BB:11:HIS:CB   | 1:DH:109:ASP:HB3  | 2.24                     | 0.66              |
| 1:CQ:7:THR:HG22  | 1:CQ:17:ILE:HG12  | 1.77                     | 0.66              |
| 1:DI:7:THR:HG22  | 1:DI:17:ILE:HG12  | 1.77                     | 0.66              |
| 1:AF:6:ILE:HD13  | 1:BY:123:ILE:HD11 | 1.78                     | 0.66              |
| 1:AI:7:THR:HG22  | 1:AI:17:ILE:HG12  | 1.77                     | 0.66              |
| 1:AK:131:GLU:CB  | 1:CI:1:PRO:HD3    | 2.27                     | 0.65              |
| 1:AQ:7:THR:HG22  | 1:AQ:17:ILE:HG12  | 1.76                     | 0.65              |
| 1:AU:7:THR:HG22  | 1:AU:17:ILE:HG12  | 1.77                     | 0.65              |
| 1:BH:32:ARG:NH1  | 1:DC:129:ASN:O    | 2.28                     | 0.65              |
| 1:BM:7:THR:HG22  | 1:BM:17:ILE:HG12  | 1.77                     | 0.65              |
| 1:BV:7:THR:HG22  | 1:BV:17:ILE:HG12  | 1.77                     | 0.65              |
| 1:DH:7:THR:HG22  | 1:DH:17:ILE:HG12  | 1.76                     | 0.65              |
| 1:AC:7:THR:HG22  | 1:AC:17:ILE:HG12  | 1.77                     | 0.65              |
| 1:BG:7:THR:HG22  | 1:BG:17:ILE:HG12  | 1.77                     | 0.65              |
| 1:AF:7:THR:HG22  | 1:AF:17:ILE:HG12  | 1.77                     | 0.65              |
| 1:AS:94:VAL:HG22 | 1:BX:94:VAL:HG13  | 1.77                     | 0.65              |
| 1:CK:7:THR:HG22  | 1:CK:17:ILE:HG12  | 1.77                     | 0.65              |
| 1:AJ:7:THR:HG22  | 1:AJ:17:ILE:HG12  | 1.79                     | 0.65              |
| 1:AP:7:THR:HG22  | 1:AP:17:ILE:HG12  | 1.79                     | 0.65              |
| 1:BN:7:THR:HG22  | 1:BN:17:ILE:HG12  | 1.79                     | 0.65              |
| 1:CB:7:THR:HG22  | 1:CB:17:ILE:HG12  | 1.77                     | 0.65              |
| 1:CF:7:THR:HG22  | 1:CF:17:ILE:HG12  | 1.79                     | 0.65              |
| 1:DD:7:THR:HG22  | 1:DD:17:ILE:HG12  | 1.79                     | 0.65              |
| 1:AM:7:THR:HG22  | 1:AM:17:ILE:HG12  | 1.79                     | 0.65              |
| 1:BH:7:THR:HG22  | 1:BH:17:ILE:HG12  | 1.79                     | 0.65              |
| 1:CO:7:THR:HG22  | 1:CO:17:ILE:HG12  | 1.79                     | 0.65              |
| 1:AB:1:PRO:HD3   | 1:DA:131:GLU:HB3  | 1.76                     | 0.65              |
| 1:AB:6:ILE:HD13  | 1:DA:123:ILE:HD11 | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AG:94:VAL:HG13 | 1:AZ:94:VAL:HG22 | 1.79                     | 0.65              |
| 1:AV:7:THR:HG22  | 1:AV:17:ILE:HG12 | 1.79                     | 0.65              |
| 1:BQ:7:THR:HG22  | 1:BQ:17:ILE:HG12 | 1.79                     | 0.65              |
| 1:CU:7:THR:HG22  | 1:CU:17:ILE:HG12 | 1.79                     | 0.65              |
| 1:DJ:7:THR:HG22  | 1:DJ:17:ILE:HG12 | 1.79                     | 0.65              |
| 1:AF:131:GLU:CB  | 1:BY:1:PRO:HD3   | 2.26                     | 0.65              |
| 1:AS:2:ALA:HA    | 1:BX:134:TYR:O   | 1.97                     | 0.65              |
| 1:CT:7:THR:HG22  | 1:CT:17:ILE:HG12 | 1.77                     | 0.65              |
| 1:AA:99:PRO:HD2  | 1:AQ:90:ASN:ND2  | 2.12                     | 0.65              |
| 1:CZ:7:THR:HG22  | 1:CZ:17:ILE:HG12 | 1.77                     | 0.65              |
| 1:CR:7:THR:HG22  | 1:CR:17:ILE:HG12 | 1.79                     | 0.65              |
| 1:AA:7:THR:HG22  | 1:AA:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:AI:131:GLU:HB3 | 1:CB:1:PRO:HD3   | 1.79                     | 0.64              |
| 1:BA:7:THR:HG22  | 1:BA:17:ILE:HG12 | 1.77                     | 0.64              |
| 1:AG:7:THR:HG22  | 1:AG:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:BP:21:THR:O    | 1:DG:132:HIS:HB2 | 1.96                     | 0.64              |
| 1:AD:7:THR:HG22  | 1:AD:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:AS:7:THR:HG22  | 1:AS:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:BK:7:THR:HG22  | 1:BK:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:CC:7:THR:HG22  | 1:CC:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:CF:11:HIS:HB2  | 1:CP:109:ASP:HB3 | 1.80                     | 0.64              |
| 1:AP:80:ASP:HB2  | 1:CH:73:THR:O    | 1.97                     | 0.64              |
| 1:AU:134:TYR:CD1 | 1:CI:3:LEU:HD23  | 2.33                     | 0.64              |
| 1:BE:7:THR:HG22  | 1:BE:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:CK:3:LEU:HD23  | 1:CR:134:TYR:HB2 | 1.78                     | 0.64              |
| 1:CL:7:THR:HG22  | 1:CL:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:AP:80:ASP:CB   | 1:CH:73:THR:N    | 2.61                     | 0.64              |
| 1:BC:1:PRO:HD3   | 1:BH:131:GLU:HB3 | 1.79                     | 0.64              |
| 1:BE:21:THR:O    | 1:CZ:132:HIS:HB2 | 1.96                     | 0.64              |
| 1:BO:1:PRO:CD    | 1:DG:131:GLU:HB3 | 2.27                     | 0.64              |
| 1:BZ:7:THR:HG22  | 1:BZ:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:DG:7:THR:HG22  | 1:DG:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:AF:1:PRO:HD3   | 1:BY:131:GLU:CB  | 2.24                     | 0.64              |
| 1:AM:11:HIS:HB2  | 1:CD:109:ASP:HB3 | 1.79                     | 0.64              |
| 1:AY:73:THR:H    | 1:BV:80:ASP:HB2  | 1.62                     | 0.64              |
| 1:BW:7:THR:HG22  | 1:BW:17:ILE:HG12 | 1.79                     | 0.64              |
| 1:BY:7:THR:HG22  | 1:BY:17:ILE:HG12 | 1.77                     | 0.64              |
| 1:AF:90:ASN:CG   | 1:BY:99:PRO:HD2  | 2.23                     | 0.64              |
| 1:AH:20:PRO:HB2  | 1:AZ:134:TYR:CZ  | 2.33                     | 0.64              |
| 1:AH:69:PRO:HB3  | 1:AH:89:THR:HG22 | 1.80                     | 0.64              |
| 1:DK:69:PRO:HB3  | 1:DK:89:THR:HG22 | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AZ:69:PRO:HB3  | 1:AZ:89:THR:HG22 | 1.80                     | 0.63              |
| 1:BR:69:PRO:HB3  | 1:BR:89:THR:HG22 | 1.80                     | 0.63              |
| 1:CI:7:THR:HG22  | 1:CI:17:ILE:HG12 | 1.79                     | 0.63              |
| 1:AE:69:PRO:HB3  | 1:AE:89:THR:HG22 | 1.80                     | 0.63              |
| 1:AJ:21:THR:O    | 1:CE:132:HIS:HB2 | 1.98                     | 0.63              |
| 1:BT:7:THR:HG22  | 1:BT:17:ILE:HG12 | 1.79                     | 0.63              |
| 1:BX:69:PRO:HB3  | 1:BX:89:THR:HG22 | 1.80                     | 0.63              |
| 1:DA:7:THR:HG22  | 1:DA:17:ILE:HG12 | 1.79                     | 0.63              |
| 1:AH:94:VAL:HG22 | 1:CX:94:VAL:HG13 | 1.79                     | 0.63              |
| 1:BI:69:PRO:HB3  | 1:BI:89:THR:HG22 | 1.80                     | 0.63              |
| 1:CP:69:PRO:HB3  | 1:CP:89:THR:HG22 | 1.80                     | 0.63              |
| 1:DB:69:PRO:HB3  | 1:DB:89:THR:HG22 | 1.80                     | 0.63              |
| 1:AN:69:PRO:HB3  | 1:AN:89:THR:HG22 | 1.80                     | 0.63              |
| 1:AR:1:PRO:HD3   | 1:CH:131:GLU:CB  | 2.21                     | 0.63              |
| 1:CX:7:THR:HG22  | 1:CX:17:ILE:HG12 | 1.79                     | 0.63              |
| 1:AF:1:PRO:CD    | 1:BY:131:GLU:HB3 | 2.26                     | 0.63              |
| 1:AK:69:PRO:HB3  | 1:AK:89:THR:HG22 | 1.80                     | 0.63              |
| 1:AQ:20:PRO:HB2  | 1:AT:134:TYR:CZ  | 2.34                     | 0.63              |
| 1:AY:7:THR:HG22  | 1:AY:17:ILE:HG12 | 1.79                     | 0.63              |
| 1:CG:69:PRO:HB3  | 1:CG:89:THR:HG22 | 1.80                     | 0.63              |
| 1:AF:131:GLU:HB3 | 1:BY:1:PRO:CD    | 2.28                     | 0.63              |
| 1:BB:7:THR:HG22  | 1:BB:17:ILE:HG12 | 1.79                     | 0.63              |
| 1:BL:69:PRO:HB3  | 1:BL:89:THR:HG22 | 1.80                     | 0.63              |
| 1:AP:134:TYR:HD1 | 1:AU:3:LEU:HD23  | 1.59                     | 0.63              |
| 1:AQ:69:PRO:HB3  | 1:AQ:89:THR:HG22 | 1.80                     | 0.63              |
| 1:AS:11:HIS:HB2  | 1:BX:109:ASP:HB3 | 1.80                     | 0.63              |
| 1:CJ:69:PRO:HB3  | 1:CJ:89:THR:HG22 | 1.80                     | 0.63              |
| 1:CJ:132:HIS:HE1 | 1:CR:52:GLU:HG3  | 1.64                     | 0.63              |
| 1:AM:131:GLU:HB3 | 1:CD:1:PRO:HD3   | 1.81                     | 0.63              |
| 1:AS:1:PRO:HD2   | 1:BX:132:HIS:O   | 1.99                     | 0.63              |
| 1:AY:134:TYR:HB2 | 1:BV:3:LEU:HD23  | 1.81                     | 0.63              |
| 1:CF:131:GLU:HB3 | 1:CP:1:PRO:CD    | 2.27                     | 0.63              |
| 1:AB:69:PRO:HB3  | 1:AB:89:THR:HG22 | 1.80                     | 0.62              |
| 1:AP:73:THR:H    | 1:AU:80:ASP:HB2  | 1.63                     | 0.62              |
| 1:AB:131:GLU:HB3 | 1:DA:1:PRO:HD3   | 1.81                     | 0.62              |
| 1:AG:52:GLU:HG3  | 1:AZ:132:HIS:HE1 | 1.64                     | 0.62              |
| 1:AK:132:HIS:CE1 | 1:CI:50:VAL:HG23 | 2.33                     | 0.62              |
| 1:BC:69:PRO:HB3  | 1:BC:89:THR:HG22 | 1.80                     | 0.62              |
| 1:BD:131:GLU:HB3 | 1:CW:1:PRO:HD3   | 1.81                     | 0.62              |
| 1:CD:69:PRO:HB3  | 1:CD:89:THR:HG22 | 1.80                     | 0.62              |
| 1:CS:69:PRO:HB3  | 1:CS:89:THR:HG22 | 1.80                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DH:69:PRO:HB3   | 1:DH:89:THR:HG22  | 1.80                     | 0.62              |
| 1:AU:94:VAL:HG22  | 1:CK:94:VAL:HG13  | 1.81                     | 0.62              |
| 1:BF:1:PRO:HD3    | 1:BK:131:GLU:HB3  | 1.79                     | 0.62              |
| 1:AE:109:ASP:HB3  | 1:CU:11:HIS:H     | 1.64                     | 0.62              |
| 1:AW:69:PRO:HB3   | 1:AW:89:THR:HG22  | 1.80                     | 0.62              |
| 1:BF:69:PRO:HB3   | 1:BF:89:THR:HG22  | 1.80                     | 0.62              |
| 1:CC:131:GLU:HB3  | 1:CG:1:PRO:CD     | 2.29                     | 0.62              |
| 1:DE:69:PRO:HB3   | 1:DE:89:THR:HG22  | 1.80                     | 0.62              |
| 1:AP:21:THR:O     | 1:CH:132:HIS:HB2  | 1.99                     | 0.62              |
| 1:AT:69:PRO:HB3   | 1:AT:89:THR:HG22  | 1.80                     | 0.62              |
| 1:BU:69:PRO:HB3   | 1:BU:89:THR:HG22  | 1.80                     | 0.62              |
| 1:CY:69:PRO:HB3   | 1:CY:89:THR:HG22  | 1.80                     | 0.62              |
| 1:AG:134:TYR:CD1  | 1:BA:3:LEU:HD23   | 2.34                     | 0.62              |
| 1:CV:69:PRO:HB3   | 1:CV:89:THR:HG22  | 1.80                     | 0.62              |
| 1:AK:109:ASP:CB   | 1:CI:11:HIS:HB2   | 2.29                     | 0.62              |
| 1:CA:69:PRO:HB3   | 1:CA:89:THR:HG22  | 1.80                     | 0.62              |
| 1:AK:6:ILE:HD13   | 1:CI:123:ILE:HD11 | 1.80                     | 0.61              |
| 1:BE:94:VAL:HG13  | 1:DE:94:VAL:HG22  | 1.80                     | 0.61              |
| 1:BO:69:PRO:HB3   | 1:BO:89:THR:HG22  | 1.80                     | 0.61              |
| 1:CF:94:VAL:HG13  | 1:CP:94:VAL:HG22  | 1.82                     | 0.61              |
| 1:AK:134:TYR:O    | 1:CI:3:LEU:N      | 2.26                     | 0.61              |
| 1:AB:1:PRO:CD     | 1:DA:131:GLU:HB3  | 2.30                     | 0.61              |
| 1:AV:94:VAL:HG13  | 1:CA:94:VAL:HG22  | 1.82                     | 0.61              |
| 1:BB:131:GLU:HB3  | 1:DH:1:PRO:HD3    | 1.82                     | 0.61              |
| 1:AH:90:ASN:ND2   | 1:CX:99:PRO:HD2   | 2.15                     | 0.61              |
| 1:BC:1:PRO:CD     | 1:BH:131:GLU:HB3  | 2.30                     | 0.61              |
| 1:AR:132:HIS:NE2  | 1:CH:52:GLU:OE2   | 2.33                     | 0.61              |
| 1:CM:69:PRO:HB3   | 1:CM:89:THR:HG22  | 1.80                     | 0.61              |
| 1:AR:94:VAL:HG22  | 1:CH:94:VAL:HG13  | 1.81                     | 0.61              |
| 1:AC:1:PRO:HD3    | 1:BV:131:GLU:CB   | 2.27                     | 0.61              |
| 1:AU:88:ARG:HD2   | 1:CK:99:PRO:HB2   | 1.83                     | 0.61              |
| 1:AV:134:TYR:HB2  | 1:CB:3:LEU:HD23   | 1.81                     | 0.61              |
| 1:BT:131:GLU:HB3  | 1:DK:1:PRO:CD     | 2.31                     | 0.61              |
| 1:CM:1:PRO:HD3    | 1:CO:131:GLU:HB3  | 1.83                     | 0.61              |
| 1:BF:109:ASP:HB3  | 1:BK:11:HIS:HB2   | 1.83                     | 0.60              |
| 1:BN:11:HIS:HB2   | 1:BR:109:ASP:HB3  | 1.82                     | 0.60              |
| 1:AN:132:HIS:CE1  | 1:CL:50:VAL:HG23  | 2.36                     | 0.60              |
| 1:BT:123:ILE:HD11 | 1:DK:6:ILE:HD13   | 1.83                     | 0.60              |
| 1:AA:99:PRO:HD2   | 1:AQ:90:ASN:CG    | 2.26                     | 0.60              |
| 1:AI:3:LEU:HD23   | 1:CX:134:TYR:HB2  | 1.84                     | 0.60              |
| 1:BD:1:PRO:HD3    | 1:CW:131:GLU:OE1  | 2.01                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AV:131:GLU:HB3  | 1:CA:1:PRO:HD3   | 1.82                     | 0.60              |
| 1:CJ:1:PRO:CD     | 1:CR:131:GLU:HB3 | 2.32                     | 0.60              |
| 1:AY:94:VAL:HG13  | 1:BU:94:VAL:HG22 | 1.84                     | 0.60              |
| 1:CC:94:VAL:HG13  | 1:CG:94:VAL:HG22 | 1.84                     | 0.60              |
| 1:CY:132:HIS:CE1  | 1:DJ:50:VAL:HG23 | 2.37                     | 0.59              |
| 1:AB:123:ILE:HD11 | 1:DA:6:ILE:HD13  | 1.83                     | 0.59              |
| 1:BB:3:LEU:HD23   | 1:CW:134:TYR:CD1 | 2.37                     | 0.59              |
| 1:BD:78:GLY:O     | 1:BH:74:ILE:HA   | 2.01                     | 0.59              |
| 1:AI:80:ASP:HB2   | 1:CX:73:THR:H    | 1.67                     | 0.59              |
| 1:AS:74:ILE:HA    | 1:BY:78:GLY:O    | 2.01                     | 0.59              |
| 1:AB:132:HIS:CE1  | 1:DA:50:VAL:HG23 | 2.37                     | 0.59              |
| 1:AU:10:ASP:HB2   | 1:CK:109:ASP:HB2 | 1.83                     | 0.59              |
| 1:BD:21:THR:O     | 1:BH:132:HIS:HB2 | 2.02                     | 0.59              |
| 1:AP:79:SER:HA    | 1:CH:74:ILE:HG12 | 1.85                     | 0.59              |
| 1:BI:94:VAL:HG22  | 1:BQ:94:VAL:HG13 | 1.84                     | 0.59              |
| 1:AE:8:LEU:HB3    | 1:CU:116:SER:OG  | 2.02                     | 0.59              |
| 1:AE:99:PRO:HD2   | 1:CU:90:ASN:CG   | 2.28                     | 0.59              |
| 1:AR:132:HIS:HB2  | 1:CF:21:THR:O    | 2.02                     | 0.59              |
| 1:AU:11:HIS:H     | 1:CK:109:ASP:CB  | 2.13                     | 0.59              |
| 1:BT:73:THR:H     | 1:DL:80:ASP:HB2  | 1.66                     | 0.59              |
| 1:AH:1:PRO:CD     | 1:CX:131:GLU:HB3 | 2.33                     | 0.59              |
| 1:BD:41:ILE:HG23  | 1:BD:42:GLY:H    | 1.68                     | 0.59              |
| 1:BJ:50:VAL:HG23  | 1:DC:132:HIS:CE1 | 2.38                     | 0.59              |
| 1:AL:41:ILE:HG23  | 1:AL:42:GLY:H    | 1.68                     | 0.59              |
| 1:BC:94:VAL:HG22  | 1:BH:94:VAL:HG13 | 1.85                     | 0.59              |
| 1:CC:62:VAL:CG2   | 1:CC:96:PHE:HB2  | 2.33                     | 0.59              |
| 1:CH:41:ILE:HG23  | 1:CH:42:GLY:H    | 1.68                     | 0.59              |
| 1:CW:41:ILE:HG23  | 1:CW:42:GLY:H    | 1.68                     | 0.59              |
| 1:AF:41:ILE:HG23  | 1:AF:42:GLY:H    | 1.68                     | 0.59              |
| 1:AJ:62:VAL:CG2   | 1:AJ:96:PHE:HB2  | 2.33                     | 0.59              |
| 1:AP:80:ASP:HB3   | 1:CH:73:THR:N    | 2.17                     | 0.59              |
| 1:BA:41:ILE:HG23  | 1:BA:42:GLY:H    | 1.68                     | 0.59              |
| 1:BE:123:ILE:HD11 | 1:DE:6:ILE:HD13  | 1.83                     | 0.59              |
| 1:BJ:41:ILE:HG23  | 1:BJ:42:GLY:H    | 1.68                     | 0.59              |
| 1:DI:41:ILE:HG23  | 1:DI:42:GLY:H    | 1.68                     | 0.59              |
| 1:AG:62:VAL:CG2   | 1:AG:96:PHE:HB2  | 2.33                     | 0.58              |
| 1:AI:41:ILE:HG23  | 1:AI:42:GLY:H    | 1.68                     | 0.58              |
| 1:AY:1:PRO:HD3    | 1:BU:131:GLU:HB3 | 1.84                     | 0.58              |
| 1:BP:80:ASP:CB    | 1:DG:73:THR:H    | 2.14                     | 0.58              |
| 1:CF:123:ILE:HD11 | 1:CP:6:ILE:HD13  | 1.85                     | 0.58              |
| 1:DD:62:VAL:CG2   | 1:DD:96:PHE:HB2  | 2.33                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AP:62:VAL:CG2  | 1:AP:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:AU:41:ILE:HG23 | 1:AU:42:GLY:H     | 1.68                     | 0.58              |
| 1:BH:62:VAL:CG2  | 1:BH:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:CF:62:VAL:CG2  | 1:CF:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:CO:62:VAL:CG2  | 1:CO:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:DG:62:VAL:CG2  | 1:DG:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:AH:132:HIS:HE1 | 1:CX:52:GLU:HG3   | 1.69                     | 0.58              |
| 1:AM:94:VAL:HG13 | 1:CD:94:VAL:HG22  | 1.86                     | 0.58              |
| 1:AV:62:VAL:CG2  | 1:AV:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:BQ:62:VAL:CG2  | 1:BQ:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:BT:62:VAL:CG2  | 1:BT:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:CT:41:ILE:HG23 | 1:CT:42:GLY:H     | 1.68                     | 0.58              |
| 1:DL:41:ILE:HG23 | 1:DL:42:GLY:H     | 1.68                     | 0.58              |
| 1:AD:62:VAL:CG2  | 1:AD:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:AS:62:VAL:CG2  | 1:AS:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:AX:41:ILE:HG23 | 1:AX:42:GLY:H     | 1.68                     | 0.58              |
| 1:BG:41:ILE:HG23 | 1:BG:42:GLY:H     | 1.68                     | 0.58              |
| 1:BN:62:VAL:CG2  | 1:BN:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:BW:131:GLU:HB3 | 1:DB:1:PRO:HD3    | 1.84                     | 0.58              |
| 1:CB:41:ILE:HG23 | 1:CB:42:GLY:H     | 1.68                     | 0.58              |
| 1:DA:62:VAL:CG2  | 1:DA:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:DF:41:ILE:HG23 | 1:DF:42:GLY:H     | 1.68                     | 0.58              |
| 1:AA:131:GLU:HB3 | 1:AQ:1:PRO:HD3    | 1.84                     | 0.58              |
| 1:AE:99:PRO:HD2  | 1:CU:90:ASN:OD1   | 2.03                     | 0.58              |
| 1:AK:50:VAL:HG23 | 1:CI:132:HIS:CE1  | 2.39                     | 0.58              |
| 1:AM:62:VAL:CG2  | 1:AM:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:CK:41:ILE:HG23 | 1:CK:42:GLY:H     | 1.68                     | 0.58              |
| 1:AF:88:ARG:HD2  | 1:BY:99:PRO:HB2   | 1.84                     | 0.58              |
| 1:BK:62:VAL:CG2  | 1:BK:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:BM:41:ILE:HG23 | 1:BM:42:GLY:H     | 1.68                     | 0.58              |
| 1:CU:62:VAL:CG2  | 1:CU:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:CZ:41:ILE:HG23 | 1:CZ:42:GLY:H     | 1.68                     | 0.58              |
| 1:AA:62:VAL:CG2  | 1:AA:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:CL:62:VAL:CG2  | 1:CL:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:AH:6:ILE:HD13  | 1:CX:123:ILE:HD11 | 1.86                     | 0.58              |
| 1:AW:21:THR:O    | 1:CA:132:HIS:HB2  | 2.04                     | 0.58              |
| 1:BI:131:GLU:HB3 | 1:BQ:1:PRO:HD3    | 1.85                     | 0.58              |
| 1:CI:62:VAL:CG2  | 1:CI:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:DC:41:ILE:HG23 | 1:DC:42:GLY:H     | 1.68                     | 0.58              |
| 1:BB:62:VAL:CG2  | 1:BB:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:BE:134:TYR:HB2 | 1:DF:3:LEU:HD23   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BS:41:ILE:HG23  | 1:BS:42:GLY:H     | 1.68                     | 0.58              |
| 1:CC:73:THR:H     | 1:CH:80:ASP:CB    | 2.16                     | 0.58              |
| 1:AA:11:HIS:CB    | 1:AQ:109:ASP:HB3  | 2.34                     | 0.58              |
| 1:AH:134:TYR:CD1  | 1:CY:3:LEU:HD23   | 2.39                     | 0.58              |
| 1:AR:41:ILE:HG23  | 1:AR:42:GLY:H     | 1.68                     | 0.58              |
| 1:BE:62:VAL:CG2   | 1:BE:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:BE:132:HIS:HB2  | 1:DF:21:THR:O     | 2.04                     | 0.58              |
| 1:BZ:62:VAL:CG2   | 1:BZ:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:CE:41:ILE:HG23  | 1:CE:42:GLY:H     | 1.68                     | 0.58              |
| 1:DJ:62:VAL:CG2   | 1:DJ:96:PHE:HB2   | 2.33                     | 0.58              |
| 1:AF:123:ILE:HD11 | 1:BY:6:ILE:HD13   | 1.83                     | 0.57              |
| 1:AL:50:VAL:HG23  | 1:CE:132:HIS:CE1  | 2.39                     | 0.57              |
| 1:CR:62:VAL:CG2   | 1:CR:96:PHE:HB2   | 2.33                     | 0.57              |
| 1:AK:1:PRO:CD     | 1:CI:131:GLU:HB3  | 2.34                     | 0.57              |
| 1:AV:1:PRO:HD3    | 1:CA:131:GLU:HB3  | 1.85                     | 0.57              |
| 1:AY:11:HIS:HB2   | 1:BU:109:ASP:HB3  | 1.85                     | 0.57              |
| 1:BP:41:ILE:HG23  | 1:BP:42:GLY:H     | 1.68                     | 0.57              |
| 1:BW:62:VAL:CG2   | 1:BW:96:PHE:HB2   | 2.33                     | 0.57              |
| 1:AE:132:HIS:CE1  | 1:CU:50:VAL:HG23  | 2.39                     | 0.57              |
| 1:BD:1:PRO:HD3    | 1:CW:131:GLU:HB3  | 1.85                     | 0.57              |
| 1:BD:134:TYR:CD1  | 1:CU:3:LEU:HD23   | 2.39                     | 0.57              |
| 1:BV:41:ILE:HG23  | 1:BV:42:GLY:H     | 1.68                     | 0.57              |
| 1:CN:41:ILE:HG23  | 1:CN:42:GLY:H     | 1.68                     | 0.57              |
| 1:CX:62:VAL:CG2   | 1:CX:96:PHE:HB2   | 2.33                     | 0.57              |
| 1:AR:98:LEU:HD13  | 1:AR:107:ARG:HD2  | 1.87                     | 0.57              |
| 1:BJ:3:LEU:HD23   | 1:BQ:134:TYR:HB2  | 1.86                     | 0.57              |
| 1:AR:1:PRO:HD2    | 1:CH:132:HIS:O    | 2.05                     | 0.57              |
| 1:AY:62:VAL:CG2   | 1:AY:96:PHE:HB2   | 2.33                     | 0.57              |
| 1:BP:98:LEU:HD13  | 1:BP:107:ARG:HD2  | 1.87                     | 0.57              |
| 1:BF:1:PRO:CD     | 1:BK:131:GLU:HB3  | 2.35                     | 0.57              |
| 1:BV:98:LEU:HD13  | 1:BV:107:ARG:HD2  | 1.87                     | 0.57              |
| 1:BD:98:LEU:HD13  | 1:BD:107:ARG:HD2  | 1.87                     | 0.57              |
| 1:BG:98:LEU:HD13  | 1:BG:107:ARG:HD2  | 1.87                     | 0.57              |
| 1:BJ:21:THR:O     | 1:BQ:132:HIS:HB2  | 2.05                     | 0.57              |
| 1:BY:41:ILE:HG23  | 1:BY:42:GLY:H     | 1.68                     | 0.57              |
| 1:AI:21:THR:O     | 1:CX:132:HIS:HB2  | 2.03                     | 0.57              |
| 1:AI:24:ASP:OD1   | 1:AI:25:LYS:N     | 2.38                     | 0.57              |
| 1:AO:41:ILE:HG23  | 1:AO:42:GLY:H     | 1.68                     | 0.57              |
| 1:AU:98:LEU:HD13  | 1:AU:107:ARG:HD2  | 1.87                     | 0.57              |
| 1:BF:6:ILE:HD13   | 1:BK:123:ILE:HD11 | 1.85                     | 0.57              |
| 1:BY:24:ASP:OD1   | 1:BY:25:LYS:N     | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CN:98:LEU:HD13  | 1:CN:107:ARG:HD2  | 1.87                     | 0.57              |
| 1:DL:98:LEU:HD13  | 1:DL:107:ARG:HD2  | 1.87                     | 0.57              |
| 1:AU:24:ASP:OD1   | 1:AU:25:LYS:N     | 2.38                     | 0.57              |
| 1:AX:24:ASP:OD1   | 1:AX:25:LYS:N     | 2.38                     | 0.57              |
| 1:BG:24:ASP:OD1   | 1:BG:25:LYS:N     | 2.38                     | 0.57              |
| 1:CQ:41:ILE:HG23  | 1:CQ:42:GLY:H     | 1.68                     | 0.57              |
| 1:AC:41:ILE:HG23  | 1:AC:42:GLY:H     | 1.68                     | 0.56              |
| 1:AL:132:HIS:HB2  | 1:CC:21:THR:O     | 2.04                     | 0.56              |
| 1:AM:132:HIS:HB2  | 1:CE:21:THR:O     | 2.04                     | 0.56              |
| 1:BT:11:HIS:HB2   | 1:DK:109:ASP:HB3  | 1.87                     | 0.56              |
| 1:BW:50:VAL:HG23  | 1:DB:132:HIS:CE1  | 2.39                     | 0.56              |
| 1:CE:98:LEU:HD13  | 1:CE:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:AC:98:LEU:HD13  | 1:AC:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:AB:109:ASP:HB3  | 1:DA:11:HIS:CB    | 2.35                     | 0.56              |
| 1:AB:131:GLU:CB   | 1:DA:1:PRO:HD3    | 2.35                     | 0.56              |
| 1:AG:11:HIS:NE2   | 1:AZ:108:GLU:OE1  | 2.39                     | 0.56              |
| 1:AV:11:HIS:HB2   | 1:CA:109:ASP:HB3  | 1.87                     | 0.56              |
| 1:BG:50:VAL:HG23  | 1:CZ:132:HIS:CE1  | 2.40                     | 0.56              |
| 1:BG:132:HIS:HB2  | 1:CX:21:THR:O     | 2.05                     | 0.56              |
| 1:BJ:24:ASP:OD1   | 1:BJ:25:LYS:N     | 2.38                     | 0.56              |
| 1:BM:24:ASP:OD1   | 1:BM:25:LYS:N     | 2.38                     | 0.56              |
| 1:BN:50:VAL:HG23  | 1:BR:132:HIS:CE1  | 2.40                     | 0.56              |
| 1:BN:131:GLU:HB3  | 1:BR:1:PRO:HD3    | 1.87                     | 0.56              |
| 1:BP:24:ASP:OD1   | 1:BP:25:LYS:N     | 2.38                     | 0.56              |
| 1:BW:73:THR:H     | 1:DC:80:ASP:HB2   | 1.70                     | 0.56              |
| 1:AA:94:VAL:HG13  | 1:AQ:94:VAL:HG22  | 1.88                     | 0.56              |
| 1:AR:94:VAL:HG13  | 1:CH:94:VAL:HG22  | 1.87                     | 0.56              |
| 1:AT:62:VAL:CG2   | 1:AT:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:AW:62:VAL:CG2   | 1:AW:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:BI:6:ILE:HD13   | 1:BQ:123:ILE:HD11 | 1.87                     | 0.56              |
| 1:BR:62:VAL:CG2   | 1:BR:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:CT:98:LEU:HD13  | 1:CT:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:AG:73:THR:H     | 1:BA:80:ASP:HB2   | 1.69                     | 0.56              |
| 1:CC:132:HIS:HB2  | 1:CH:21:THR:O     | 2.06                     | 0.56              |
| 1:CK:24:ASP:OD1   | 1:CK:25:LYS:N     | 2.38                     | 0.56              |
| 1:CM:62:VAL:CG2   | 1:CM:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:CW:24:ASP:OD1   | 1:CW:25:LYS:N     | 2.38                     | 0.56              |
| 1:AG:130:VAL:HG11 | 1:AZ:60:PHE:CD1   | 2.40                     | 0.56              |
| 1:AQ:62:VAL:CG2   | 1:AQ:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:AS:1:PRO:HD3    | 1:BX:131:GLU:HB3  | 1.87                     | 0.56              |
| 1:AZ:62:VAL:CG2   | 1:AZ:96:PHE:HB2   | 2.36                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BC:62:VAL:CG2   | 1:BC:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:BS:24:ASP:OD1   | 1:BS:25:LYS:N     | 2.38                     | 0.56              |
| 1:BY:98:LEU:HD13  | 1:BY:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:CH:98:LEU:HD13  | 1:CH:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:CM:94:VAL:HG22  | 1:CO:94:VAL:HG13  | 1.88                     | 0.56              |
| 1:DB:62:VAL:CG2   | 1:DB:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:DE:62:VAL:CG2   | 1:DE:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:DK:62:VAL:CG2   | 1:DK:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:AE:62:VAL:CG2   | 1:AE:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:AK:62:VAL:CG2   | 1:AK:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:AO:98:LEU:HD13  | 1:AO:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:AU:126:THR:HG21 | 1:CK:48:SER:OG    | 2.06                     | 0.56              |
| 1:BL:62:VAL:CG2   | 1:BL:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:CA:62:VAL:CG2   | 1:CA:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:CG:62:VAL:CG2   | 1:CG:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:AB:50:VAL:HG23  | 1:DA:132:HIS:CE1  | 2.40                     | 0.56              |
| 1:AB:62:VAL:CG2   | 1:AB:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:AG:109:ASP:HB3  | 1:AZ:11:HIS:H     | 1.70                     | 0.56              |
| 1:AK:1:PRO:HD3    | 1:CI:131:GLU:HB3  | 1.87                     | 0.56              |
| 1:AX:98:LEU:HD13  | 1:AX:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:BC:132:HIS:HB2  | 1:BI:21:THR:O     | 2.06                     | 0.56              |
| 1:BF:62:VAL:CG2   | 1:BF:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:BJ:98:LEU:HD13  | 1:BJ:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:BP:1:PRO:HD3    | 1:DF:131:GLU:HB3  | 1.87                     | 0.56              |
| 1:CB:24:ASP:OD1   | 1:CB:25:LYS:N     | 2.38                     | 0.56              |
| 1:CS:62:VAL:CG2   | 1:CS:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:CZ:24:ASP:OD1   | 1:CZ:25:LYS:N     | 2.38                     | 0.56              |
| 1:DH:62:VAL:CG2   | 1:DH:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:DI:24:ASP:OD1   | 1:DI:25:LYS:N     | 2.38                     | 0.56              |
| 1:AA:134:TYR:HB2  | 1:AR:3:LEU:HD23   | 1.88                     | 0.56              |
| 1:BN:3:LEU:HD23   | 1:DF:134:TYR:CD1  | 2.41                     | 0.56              |
| 1:BU:62:VAL:CG2   | 1:BU:96:PHE:HB2   | 2.36                     | 0.56              |
| 1:CZ:98:LEU:HD13  | 1:CZ:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:AF:90:ASN:ND2   | 1:BY:99:PRO:HD2   | 2.20                     | 0.56              |
| 1:BA:98:LEU:HD13  | 1:BA:107:ARG:HD2  | 1.87                     | 0.56              |
| 1:BB:94:VAL:HG13  | 1:DH:94:VAL:HG22  | 1.88                     | 0.56              |
| 1:BB:109:ASP:HB3  | 1:DH:11:HIS:H     | 1.71                     | 0.56              |
| 1:BI:3:LEU:N      | 1:BQ:134:TYR:O    | 2.25                     | 0.56              |
| 1:BN:123:ILE:HD11 | 1:BR:6:ILE:HD13   | 1.88                     | 0.56              |
| 1:BO:6:ILE:HD13   | 1:DG:123:ILE:HD11 | 1.88                     | 0.56              |
| 1:BO:62:VAL:CG2   | 1:BO:96:PHE:HB2   | 2.36                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BW:11:HIS:HB2   | 1:DB:109:ASP:HB3 | 1.87                     | 0.56              |
| 1:CQ:24:ASP:OD1   | 1:CQ:25:LYS:N    | 2.38                     | 0.56              |
| 1:CW:98:LEU:HD13  | 1:CW:107:ARG:HD2 | 1.87                     | 0.56              |
| 1:DC:24:ASP:OD1   | 1:DC:25:LYS:N    | 2.38                     | 0.56              |
| 1:DC:98:LEU:HD13  | 1:DC:107:ARG:HD2 | 1.87                     | 0.56              |
| 1:DI:98:LEU:HD13  | 1:DI:107:ARG:HD2 | 1.87                     | 0.56              |
| 1:AI:98:LEU:HD13  | 1:AI:107:ARG:HD2 | 1.87                     | 0.55              |
| 1:AL:132:HIS:NE2  | 1:CE:52:GLU:OE2  | 2.36                     | 0.55              |
| 1:AU:133:PHE:CD1  | 1:CK:3:LEU:HD12  | 2.41                     | 0.55              |
| 1:CB:98:LEU:HD13  | 1:CB:107:ARG:HD2 | 1.87                     | 0.55              |
| 1:CF:132:HIS:HB2  | 1:CQ:21:THR:O    | 2.06                     | 0.55              |
| 1:CH:24:ASP:OD1   | 1:CH:25:LYS:N    | 2.38                     | 0.55              |
| 1:CV:62:VAL:CG2   | 1:CV:96:PHE:HB2  | 2.36                     | 0.55              |
| 1:DL:24:ASP:OD1   | 1:DL:25:LYS:N    | 2.38                     | 0.55              |
| 1:AL:1:PRO:HD2    | 1:CE:132:HIS:O   | 2.05                     | 0.55              |
| 1:AS:20:PRO:HB2   | 1:CK:134:TYR:CZ  | 2.41                     | 0.55              |
| 1:BA:24:ASP:OD1   | 1:BA:25:LYS:N    | 2.38                     | 0.55              |
| 1:BG:1:PRO:HD2    | 1:CZ:132:HIS:O   | 2.06                     | 0.55              |
| 1:BI:62:VAL:CG2   | 1:BI:96:PHE:HB2  | 2.36                     | 0.55              |
| 1:BM:98:LEU:HD13  | 1:BM:107:ARG:HD2 | 1.87                     | 0.55              |
| 1:BX:62:VAL:CG2   | 1:BX:96:PHE:HB2  | 2.36                     | 0.55              |
| 1:CK:98:LEU:HD13  | 1:CK:107:ARG:HD2 | 1.87                     | 0.55              |
| 1:CN:21:THR:O     | 1:CO:132:HIS:HB2 | 2.06                     | 0.55              |
| 1:AJ:80:ASP:CB    | 1:CE:73:THR:H    | 2.19                     | 0.55              |
| 1:AR:1:PRO:CD     | 1:CH:131:GLU:HB3 | 2.26                     | 0.55              |
| 1:BS:98:LEU:HD13  | 1:BS:107:ARG:HD2 | 1.87                     | 0.55              |
| 1:CE:24:ASP:OD1   | 1:CE:25:LYS:N    | 2.38                     | 0.55              |
| 1:DF:98:LEU:HD13  | 1:DF:107:ARG:HD2 | 1.87                     | 0.55              |
| 1:AH:90:ASN:CG    | 1:CX:99:PRO:HD2  | 2.31                     | 0.55              |
| 1:AP:94:VAL:HG13  | 1:AT:94:VAL:HG22 | 1.88                     | 0.55              |
| 1:BI:1:PRO:CD     | 1:BQ:131:GLU:HB3 | 2.35                     | 0.55              |
| 1:BT:132:HIS:NE2  | 1:DK:50:VAL:HG23 | 2.22                     | 0.55              |
| 1:CC:123:ILE:HD11 | 1:CG:6:ILE:HD13  | 1.87                     | 0.55              |
| 1:AH:62:VAL:CG2   | 1:AH:96:PHE:HB2  | 2.36                     | 0.55              |
| 1:BT:52:GLU:HG3   | 1:DK:132:HIS:HE1 | 1.71                     | 0.55              |
| 1:CF:134:TYR:HB2  | 1:CQ:3:LEU:HD23  | 1.89                     | 0.55              |
| 1:CQ:98:LEU:HD13  | 1:CQ:107:ARG:HD2 | 1.87                     | 0.55              |
| 1:CY:62:VAL:CG2   | 1:CY:96:PHE:HB2  | 2.36                     | 0.55              |
| 1:AN:109:ASP:HB3  | 1:CL:11:HIS:CB   | 2.36                     | 0.55              |
| 1:AR:24:ASP:OD1   | 1:AR:25:LYS:N    | 2.38                     | 0.55              |
| 1:CP:62:VAL:CG2   | 1:CP:96:PHE:HB2  | 2.36                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:CT:24:ASP:OD1   | 1:CT:25:LYS:N    | 2.38                     | 0.55              |
| 1:AG:80:ASP:CB    | 1:CB:73:THR:H    | 2.20                     | 0.55              |
| 1:AR:62:VAL:CG2   | 1:AR:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:BJ:62:VAL:CG2   | 1:BJ:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:BM:62:VAL:CG2   | 1:BM:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:CQ:62:VAL:CG2   | 1:CQ:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:CW:62:VAL:CG2   | 1:CW:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:CZ:62:VAL:CG2   | 1:CZ:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:BN:131:GLU:HB3  | 1:BR:1:PRO:CD    | 2.37                     | 0.55              |
| 1:CD:62:VAL:CG2   | 1:CD:96:PHE:HB2  | 2.36                     | 0.55              |
| 1:CH:62:VAL:CG2   | 1:CH:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:CJ:62:VAL:CG2   | 1:CJ:96:PHE:HB2  | 2.36                     | 0.55              |
| 1:CN:62:VAL:CG2   | 1:CN:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:CY:109:ASP:HB3  | 1:DJ:11:HIS:CB   | 2.36                     | 0.55              |
| 1:AA:123:ILE:HD11 | 1:AQ:6:ILE:HD13  | 1.88                     | 0.55              |
| 1:AF:99:PRO:HD2   | 1:BY:90:ASN:CG   | 2.31                     | 0.55              |
| 1:AH:134:TYR:CZ   | 1:CY:20:PRO:HB2  | 2.42                     | 0.55              |
| 1:AL:98:LEU:HD13  | 1:AL:107:ARG:HD2 | 1.87                     | 0.55              |
| 1:AO:24:ASP:OD1   | 1:AO:25:LYS:N    | 2.38                     | 0.55              |
| 1:AO:62:VAL:CG2   | 1:AO:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:AU:131:GLU:HB3  | 1:CK:1:PRO:HD3   | 1.88                     | 0.55              |
| 1:BN:52:GLU:HG3   | 1:BR:132:HIS:HE1 | 1.71                     | 0.55              |
| 1:BS:62:VAL:CG2   | 1:BS:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:CB:62:VAL:CG2   | 1:CB:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:DL:62:VAL:CG2   | 1:DL:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:AE:123:ILE:HD11 | 1:CU:6:ILE:HD13  | 1.90                     | 0.55              |
| 1:AF:62:VAL:CG2   | 1:AF:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:AL:62:VAL:CG2   | 1:AL:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:AL:94:VAL:HG22  | 1:CE:94:VAL:HG13 | 1.89                     | 0.55              |
| 1:AM:134:TYR:HB2  | 1:CE:3:LEU:HD23  | 1.89                     | 0.55              |
| 1:AS:73:THR:H     | 1:BY:80:ASP:CB   | 2.20                     | 0.55              |
| 1:AU:62:VAL:CG2   | 1:AU:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:BA:62:VAL:CG2   | 1:BA:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:BD:62:VAL:CG2   | 1:BD:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:CN:24:ASP:OD1   | 1:CN:25:LYS:N    | 2.38                     | 0.55              |
| 1:CT:62:VAL:CG2   | 1:CT:96:PHE:HB2  | 2.37                     | 0.55              |
| 1:AC:24:ASP:OD1   | 1:AC:25:LYS:N    | 2.38                     | 0.54              |
| 1:AF:24:ASP:OD1   | 1:AF:25:LYS:N    | 2.38                     | 0.54              |
| 1:AG:134:TYR:HB2  | 1:BA:3:LEU:HD23  | 1.88                     | 0.54              |
| 1:BZ:62:VAL:HG23  | 1:BZ:96:PHE:HB2  | 1.90                     | 0.54              |
| 1:DA:62:VAL:HG23  | 1:DA:96:PHE:HB2  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AF:91:ARG:O     | 1:BY:96:PHE:HA    | 2.07                     | 0.54              |
| 1:AF:98:LEU:HD13  | 1:AF:107:ARG:HD2  | 1.87                     | 0.54              |
| 1:AI:62:VAL:CG2   | 1:AI:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:AN:62:VAL:CG2   | 1:AN:96:PHE:HB2   | 2.36                     | 0.54              |
| 1:AA:62:VAL:HG23  | 1:AA:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:AC:62:VAL:CG2   | 1:AC:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:AG:116:SER:OG   | 1:AZ:8:LEU:HB3    | 2.07                     | 0.54              |
| 1:AL:24:ASP:OD1   | 1:AL:25:LYS:N     | 2.38                     | 0.54              |
| 1:AS:6:ILE:HD13   | 1:BX:123:ILE:HD11 | 1.88                     | 0.54              |
| 1:BQ:62:VAL:HG23  | 1:BQ:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:CC:52:GLU:HG3   | 1:CG:132:HIS:HE1  | 1.70                     | 0.54              |
| 1:CL:62:VAL:HG23  | 1:CL:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:AC:132:HIS:HB2  | 1:BT:21:THR:O     | 2.08                     | 0.54              |
| 1:AG:62:VAL:HG23  | 1:AG:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:AM:62:VAL:HG23  | 1:AM:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:AY:62:VAL:HG23  | 1:AY:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:BF:132:HIS:CE1  | 1:BK:50:VAL:HG23  | 2.42                     | 0.54              |
| 1:BV:24:ASP:OD1   | 1:BV:25:LYS:N     | 2.38                     | 0.54              |
| 1:DC:62:VAL:CG2   | 1:DC:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:AF:99:PRO:HB2   | 1:BY:88:ARG:HD2   | 1.88                     | 0.54              |
| 1:AS:62:VAL:HG23  | 1:AS:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:BG:62:VAL:CG2   | 1:BG:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:DG:62:VAL:HG23  | 1:DG:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:AP:1:PRO:HG3    | 1:AT:125:SER:HB3  | 1.90                     | 0.54              |
| 1:BT:62:VAL:HG23  | 1:BT:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:BY:62:VAL:CG2   | 1:BY:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:CO:62:VAL:HG23  | 1:CO:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:CX:62:VAL:HG23  | 1:CX:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:AP:62:VAL:HG23  | 1:AP:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:BE:73:THR:H     | 1:DF:80:ASP:CB    | 2.19                     | 0.54              |
| 1:CU:62:VAL:HG23  | 1:CU:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:DJ:62:VAL:HG23  | 1:DJ:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:AA:132:HIS:HB2  | 1:AR:21:THR:O     | 2.07                     | 0.54              |
| 1:AP:132:HIS:HB2  | 1:AU:21:THR:O     | 2.08                     | 0.54              |
| 1:AU:130:VAL:HG11 | 1:CK:60:PHE:CD1   | 2.42                     | 0.54              |
| 1:BP:62:VAL:CG2   | 1:BP:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:CJ:132:HIS:HB2  | 1:CS:21:THR:O     | 2.08                     | 0.54              |
| 1:CK:62:VAL:CG2   | 1:CK:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:AY:1:PRO:HD3    | 1:BU:131:GLU:CB   | 2.38                     | 0.54              |
| 1:BV:62:VAL:CG2   | 1:BV:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:AT:21:THR:OG1   | 1:AT:32:ARG:HB3   | 2.08                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AV:6:ILE:HD13  | 1:CA:123:ILE:HD11 | 1.90                     | 0.54              |
| 1:BH:62:VAL:HG23 | 1:BH:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:CF:62:VAL:HG23 | 1:CF:96:PHE:HB2   | 1.90                     | 0.54              |
| 1:DB:21:THR:OG1  | 1:DB:32:ARG:HB3   | 2.08                     | 0.54              |
| 1:DF:24:ASP:OD1  | 1:DF:25:LYS:N     | 2.38                     | 0.54              |
| 1:DI:62:VAL:CG2  | 1:DI:96:PHE:HB2   | 2.37                     | 0.54              |
| 1:AB:21:THR:OG1  | 1:AB:32:ARG:HB3   | 2.09                     | 0.53              |
| 1:AE:21:THR:OG1  | 1:AE:32:ARG:HB3   | 2.09                     | 0.53              |
| 1:AM:73:THR:H    | 1:CE:80:ASP:HB2   | 1.73                     | 0.53              |
| 1:BB:131:GLU:HB3 | 1:DH:1:PRO:CD     | 2.37                     | 0.53              |
| 1:BD:24:ASP:OD1  | 1:BD:25:LYS:N     | 2.38                     | 0.53              |
| 1:CJ:21:THR:OG1  | 1:CJ:32:ARG:HB3   | 2.09                     | 0.53              |
| 1:DH:21:THR:OG1  | 1:DH:32:ARG:HB3   | 2.08                     | 0.53              |
| 1:AA:109:ASP:CB  | 1:AQ:11:HIS:H     | 2.19                     | 0.53              |
| 1:AF:96:PHE:HA   | 1:BY:91:ARG:O     | 2.08                     | 0.53              |
| 1:AN:1:PRO:HD3   | 1:CL:131:GLU:HB3  | 1.89                     | 0.53              |
| 1:AQ:21:THR:OG1  | 1:AQ:32:ARG:HB3   | 2.09                     | 0.53              |
| 1:AX:62:VAL:CG2  | 1:AX:96:PHE:HB2   | 2.37                     | 0.53              |
| 1:BI:131:GLU:CB  | 1:BQ:1:PRO:HD3    | 2.38                     | 0.53              |
| 1:BO:21:THR:OG1  | 1:BO:32:ARG:HB3   | 2.08                     | 0.53              |
| 1:DF:62:VAL:CG2  | 1:DF:96:PHE:HB2   | 2.37                     | 0.53              |
| 1:AU:11:HIS:NE2  | 1:CK:108:GLU:OE1  | 2.41                     | 0.53              |
| 1:AY:6:ILE:HD13  | 1:BU:123:ILE:HD11 | 1.90                     | 0.53              |
| 1:BK:62:VAL:HG23 | 1:BK:96:PHE:HB2   | 1.90                     | 0.53              |
| 1:BC:21:THR:OG1  | 1:BC:32:ARG:HB3   | 2.09                     | 0.53              |
| 1:BN:132:HIS:CE1 | 1:BR:50:VAL:HG23  | 2.43                     | 0.53              |
| 1:BW:62:VAL:HG23 | 1:BW:96:PHE:HB2   | 1.90                     | 0.53              |
| 1:CE:62:VAL:CG2  | 1:CE:96:PHE:HB2   | 2.37                     | 0.53              |
| 1:CR:62:VAL:HG23 | 1:CR:96:PHE:HB2   | 1.90                     | 0.53              |
| 1:AJ:62:VAL:HG23 | 1:AJ:96:PHE:HB2   | 1.90                     | 0.53              |
| 1:AZ:21:THR:OG1  | 1:AZ:32:ARG:HB3   | 2.09                     | 0.53              |
| 1:BL:21:THR:OG1  | 1:BL:32:ARG:HB3   | 2.08                     | 0.53              |
| 1:CM:21:THR:OG1  | 1:CM:32:ARG:HB3   | 2.09                     | 0.53              |
| 1:CM:132:HIS:CE1 | 1:CO:50:VAL:HG23  | 2.43                     | 0.53              |
| 1:CS:44:TYR:HE1  | 1:CS:68:VAL:HG13  | 1.74                     | 0.53              |
| 1:DK:21:THR:OG1  | 1:DK:32:ARG:HB3   | 2.08                     | 0.53              |
| 1:AC:6:ILE:HD13  | 1:BV:123:ILE:HD11 | 1.91                     | 0.53              |
| 1:AH:44:TYR:HE1  | 1:AH:68:VAL:HG13  | 1.74                     | 0.53              |
| 1:AK:109:ASP:CA  | 1:CI:11:HIS:HB2   | 2.39                     | 0.53              |
| 1:BB:50:VAL:HG23 | 1:DH:132:HIS:CE1  | 2.44                     | 0.53              |
| 1:BB:62:VAL:HG23 | 1:BB:96:PHE:HB2   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BI:123:ILE:HD11 | 1:BQ:6:ILE:HD13  | 1.91                     | 0.53              |
| 1:BN:62:VAL:HG23  | 1:BN:96:PHE:HB2  | 1.90                     | 0.53              |
| 1:CD:21:THR:OG1   | 1:CD:32:ARG:HB3  | 2.08                     | 0.53              |
| 1:AK:44:TYR:HE1   | 1:AK:68:VAL:HG13 | 1.74                     | 0.53              |
| 1:AN:21:THR:OG1   | 1:AN:32:ARG:HB3  | 2.09                     | 0.53              |
| 1:AQ:44:TYR:HE1   | 1:AQ:68:VAL:HG13 | 1.74                     | 0.53              |
| 1:AT:44:TYR:HE1   | 1:AT:68:VAL:HG13 | 1.74                     | 0.53              |
| 1:BI:21:THR:OG1   | 1:BI:32:ARG:HB3  | 2.09                     | 0.53              |
| 1:CD:44:TYR:HE1   | 1:CD:68:VAL:HG13 | 1.74                     | 0.53              |
| 1:CP:21:THR:OG1   | 1:CP:32:ARG:HB3  | 2.09                     | 0.53              |
| 1:AF:21:THR:O     | 1:CU:132:HIS:HB2 | 2.09                     | 0.53              |
| 1:BD:3:LEU:HD23   | 1:BH:134:TYR:HB2 | 1.91                     | 0.53              |
| 1:CV:44:TYR:HE1   | 1:CV:68:VAL:HG13 | 1.74                     | 0.53              |
| 1:DD:62:VAL:HG23  | 1:DD:96:PHE:HB2  | 1.90                     | 0.53              |
| 1:AD:62:VAL:HG23  | 1:AD:96:PHE:HB2  | 1.90                     | 0.53              |
| 1:AE:108:GLU:OE1  | 1:CU:11:HIS:CE1  | 2.62                     | 0.53              |
| 1:BT:50:VAL:HG23  | 1:DK:132:HIS:CE1 | 2.43                     | 0.53              |
| 1:CA:21:THR:OG1   | 1:CA:32:ARG:HB3  | 2.09                     | 0.53              |
| 1:AV:62:VAL:HG23  | 1:AV:96:PHE:HB2  | 1.90                     | 0.53              |
| 1:BJ:1:PRO:HD3    | 1:DC:131:GLU:CB  | 2.32                     | 0.53              |
| 1:BX:44:TYR:HE1   | 1:BX:68:VAL:HG13 | 1.74                     | 0.53              |
| 1:CI:62:VAL:HG23  | 1:CI:96:PHE:HB2  | 1.90                     | 0.53              |
| 1:CJ:44:TYR:HE1   | 1:CJ:68:VAL:HG13 | 1.74                     | 0.53              |
| 1:AE:44:TYR:HE1   | 1:AE:68:VAL:HG13 | 1.74                     | 0.52              |
| 1:AP:134:TYR:CZ   | 1:AU:20:PRO:HB2  | 2.42                     | 0.52              |
| 1:AV:73:THR:H     | 1:CB:80:ASP:CB   | 2.22                     | 0.52              |
| 1:BB:123:ILE:HD11 | 1:DH:6:ILE:HD13  | 1.90                     | 0.52              |
| 1:BG:94:VAL:HG22  | 1:CZ:94:VAL:HG13 | 1.91                     | 0.52              |
| 1:BO:44:TYR:HE1   | 1:BO:68:VAL:HG13 | 1.74                     | 0.52              |
| 1:CG:44:TYR:HE1   | 1:CG:68:VAL:HG13 | 1.74                     | 0.52              |
| 1:CJ:134:TYR:CZ   | 1:CS:20:PRO:HB2  | 2.44                     | 0.52              |
| 1:AI:132:HIS:NE2  | 1:CB:52:GLU:OE2  | 2.43                     | 0.52              |
| 1:AW:44:TYR:HE1   | 1:AW:68:VAL:HG13 | 1.74                     | 0.52              |
| 1:BD:58:ASP:O     | 1:BD:100:ALA:N   | 2.43                     | 0.52              |
| 1:BF:21:THR:OG1   | 1:BF:32:ARG:HB3  | 2.09                     | 0.52              |
| 1:BU:21:THR:OG1   | 1:BU:32:ARG:HB3  | 2.09                     | 0.52              |
| 1:CC:62:VAL:HG23  | 1:CC:96:PHE:HB2  | 1.90                     | 0.52              |
| 1:CF:73:THR:H     | 1:CQ:80:ASP:HB2  | 1.74                     | 0.52              |
| 1:CK:58:ASP:O     | 1:CK:100:ALA:N   | 2.43                     | 0.52              |
| 1:CP:44:TYR:HE1   | 1:CP:68:VAL:HG13 | 1.74                     | 0.52              |
| 1:AN:44:TYR:HE1   | 1:AN:68:VAL:HG13 | 1.74                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AS:11:HIS:CB   | 1:BX:109:ASP:HB3  | 2.39                     | 0.52              |
| 1:BX:21:THR:OG1  | 1:BX:32:ARG:HB3   | 2.09                     | 0.52              |
| 1:BY:58:ASP:O    | 1:BY:100:ALA:N    | 2.43                     | 0.52              |
| 1:DE:21:THR:OG1  | 1:DE:32:ARG:HB3   | 2.09                     | 0.52              |
| 1:DH:44:TYR:HE1  | 1:DH:68:VAL:HG13  | 1.74                     | 0.52              |
| 1:DI:58:ASP:O    | 1:DI:100:ALA:N    | 2.43                     | 0.52              |
| 1:AO:21:THR:O    | 1:CL:132:HIS:HB2  | 2.10                     | 0.52              |
| 1:AY:50:VAL:HG23 | 1:BU:132:HIS:CE1  | 2.44                     | 0.52              |
| 1:BE:62:VAL:HG23 | 1:BE:96:PHE:HB2   | 1.90                     | 0.52              |
| 1:BE:131:GLU:CB  | 1:DE:1:PRO:HD3    | 2.37                     | 0.52              |
| 1:BF:44:TYR:HE1  | 1:BF:68:VAL:HG13  | 1.74                     | 0.52              |
| 1:BR:21:THR:OG1  | 1:BR:32:ARG:HB3   | 2.09                     | 0.52              |
| 1:CN:58:ASP:O    | 1:CN:100:ALA:N    | 2.43                     | 0.52              |
| 1:AS:108:GLU:HG3 | 1:BX:128:VAL:HG13 | 1.92                     | 0.52              |
| 1:AW:21:THR:OG1  | 1:AW:32:ARG:HB3   | 2.08                     | 0.52              |
| 1:BJ:58:ASP:O    | 1:BJ:100:ALA:N    | 2.43                     | 0.52              |
| 1:BN:50:VAL:O    | 1:BR:132:HIS:NE2  | 2.43                     | 0.52              |
| 1:BS:58:ASP:O    | 1:BS:100:ALA:N    | 2.43                     | 0.52              |
| 1:CY:131:GLU:HB3 | 1:DJ:1:PRO:HD3    | 1.91                     | 0.52              |
| 1:AC:58:ASP:O    | 1:AC:100:ALA:N    | 2.43                     | 0.52              |
| 1:AO:58:ASP:O    | 1:AO:100:ALA:N    | 2.43                     | 0.52              |
| 1:BI:44:TYR:HE1  | 1:BI:68:VAL:HG13  | 1.74                     | 0.52              |
| 1:BO:131:GLU:HB3 | 1:DG:1:PRO:HD3    | 1.91                     | 0.52              |
| 1:BO:132:HIS:HB2 | 1:DH:21:THR:O     | 2.09                     | 0.52              |
| 1:CC:134:TYR:HB2 | 1:CH:3:LEU:HD23   | 1.90                     | 0.52              |
| 1:CT:58:ASP:O    | 1:CT:100:ALA:N    | 2.43                     | 0.52              |
| 1:CV:21:THR:OG1  | 1:CV:32:ARG:HB3   | 2.08                     | 0.52              |
| 1:CY:21:THR:OG1  | 1:CY:32:ARG:HB3   | 2.09                     | 0.52              |
| 1:AM:131:GLU:HB3 | 1:CD:1:PRO:CD     | 2.39                     | 0.52              |
| 1:AP:22:GLN:HB2  | 1:CH:132:HIS:CD2  | 2.45                     | 0.52              |
| 1:AQ:101:GLN:HG3 | 1:AR:84:VAL:HG22  | 1.92                     | 0.52              |
| 1:BC:132:HIS:CE1 | 1:BH:50:VAL:HG23  | 2.44                     | 0.52              |
| 1:CM:44:TYR:HE1  | 1:CM:68:VAL:HG13  | 1.74                     | 0.52              |
| 1:CZ:58:ASP:O    | 1:CZ:100:ALA:N    | 2.43                     | 0.52              |
| 1:AI:58:ASP:O    | 1:AI:100:ALA:N    | 2.43                     | 0.52              |
| 1:AK:21:THR:OG1  | 1:AK:32:ARG:HB3   | 2.08                     | 0.52              |
| 1:AV:131:GLU:HB3 | 1:CA:1:PRO:CD     | 2.40                     | 0.52              |
| 1:AW:101:GLN:HG3 | 1:AX:84:VAL:HG22  | 1.92                     | 0.52              |
| 1:AZ:44:TYR:HE1  | 1:AZ:68:VAL:HG13  | 1.74                     | 0.52              |
| 1:AZ:101:GLN:HG3 | 1:BA:84:VAL:HG22  | 1.92                     | 0.52              |
| 1:BC:101:GLN:HG3 | 1:BD:84:VAL:HG22  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:BO:1:PRO:HD3   | 1:DG:131:GLU:CB  | 2.36                     | 0.52              |
| 1:BR:101:GLN:HG3 | 1:BS:84:VAL:HG22 | 1.92                     | 0.52              |
| 1:BU:101:GLN:HG3 | 1:BV:84:VAL:HG22 | 1.92                     | 0.52              |
| 1:CB:58:ASP:O    | 1:CB:100:ALA:N   | 2.43                     | 0.52              |
| 1:CG:21:THR:OG1  | 1:CG:32:ARG:HB3  | 2.09                     | 0.52              |
| 1:CG:101:GLN:HG3 | 1:CH:84:VAL:HG22 | 1.92                     | 0.52              |
| 1:CN:3:LEU:HD23  | 1:CO:134:TYR:HB2 | 1.91                     | 0.52              |
| 1:CS:21:THR:OG1  | 1:CS:32:ARG:HB3  | 2.09                     | 0.52              |
| 1:AP:81:THR:OG1  | 1:CH:72:ALA:HB2  | 2.10                     | 0.52              |
| 1:AP:132:HIS:HE1 | 1:AT:52:GLU:HG3  | 1.75                     | 0.52              |
| 1:AS:21:THR:O    | 1:CK:132:HIS:HB2 | 2.11                     | 0.52              |
| 1:AU:94:VAL:HG13 | 1:CK:94:VAL:HG22 | 1.91                     | 0.52              |
| 1:BF:101:GLN:HG3 | 1:BG:84:VAL:HG22 | 1.92                     | 0.52              |
| 1:BJ:132:HIS:CE1 | 1:DC:50:VAL:HG23 | 2.45                     | 0.52              |
| 1:BR:44:TYR:HE1  | 1:BR:68:VAL:HG13 | 1.74                     | 0.52              |
| 1:CQ:58:ASP:O    | 1:CQ:100:ALA:N   | 2.43                     | 0.52              |
| 1:DE:44:TYR:HE1  | 1:DE:68:VAL:HG13 | 1.74                     | 0.52              |
| 1:DK:44:TYR:HE1  | 1:DK:68:VAL:HG13 | 1.74                     | 0.52              |
| 1:DK:101:GLN:HG3 | 1:DL:84:VAL:HG22 | 1.92                     | 0.52              |
| 1:AB:44:TYR:HE1  | 1:AB:68:VAL:HG13 | 1.74                     | 0.51              |
| 1:AH:21:THR:OG1  | 1:AH:32:ARG:HB3  | 2.09                     | 0.51              |
| 1:AT:101:GLN:HG3 | 1:AU:84:VAL:HG22 | 1.92                     | 0.51              |
| 1:BT:94:VAL:HG13 | 1:DK:94:VAL:HG22 | 1.92                     | 0.51              |
| 1:BX:101:GLN:HG3 | 1:BY:84:VAL:HG22 | 1.92                     | 0.51              |
| 1:BZ:98:LEU:HD13 | 1:BZ:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:CE:58:ASP:O    | 1:CE:100:ALA:N   | 2.43                     | 0.51              |
| 1:CH:58:ASP:O    | 1:CH:100:ALA:N   | 2.43                     | 0.51              |
| 1:DG:98:LEU:HD13 | 1:DG:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:AA:131:GLU:HB3 | 1:AQ:1:PRO:CD    | 2.40                     | 0.51              |
| 1:AH:101:GLN:HG3 | 1:AI:84:VAL:HG22 | 1.92                     | 0.51              |
| 1:AI:1:PRO:HD3   | 1:CB:131:GLU:CB  | 2.36                     | 0.51              |
| 1:AU:11:HIS:CG   | 1:CK:108:GLU:HB3 | 2.46                     | 0.51              |
| 1:CD:101:GLN:HG3 | 1:CE:84:VAL:HG22 | 1.92                     | 0.51              |
| 1:CF:98:LEU:HD13 | 1:CF:107:ARG:HD2 | 1.92                     | 0.51              |
| 1:DB:101:GLN:HG3 | 1:DC:84:VAL:HG22 | 1.92                     | 0.51              |
| 1:AH:11:HIS:H    | 1:CX:109:ASP:CB  | 2.22                     | 0.51              |
| 1:AM:50:VAL:HG23 | 1:CD:132:HIS:CE1 | 2.45                     | 0.51              |
| 1:AN:101:GLN:HG3 | 1:AO:84:VAL:HG22 | 1.92                     | 0.51              |
| 1:AU:91:ARG:O    | 1:CK:96:PHE:HA   | 2.10                     | 0.51              |
| 1:BC:132:HIS:HE1 | 1:BH:52:GLU:HG3  | 1.76                     | 0.51              |
| 1:BV:58:ASP:O    | 1:BV:100:ALA:N   | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CM:101:GLN:HG3  | 1:CN:84:VAL:HG22  | 1.92                     | 0.51              |
| 1:CO:98:LEU:HD13  | 1:CO:107:ARG:HD2  | 1.93                     | 0.51              |
| 1:CS:34:LEU:HD23  | 1:CS:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:CU:98:LEU:HD13  | 1:CU:107:ARG:HD2  | 1.93                     | 0.51              |
| 1:CY:101:GLN:HG3  | 1:CZ:84:VAL:HG22  | 1.92                     | 0.51              |
| 1:DB:44:TYR:HE1   | 1:DB:68:VAL:HG13  | 1.74                     | 0.51              |
| 1:DH:34:LEU:HD23  | 1:DH:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:AP:98:LEU:HD13  | 1:AP:107:ARG:HD2  | 1.93                     | 0.51              |
| 1:AS:131:GLU:HB3  | 1:BX:1:PRO:HD3    | 1.93                     | 0.51              |
| 1:BB:132:HIS:HB2  | 1:DI:21:THR:O     | 2.09                     | 0.51              |
| 1:BC:44:TYR:HE1   | 1:BC:68:VAL:HG13  | 1.74                     | 0.51              |
| 1:BF:34:LEU:HD23  | 1:BF:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:BP:58:ASP:O     | 1:BP:100:ALA:N    | 2.43                     | 0.51              |
| 1:BU:44:TYR:HE1   | 1:BU:68:VAL:HG13  | 1.74                     | 0.51              |
| 1:CA:44:TYR:HE1   | 1:CA:68:VAL:HG13  | 1.74                     | 0.51              |
| 1:CX:98:LEU:HD13  | 1:CX:107:ARG:HD2  | 1.93                     | 0.51              |
| 1:AR:6:ILE:HD13   | 1:CH:123:ILE:HD11 | 1.93                     | 0.51              |
| 1:AS:130:VAL:HG11 | 1:BX:60:PHE:CE1   | 2.46                     | 0.51              |
| 1:AV:98:LEU:HD13  | 1:AV:107:ARG:HD2  | 1.93                     | 0.51              |
| 1:BA:90:ASN:CG    | 1:CQ:99:PRO:HD2   | 2.35                     | 0.51              |
| 1:BX:34:LEU:HD23  | 1:BX:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:CI:98:LEU:HD13  | 1:CI:107:ARG:HD2  | 1.93                     | 0.51              |
| 1:CM:1:PRO:CD     | 1:CO:131:GLU:HB3  | 2.41                     | 0.51              |
| 1:CY:44:TYR:HE1   | 1:CY:68:VAL:HG13  | 1.74                     | 0.51              |
| 1:DH:101:GLN:HG3  | 1:DI:84:VAL:HG22  | 1.92                     | 0.51              |
| 1:AD:98:LEU:HD13  | 1:AD:107:ARG:HD2  | 1.93                     | 0.51              |
| 1:AH:34:LEU:HD23  | 1:AH:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:AN:34:LEU:HD23  | 1:AN:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:AN:131:GLU:HB3  | 1:CL:1:PRO:HD3    | 1.91                     | 0.51              |
| 1:AT:34:LEU:HD23  | 1:AT:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:AX:131:GLU:CB   | 1:CN:1:PRO:HD3    | 2.36                     | 0.51              |
| 1:BG:52:GLU:OE2   | 1:CZ:132:HIS:NE2  | 2.40                     | 0.51              |
| 1:CJ:34:LEU:HD23  | 1:CJ:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:CV:101:GLN:HG3  | 1:CW:84:VAL:HG22  | 1.92                     | 0.51              |
| 1:CX:47:SER:HB2   | 1:CX:65:PHE:HB2   | 1.93                     | 0.51              |
| 1:DD:47:SER:HB2   | 1:DD:65:PHE:HB2   | 1.93                     | 0.51              |
| 1:DE:101:GLN:HG3  | 1:DF:84:VAL:HG22  | 1.92                     | 0.51              |
| 1:DF:58:ASP:O     | 1:DF:100:ALA:N    | 2.43                     | 0.51              |
| 1:AB:101:GLN:HG3  | 1:AC:84:VAL:HG22  | 1.92                     | 0.51              |
| 1:AJ:47:SER:HB2   | 1:AJ:65:PHE:HB2   | 1.93                     | 0.51              |
| 1:AV:1:PRO:HD2    | 1:CA:132:HIS:O    | 2.11                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AV:47:SER:HB2   | 1:AV:65:PHE:HB2  | 1.93                     | 0.51              |
| 1:BL:44:TYR:HE1   | 1:BL:68:VAL:HG13 | 1.74                     | 0.51              |
| 1:BW:132:HIS:HB2  | 1:DC:21:THR:O    | 2.10                     | 0.51              |
| 1:CD:34:LEU:HD23  | 1:CD:43:ALA:HB2  | 1.93                     | 0.51              |
| 1:CI:47:SER:HB2   | 1:CI:65:PHE:HB2  | 1.93                     | 0.51              |
| 1:CM:34:LEU:HD23  | 1:CM:43:ALA:HB2  | 1.93                     | 0.51              |
| 1:DJ:98:LEU:HD13  | 1:DJ:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:AG:98:LEU:HD13  | 1:AG:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:AR:134:TYR:CD1  | 1:CF:3:LEU:HD23  | 2.46                     | 0.51              |
| 1:BE:47:SER:HB2   | 1:BE:65:PHE:HB2  | 1.93                     | 0.51              |
| 1:BE:52:GLU:HG3   | 1:DE:132:HIS:HE1 | 1.75                     | 0.51              |
| 1:BL:34:LEU:HD23  | 1:BL:43:ALA:HB2  | 1.93                     | 0.51              |
| 1:BQ:98:LEU:HD13  | 1:BQ:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:BW:52:GLU:HG3   | 1:DB:132:HIS:HE1 | 1.75                     | 0.51              |
| 1:BW:98:LEU:HD13  | 1:BW:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:CF:131:GLU:CB   | 1:CP:1:PRO:HD3   | 2.39                     | 0.51              |
| 1:CJ:1:PRO:HD3    | 1:CR:131:GLU:CB  | 2.41                     | 0.51              |
| 1:CY:1:PRO:HD3    | 1:DJ:131:GLU:HB3 | 1.92                     | 0.51              |
| 1:AD:47:SER:HB2   | 1:AD:65:PHE:HB2  | 1.93                     | 0.51              |
| 1:AF:126:THR:HG21 | 1:BY:48:SER:OG   | 2.10                     | 0.51              |
| 1:AM:98:LEU:HD13  | 1:AM:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:AR:58:ASP:O     | 1:AR:100:ALA:N   | 2.43                     | 0.51              |
| 1:AY:98:LEU:HD13  | 1:AY:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:BC:34:LEU:HD23  | 1:BC:43:ALA:HB2  | 1.93                     | 0.51              |
| 1:BI:34:LEU:HD23  | 1:BI:43:ALA:HB2  | 1.93                     | 0.51              |
| 1:CG:34:LEU:HD23  | 1:CG:43:ALA:HB2  | 1.93                     | 0.51              |
| 1:CR:47:SER:HB2   | 1:CR:65:PHE:HB2  | 1.93                     | 0.51              |
| 1:CU:47:SER:HB2   | 1:CU:65:PHE:HB2  | 1.93                     | 0.51              |
| 1:AJ:98:LEU:HD13  | 1:AJ:107:ARG:HD2 | 1.93                     | 0.51              |
| 1:AV:1:PRO:HD3    | 1:CA:131:GLU:CB  | 2.41                     | 0.51              |
| 1:AX:58:ASP:O     | 1:AX:100:ALA:N   | 2.43                     | 0.51              |
| 1:BB:109:ASP:HB3  | 1:DH:11:HIS:CB   | 2.41                     | 0.51              |
| 1:BI:101:GLN:HG3  | 1:BJ:84:VAL:HG22 | 1.92                     | 0.51              |
| 1:BO:101:GLN:HG3  | 1:BP:84:VAL:HG22 | 1.92                     | 0.51              |
| 1:AI:50:VAL:HG23  | 1:CB:132:HIS:CE1 | 2.46                     | 0.50              |
| 1:BB:134:TYR:HB2  | 1:DI:3:LEU:HD23  | 1.93                     | 0.50              |
| 1:BK:47:SER:HB2   | 1:BK:65:PHE:HB2  | 1.93                     | 0.50              |
| 1:BK:98:LEU:HD13  | 1:BK:107:ARG:HD2 | 1.92                     | 0.50              |
| 1:BN:98:LEU:HD13  | 1:BN:107:ARG:HD2 | 1.93                     | 0.50              |
| 1:BS:50:VAL:HG23  | 1:DL:132:HIS:CE1 | 2.45                     | 0.50              |
| 1:BT:47:SER:HB2   | 1:BT:65:PHE:HB2  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BT:98:LEU:HD13  | 1:BT:107:ARG:HD2 | 1.93                     | 0.50              |
| 1:CJ:101:GLN:HG3  | 1:CK:84:VAL:HG22 | 1.92                     | 0.50              |
| 1:CY:123:ILE:HD11 | 1:DJ:6:ILE:HD13  | 1.93                     | 0.50              |
| 1:DL:58:ASP:O     | 1:DL:100:ALA:N   | 2.43                     | 0.50              |
| 1:AA:98:LEU:HD13  | 1:AA:107:ARG:HD2 | 1.93                     | 0.50              |
| 1:AK:101:GLN:HG3  | 1:AL:84:VAL:HG22 | 1.92                     | 0.50              |
| 1:AU:73:THR:H     | 1:CI:80:ASP:HB3  | 1.75                     | 0.50              |
| 1:AV:50:VAL:HG23  | 1:CA:132:HIS:CE1 | 2.46                     | 0.50              |
| 1:BE:98:LEU:HD13  | 1:BE:107:ARG:HD2 | 1.93                     | 0.50              |
| 1:BM:58:ASP:O     | 1:BM:100:ALA:N   | 2.43                     | 0.50              |
| 1:BO:34:LEU:HD23  | 1:BO:43:ALA:HB2  | 1.93                     | 0.50              |
| 1:CZ:21:THR:O     | 1:DJ:132:HIS:HB2 | 2.11                     | 0.50              |
| 1:AA:47:SER:HB2   | 1:AA:65:PHE:HB2  | 1.93                     | 0.50              |
| 1:AE:109:ASP:HB3  | 1:CU:11:HIS:CB   | 2.41                     | 0.50              |
| 1:AK:34:LEU:HD23  | 1:AK:43:ALA:HB2  | 1.93                     | 0.50              |
| 1:AU:75:THR:HG22  | 1:CI:78:GLY:O    | 2.11                     | 0.50              |
| 1:BL:101:GLN:HG3  | 1:BM:84:VAL:HG22 | 1.92                     | 0.50              |
| 1:BW:131:GLU:HB3  | 1:DB:1:PRO:CD    | 2.42                     | 0.50              |
| 1:DA:98:LEU:HD13  | 1:DA:107:ARG:HD2 | 1.93                     | 0.50              |
| 1:AF:133:PHE:CD1  | 1:BY:3:LEU:HD12  | 2.47                     | 0.50              |
| 1:AP:47:SER:HB2   | 1:AP:65:PHE:HB2  | 1.93                     | 0.50              |
| 1:BU:34:LEU:HD23  | 1:BU:43:ALA:HB2  | 1.93                     | 0.50              |
| 1:CM:109:ASP:HB3  | 1:CO:11:HIS:CB   | 2.41                     | 0.50              |
| 1:CV:34:LEU:HD23  | 1:CV:43:ALA:HB2  | 1.93                     | 0.50              |
| 1:AF:58:ASP:O     | 1:AF:100:ALA:N   | 2.43                     | 0.50              |
| 1:AN:123:ILE:HD11 | 1:CL:6:ILE:HD13  | 1.94                     | 0.50              |
| 1:BF:50:VAL:HG23  | 1:BK:132:HIS:CE1 | 2.46                     | 0.50              |
| 1:CL:47:SER:HB2   | 1:CL:65:PHE:HB2  | 1.93                     | 0.50              |
| 1:CR:98:LEU:HD13  | 1:CR:107:ARG:HD2 | 1.93                     | 0.50              |
| 1:DB:34:LEU:HD23  | 1:DB:43:ALA:HB2  | 1.93                     | 0.50              |
| 1:DE:34:LEU:HD23  | 1:DE:43:ALA:HB2  | 1.93                     | 0.50              |
| 1:AC:132:HIS:O    | 1:BV:1:PRO:HD2   | 2.12                     | 0.50              |
| 1:AE:34:LEU:HD23  | 1:AE:43:ALA:HB2  | 1.93                     | 0.50              |
| 1:AK:94:VAL:HG22  | 1:CI:94:VAL:HG22 | 1.94                     | 0.50              |
| 1:AR:134:TYR:CZ   | 1:CF:20:PRO:HB2  | 2.46                     | 0.50              |
| 1:BW:94:VAL:HG13  | 1:DB:94:VAL:HG22 | 1.94                     | 0.50              |
| 1:BW:123:ILE:HD11 | 1:DB:6:ILE:HD13  | 1.93                     | 0.50              |
| 1:CA:101:GLN:HG3  | 1:CB:84:VAL:HG22 | 1.92                     | 0.50              |
| 1:CC:47:SER:HB2   | 1:CC:65:PHE:HB2  | 1.93                     | 0.50              |
| 1:CF:47:SER:HB2   | 1:CF:65:PHE:HB2  | 1.93                     | 0.50              |
| 1:CO:47:SER:HB2   | 1:CO:65:PHE:HB2  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AE:101:GLN:HG3  | 1:AF:84:VAL:HG22  | 1.92                     | 0.50              |
| 1:AK:60:PHE:CE1   | 1:CI:130:VAL:HG11 | 2.47                     | 0.50              |
| 1:AL:58:ASP:O     | 1:AL:100:ALA:N    | 2.43                     | 0.50              |
| 1:AM:123:ILE:HD11 | 1:CD:6:ILE:HD13   | 1.94                     | 0.50              |
| 1:BA:58:ASP:O     | 1:BA:100:ALA:N    | 2.43                     | 0.50              |
| 1:BD:8:LEU:HB3    | 1:CW:116:SER:OG   | 2.12                     | 0.50              |
| 1:BG:108:GLU:HG3  | 1:CZ:128:VAL:HG11 | 1.94                     | 0.50              |
| 1:CA:34:LEU:HD23  | 1:CA:43:ALA:HB2   | 1.93                     | 0.50              |
| 1:CK:80:ASP:HB3   | 1:CR:72:ALA:HA    | 1.94                     | 0.50              |
| 1:CP:34:LEU:HD23  | 1:CP:43:ALA:HB2   | 1.93                     | 0.50              |
| 1:CP:101:GLN:HG3  | 1:CQ:84:VAL:HG22  | 1.92                     | 0.50              |
| 1:CS:101:GLN:HG3  | 1:CT:84:VAL:HG22  | 1.92                     | 0.50              |
| 1:CW:58:ASP:O     | 1:CW:100:ALA:N    | 2.43                     | 0.50              |
| 1:AY:47:SER:HB2   | 1:AY:65:PHE:HB2   | 1.93                     | 0.50              |
| 1:BH:98:LEU:HD13  | 1:BH:107:ARG:HD2  | 1.93                     | 0.50              |
| 1:BR:34:LEU:HD23  | 1:BR:43:ALA:HB2   | 1.93                     | 0.50              |
| 1:BZ:47:SER:HB2   | 1:BZ:65:PHE:HB2   | 1.93                     | 0.50              |
| 1:CC:98:LEU:HD13  | 1:CC:107:ARG:HD2  | 1.93                     | 0.50              |
| 1:CF:11:HIS:CB    | 1:CP:109:ASP:HB3  | 2.41                     | 0.50              |
| 1:CL:98:LEU:HD13  | 1:CL:107:ARG:HD2  | 1.93                     | 0.50              |
| 1:AC:50:VAL:HG12  | 1:AC:62:VAL:HG12  | 1.94                     | 0.50              |
| 1:AG:47:SER:HB2   | 1:AG:65:PHE:HB2   | 1.93                     | 0.50              |
| 1:AH:109:ASP:HB3  | 1:CX:11:HIS:HB2   | 1.94                     | 0.50              |
| 1:AI:94:VAL:HG22  | 1:CB:94:VAL:HG13  | 1.94                     | 0.50              |
| 1:AL:94:VAL:HG13  | 1:CE:94:VAL:HG22  | 1.94                     | 0.50              |
| 1:AP:78:GLY:O     | 1:CH:75:THR:N     | 2.45                     | 0.50              |
| 1:AW:34:LEU:HD23  | 1:AW:43:ALA:HB2   | 1.93                     | 0.50              |
| 1:BW:47:SER:HB2   | 1:BW:65:PHE:HB2   | 1.93                     | 0.50              |
| 1:CM:6:ILE:HD13   | 1:CO:123:ILE:HD11 | 1.94                     | 0.50              |
| 1:DD:98:LEU:HD13  | 1:DD:107:ARG:HD2  | 1.93                     | 0.50              |
| 1:DG:47:SER:HB2   | 1:DG:65:PHE:HB2   | 1.93                     | 0.50              |
| 1:DJ:47:SER:HB2   | 1:DJ:65:PHE:HB2   | 1.93                     | 0.50              |
| 1:AM:47:SER:HB2   | 1:AM:65:PHE:HB2   | 1.93                     | 0.49              |
| 1:BA:90:ASN:ND2   | 1:CQ:99:PRO:HD2   | 2.27                     | 0.49              |
| 1:BB:98:LEU:HD13  | 1:BB:107:ARG:HD2  | 1.93                     | 0.49              |
| 1:BE:109:ASP:HB3  | 1:DE:11:HIS:H     | 1.77                     | 0.49              |
| 1:BG:132:HIS:NE2  | 1:CZ:52:GLU:OE2   | 2.43                     | 0.49              |
| 1:CN:50:VAL:HG12  | 1:CN:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:AB:34:LEU:HD23  | 1:AB:43:ALA:HB2   | 1.93                     | 0.49              |
| 1:AC:132:HIS:CE1  | 1:BV:50:VAL:HG23  | 2.47                     | 0.49              |
| 1:AE:131:GLU:HB3  | 1:CU:1:PRO:HD3    | 1.94                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AM:52:GLU:HG3  | 1:CD:132:HIS:HE1  | 1.77                     | 0.49              |
| 1:AU:11:HIS:CE1  | 1:CK:108:GLU:OE1  | 2.65                     | 0.49              |
| 1:AU:58:ASP:O    | 1:AU:100:ALA:N    | 2.43                     | 0.49              |
| 1:BH:47:SER:HB2  | 1:BH:65:PHE:HB2   | 1.93                     | 0.49              |
| 1:BJ:6:ILE:HD13  | 1:DC:123:ILE:HD11 | 1.93                     | 0.49              |
| 1:BN:47:SER:HB2  | 1:BN:65:PHE:HB2   | 1.93                     | 0.49              |
| 1:CY:34:LEU:HD23 | 1:CY:43:ALA:HB2   | 1.93                     | 0.49              |
| 1:AE:134:TYR:CD1 | 1:CV:3:LEU:HD23   | 2.47                     | 0.49              |
| 1:AO:50:VAL:HG12 | 1:AO:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:AQ:34:LEU:HD23 | 1:AQ:43:ALA:HB2   | 1.93                     | 0.49              |
| 1:AQ:98:LEU:HD13 | 1:AQ:107:ARG:HD2  | 1.95                     | 0.49              |
| 1:AZ:34:LEU:HD23 | 1:AZ:43:ALA:HB2   | 1.93                     | 0.49              |
| 1:BC:6:ILE:HD13  | 1:BH:123:ILE:HD11 | 1.94                     | 0.49              |
| 1:BS:50:VAL:HG12 | 1:BS:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:CH:50:VAL:HG12 | 1:CH:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:CY:50:VAL:HG23 | 1:DJ:132:HIS:CE1  | 2.47                     | 0.49              |
| 1:DA:47:SER:HB2  | 1:DA:65:PHE:HB2   | 1.93                     | 0.49              |
| 1:AC:1:PRO:CD    | 1:BV:131:GLU:HB3  | 2.29                     | 0.49              |
| 1:AJ:75:THR:HB   | 1:AJ:82:SER:HB3   | 1.95                     | 0.49              |
| 1:AP:50:VAL:CG1  | 1:AT:126:THR:HG23 | 2.43                     | 0.49              |
| 1:AP:80:ASP:HB3  | 1:CH:73:THR:H     | 1.74                     | 0.49              |
| 1:AS:3:LEU:N     | 1:BX:134:TYR:O    | 2.34                     | 0.49              |
| 1:BG:58:ASP:O    | 1:BG:100:ALA:N    | 2.43                     | 0.49              |
| 1:BG:108:GLU:HG3 | 1:CZ:128:VAL:CG1  | 2.43                     | 0.49              |
| 1:BV:50:VAL:HG12 | 1:BV:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:BY:50:VAL:HG12 | 1:BY:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:CC:50:VAL:HG23 | 1:CG:132:HIS:CE1  | 2.47                     | 0.49              |
| 1:AF:50:VAL:HG12 | 1:AF:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:AR:132:HIS:CD2 | 1:CF:22:GLN:HB2   | 2.48                     | 0.49              |
| 1:AS:47:SER:HB2  | 1:AS:65:PHE:HB2   | 1.93                     | 0.49              |
| 1:BA:50:VAL:HG23 | 1:CQ:132:HIS:CE1  | 2.47                     | 0.49              |
| 1:BG:94:VAL:HG13 | 1:CZ:94:VAL:HG22  | 1.94                     | 0.49              |
| 1:BQ:75:THR:HB   | 1:BQ:82:SER:HB3   | 1.95                     | 0.49              |
| 1:CF:75:THR:HB   | 1:CF:82:SER:HB3   | 1.95                     | 0.49              |
| 1:CM:98:LEU:HD13 | 1:CM:107:ARG:HD2  | 1.95                     | 0.49              |
| 1:DJ:75:THR:HB   | 1:DJ:82:SER:HB3   | 1.95                     | 0.49              |
| 1:AU:132:HIS:CD2 | 1:CI:22:GLN:HB2   | 2.48                     | 0.49              |
| 1:BH:75:THR:HB   | 1:BH:82:SER:HB3   | 1.95                     | 0.49              |
| 1:BJ:41:ILE:HG23 | 1:BJ:42:GLY:N     | 2.28                     | 0.49              |
| 1:BL:98:LEU:HD13 | 1:BL:107:ARG:HD2  | 1.95                     | 0.49              |
| 1:BM:41:ILE:HG23 | 1:BM:42:GLY:N     | 2.28                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BP:78:GLY:O     | 1:DG:74:ILE:HA   | 2.12                     | 0.49              |
| 1:CJ:94:VAL:HG13  | 1:CR:94:VAL:HG22 | 1.95                     | 0.49              |
| 1:CN:80:ASP:HB2   | 1:CO:73:THR:H    | 1.78                     | 0.49              |
| 1:AE:98:LEU:HD13  | 1:AE:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:AE:109:ASP:HB3  | 1:CU:11:HIS:HB2  | 1.94                     | 0.49              |
| 1:AJ:44:TYR:CE1   | 1:AJ:68:VAL:HG13 | 2.48                     | 0.49              |
| 1:AP:132:HIS:CE1  | 1:AT:52:GLU:HG3  | 2.47                     | 0.49              |
| 1:AS:98:LEU:HD13  | 1:AS:107:ARG:HD2 | 1.93                     | 0.49              |
| 1:BB:47:SER:HB2   | 1:BB:65:PHE:HB2  | 1.93                     | 0.49              |
| 1:BZ:75:THR:HB    | 1:BZ:82:SER:HB3  | 1.95                     | 0.49              |
| 1:CJ:98:LEU:HD13  | 1:CJ:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:CS:98:LEU:HD13  | 1:CS:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:CU:44:TYR:CE1   | 1:CU:68:VAL:HG13 | 2.48                     | 0.49              |
| 1:DE:98:LEU:HD13  | 1:DE:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:DK:34:LEU:HD23  | 1:DK:43:ALA:HB2  | 1.93                     | 0.49              |
| 1:AC:94:VAL:HG22  | 1:BV:94:VAL:HG13 | 1.95                     | 0.49              |
| 1:AK:98:LEU:HD13  | 1:AK:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:AP:75:THR:HB    | 1:AP:82:SER:HB3  | 1.95                     | 0.49              |
| 1:AV:44:TYR:CE1   | 1:AV:68:VAL:HG13 | 2.48                     | 0.49              |
| 1:AW:98:LEU:HD13  | 1:AW:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:AZ:21:THR:O     | 1:BU:132:HIS:HB2 | 2.12                     | 0.49              |
| 1:BJ:50:VAL:HG12  | 1:BJ:62:VAL:HG12 | 1.94                     | 0.49              |
| 1:BR:98:LEU:HD13  | 1:BR:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:CE:50:VAL:HG12  | 1:CE:62:VAL:HG12 | 1.94                     | 0.49              |
| 1:CG:98:LEU:HD13  | 1:CG:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:CL:44:TYR:CE1   | 1:CL:68:VAL:HG13 | 2.48                     | 0.49              |
| 1:CN:41:ILE:HG23  | 1:CN:42:GLY:N    | 2.28                     | 0.49              |
| 1:AI:50:VAL:HG12  | 1:AI:62:VAL:HG12 | 1.94                     | 0.49              |
| 1:AL:50:VAL:HG12  | 1:AL:62:VAL:HG12 | 1.94                     | 0.49              |
| 1:AN:94:VAL:HG22  | 1:CL:94:VAL:HG13 | 1.95                     | 0.49              |
| 1:AT:98:LEU:HD13  | 1:AT:107:ARG:HD2 | 1.95                     | 0.49              |
| 1:AV:75:THR:HB    | 1:AV:82:SER:HB3  | 1.95                     | 0.49              |
| 1:AY:130:VAL:HG11 | 1:BU:60:PHE:CE1  | 2.47                     | 0.49              |
| 1:BA:99:PRO:HD2   | 1:CQ:90:ASN:ND2  | 2.28                     | 0.49              |
| 1:BB:75:THR:HB    | 1:BB:82:SER:HB3  | 1.95                     | 0.49              |
| 1:BD:50:VAL:HG12  | 1:BD:62:VAL:HG12 | 1.94                     | 0.49              |
| 1:BF:94:VAL:HG22  | 1:BK:94:VAL:HG13 | 1.95                     | 0.49              |
| 1:BI:11:HIS:H     | 1:BQ:109:ASP:HB3 | 1.78                     | 0.49              |
| 1:BN:20:PRO:HB2   | 1:DF:134:TYR:CZ  | 2.48                     | 0.49              |
| 1:BW:44:TYR:CE1   | 1:BW:68:VAL:HG13 | 2.48                     | 0.49              |
| 1:CB:50:VAL:HG12  | 1:CB:62:VAL:HG12 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CE:41:ILE:HG23 | 1:CE:42:GLY:N     | 2.28                     | 0.49              |
| 1:CK:41:ILE:HG23 | 1:CK:42:GLY:N     | 2.28                     | 0.49              |
| 1:CY:6:ILE:HD13  | 1:DJ:123:ILE:HD11 | 1.95                     | 0.49              |
| 1:AC:1:PRO:HD2   | 1:BV:132:HIS:O    | 2.11                     | 0.49              |
| 1:AC:94:VAL:HG13 | 1:BV:94:VAL:HG22  | 1.95                     | 0.49              |
| 1:AF:62:VAL:HG23 | 1:AF:96:PHE:HB2   | 1.95                     | 0.49              |
| 1:BC:1:PRO:HD3   | 1:BH:131:GLU:CB   | 2.42                     | 0.49              |
| 1:BI:98:LEU:HD13 | 1:BI:107:ARG:HD2  | 1.95                     | 0.49              |
| 1:BJ:1:PRO:CD    | 1:DC:131:GLU:HB3  | 2.35                     | 0.49              |
| 1:BN:11:HIS:CB   | 1:BR:109:ASP:HB3  | 2.42                     | 0.49              |
| 1:BP:41:ILE:HG23 | 1:BP:42:GLY:N     | 2.28                     | 0.49              |
| 1:BP:50:VAL:HG12 | 1:BP:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:CK:50:VAL:HG12 | 1:CK:62:VAL:HG12  | 1.94                     | 0.49              |
| 1:CK:62:VAL:HG23 | 1:CK:96:PHE:HB2   | 1.95                     | 0.49              |
| 1:CO:75:THR:HB   | 1:CO:82:SER:HB3   | 1.95                     | 0.49              |
| 1:DG:44:TYR:CE1  | 1:DG:68:VAL:HG13  | 2.48                     | 0.49              |
| 1:AA:109:ASP:HB3 | 1:AQ:11:HIS:CB    | 2.43                     | 0.48              |
| 1:AF:11:HIS:HB3  | 1:BY:109:ASP:HB3  | 1.94                     | 0.48              |
| 1:AI:62:VAL:HG23 | 1:AI:96:PHE:HB2   | 1.95                     | 0.48              |
| 1:AM:44:TYR:CE1  | 1:AM:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:AS:3:LEU:HD23  | 1:CK:134:TYR:CD1  | 2.48                     | 0.48              |
| 1:AS:22:GLN:HB2  | 1:CK:132:HIS:CD2  | 2.47                     | 0.48              |
| 1:AU:62:VAL:HG23 | 1:AU:96:PHE:HB2   | 1.95                     | 0.48              |
| 1:AX:50:VAL:HG12 | 1:AX:62:VAL:HG12  | 1.94                     | 0.48              |
| 1:BD:116:SER:OG  | 1:CW:8:LEU:HB3    | 2.13                     | 0.48              |
| 1:BG:21:THR:O    | 1:BK:132:HIS:HB2  | 2.13                     | 0.48              |
| 1:BG:41:ILE:HG23 | 1:BG:42:GLY:N     | 2.28                     | 0.48              |
| 1:BG:50:VAL:HG12 | 1:BG:62:VAL:HG12  | 1.95                     | 0.48              |
| 1:BI:132:HIS:CE1 | 1:BQ:50:VAL:HG23  | 2.48                     | 0.48              |
| 1:BK:75:THR:HB   | 1:BK:82:SER:HB3   | 1.95                     | 0.48              |
| 1:BN:44:TYR:CE1  | 1:BN:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:BV:62:VAL:HG23 | 1:BV:96:PHE:HB2   | 1.95                     | 0.48              |
| 1:BY:62:VAL:HG23 | 1:BY:96:PHE:HB2   | 1.95                     | 0.48              |
| 1:CI:75:THR:HB   | 1:CI:82:SER:HB3   | 1.95                     | 0.48              |
| 1:CQ:41:ILE:HG23 | 1:CQ:42:GLY:N     | 2.28                     | 0.48              |
| 1:CR:44:TYR:CE1  | 1:CR:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:CU:75:THR:HB   | 1:CU:82:SER:HB3   | 1.95                     | 0.48              |
| 1:CV:98:LEU:HD13 | 1:CV:107:ARG:HD2  | 1.95                     | 0.48              |
| 1:CW:41:ILE:HG23 | 1:CW:42:GLY:N     | 2.28                     | 0.48              |
| 1:CY:98:LEU:HD13 | 1:CY:107:ARG:HD2  | 1.95                     | 0.48              |
| 1:DD:75:THR:HB   | 1:DD:82:SER:HB3   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:DL:41:ILE:HG23 | 1:DL:42:GLY:N    | 2.28                     | 0.48              |
| 1:AB:98:LEU:HD13 | 1:AB:107:ARG:HD2 | 1.95                     | 0.48              |
| 1:AF:11:HIS:CB   | 1:BY:109:ASP:HB3 | 2.42                     | 0.48              |
| 1:AK:91:ARG:O    | 1:CI:96:PHE:HA   | 2.12                     | 0.48              |
| 1:AM:11:HIS:CB   | 1:CD:109:ASP:HB3 | 2.43                     | 0.48              |
| 1:AM:75:THR:HB   | 1:AM:82:SER:HB3  | 1.95                     | 0.48              |
| 1:AU:50:VAL:HG12 | 1:AU:62:VAL:HG12 | 1.94                     | 0.48              |
| 1:BB:44:TYR:CE1  | 1:BB:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:BD:41:ILE:HG23 | 1:BD:42:GLY:N    | 2.28                     | 0.48              |
| 1:BG:132:HIS:CE1 | 1:CZ:50:VAL:HG23 | 2.47                     | 0.48              |
| 1:BP:132:HIS:CE1 | 1:DF:50:VAL:HG23 | 2.48                     | 0.48              |
| 1:BS:41:ILE:HG23 | 1:BS:42:GLY:N    | 2.28                     | 0.48              |
| 1:BZ:44:TYR:CE1  | 1:BZ:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:CA:98:LEU:HD13 | 1:CA:107:ARG:HD2 | 1.95                     | 0.48              |
| 1:CB:41:ILE:HG23 | 1:CB:42:GLY:N    | 2.28                     | 0.48              |
| 1:CB:62:VAL:HG23 | 1:CB:96:PHE:HB2  | 1.95                     | 0.48              |
| 1:CC:44:TYR:CE1  | 1:CC:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:CM:132:HIS:HE1 | 1:CO:52:GLU:HG3  | 1.78                     | 0.48              |
| 1:CP:98:LEU:HD13 | 1:CP:107:ARG:HD2 | 1.95                     | 0.48              |
| 1:CZ:50:VAL:HG12 | 1:CZ:62:VAL:HG12 | 1.94                     | 0.48              |
| 1:DA:44:TYR:CE1  | 1:DA:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:DC:41:ILE:HG23 | 1:DC:42:GLY:N    | 2.28                     | 0.48              |
| 1:DC:58:ASP:O    | 1:DC:100:ALA:N   | 2.43                     | 0.48              |
| 1:DI:41:ILE:HG23 | 1:DI:42:GLY:N    | 2.28                     | 0.48              |
| 1:DI:50:VAL:HG12 | 1:DI:62:VAL:HG12 | 1.94                     | 0.48              |
| 1:AC:50:VAL:HG23 | 1:BV:132:HIS:CE1 | 2.49                     | 0.48              |
| 1:AD:75:THR:HB   | 1:AD:82:SER:HB3  | 1.95                     | 0.48              |
| 1:BQ:44:TYR:CE1  | 1:BQ:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:BQ:47:SER:HB2  | 1:BQ:65:PHE:HB2  | 1.93                     | 0.48              |
| 1:CH:62:VAL:HG23 | 1:CH:96:PHE:HB2  | 1.95                     | 0.48              |
| 1:DG:75:THR:HB   | 1:DG:82:SER:HB3  | 1.95                     | 0.48              |
| 1:AC:62:VAL:HG23 | 1:AC:96:PHE:HB2  | 1.95                     | 0.48              |
| 1:AF:41:ILE:HG23 | 1:AF:42:GLY:N    | 2.28                     | 0.48              |
| 1:AP:80:ASP:HB2  | 1:CH:73:THR:H    | 1.78                     | 0.48              |
| 1:BA:50:VAL:HG12 | 1:BA:62:VAL:HG12 | 1.94                     | 0.48              |
| 1:BG:62:VAL:HG23 | 1:BG:96:PHE:HB2  | 1.95                     | 0.48              |
| 1:BT:18:PHE:HB3  | 1:BT:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:DC:50:VAL:HG12 | 1:DC:62:VAL:HG12 | 1.94                     | 0.48              |
| 1:AE:131:GLU:CB  | 1:CU:1:PRO:HD3   | 2.44                     | 0.48              |
| 1:AF:99:PRO:HD2  | 1:BY:90:ASN:ND2  | 2.29                     | 0.48              |
| 1:AP:18:PHE:HB3  | 1:AP:31:PHE:HB3  | 1.96                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AR:50:VAL:HG23 | 1:CH:132:HIS:CE1  | 2.48                     | 0.48              |
| 1:AS:44:TYR:CE1  | 1:AS:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:AV:18:PHE:HB3  | 1:AV:31:PHE:HB3   | 1.96                     | 0.48              |
| 1:BA:109:ASP:HB3 | 1:CQ:11:HIS:CB    | 2.44                     | 0.48              |
| 1:BF:98:LEU:HD13 | 1:BF:107:ARG:HD2  | 1.95                     | 0.48              |
| 1:BH:44:TYR:CE1  | 1:BH:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:BK:44:TYR:CE1  | 1:BK:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:BM:62:VAL:HG23 | 1:BM:96:PHE:HB2   | 1.95                     | 0.48              |
| 1:BP:73:THR:H    | 1:DD:80:ASP:CB    | 2.26                     | 0.48              |
| 1:BQ:18:PHE:HB3  | 1:BQ:31:PHE:HB3   | 1.96                     | 0.48              |
| 1:BS:90:ASN:ND2  | 1:DL:99:PRO:HD2   | 2.29                     | 0.48              |
| 1:BT:75:THR:HB   | 1:BT:82:SER:HB3   | 1.95                     | 0.48              |
| 1:BU:98:LEU:HD13 | 1:BU:107:ARG:HD2  | 1.95                     | 0.48              |
| 1:BW:75:THR:HB   | 1:BW:82:SER:HB3   | 1.95                     | 0.48              |
| 1:CC:74:ILE:HA   | 1:CH:78:GLY:O     | 2.13                     | 0.48              |
| 1:CF:18:PHE:HB3  | 1:CF:31:PHE:HB3   | 1.96                     | 0.48              |
| 1:CI:44:TYR:CE1  | 1:CI:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:CJ:6:ILE:HD13  | 1:CR:123:ILE:HD11 | 1.95                     | 0.48              |
| 1:CT:62:VAL:HG23 | 1:CT:96:PHE:HB2   | 1.95                     | 0.48              |
| 1:DF:50:VAL:HG12 | 1:DF:62:VAL:HG12  | 1.94                     | 0.48              |
| 1:AB:50:VAL:HG12 | 1:AB:62:VAL:HG12  | 1.96                     | 0.48              |
| 1:AD:18:PHE:HB3  | 1:AD:31:PHE:HB3   | 1.96                     | 0.48              |
| 1:AE:94:VAL:HG22 | 1:CU:94:VAL:HG13  | 1.95                     | 0.48              |
| 1:AH:98:LEU:HD13 | 1:AH:107:ARG:HD2  | 1.95                     | 0.48              |
| 1:AJ:18:PHE:HB3  | 1:AJ:31:PHE:HB3   | 1.96                     | 0.48              |
| 1:AN:98:LEU:HD13 | 1:AN:107:ARG:HD2  | 1.95                     | 0.48              |
| 1:AO:41:ILE:HG23 | 1:AO:42:GLY:N     | 2.28                     | 0.48              |
| 1:AY:44:TYR:CE1  | 1:AY:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:BF:131:GLU:HB3 | 1:BK:1:PRO:HD3    | 1.95                     | 0.48              |
| 1:BJ:62:VAL:HG23 | 1:BJ:96:PHE:HB2   | 1.95                     | 0.48              |
| 1:CD:98:LEU:HD13 | 1:CD:107:ARG:HD2  | 1.95                     | 0.48              |
| 1:CH:41:ILE:HG23 | 1:CH:42:GLY:N     | 2.28                     | 0.48              |
| 1:CO:44:TYR:CE1  | 1:CO:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:CQ:62:VAL:HG23 | 1:CQ:96:PHE:HB2   | 1.95                     | 0.48              |
| 1:CR:18:PHE:HB3  | 1:CR:31:PHE:HB3   | 1.96                     | 0.48              |
| 1:CX:75:THR:HB   | 1:CX:82:SER:HB3   | 1.95                     | 0.48              |
| 1:DB:98:LEU:HD13 | 1:DB:107:ARG:HD2  | 1.95                     | 0.48              |
| 1:DD:18:PHE:HB3  | 1:DD:31:PHE:HB3   | 1.96                     | 0.48              |
| 1:AA:44:TYR:CE1  | 1:AA:68:VAL:HG13  | 2.48                     | 0.48              |
| 1:AA:75:THR:HB   | 1:AA:82:SER:HB3   | 1.95                     | 0.48              |
| 1:AE:48:SER:OG   | 1:CU:126:THR:HG21 | 2.13                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AG:75:THR:HB    | 1:AG:82:SER:HB3  | 1.95                     | 0.48              |
| 1:AL:41:ILE:HG23  | 1:AL:42:GLY:N    | 2.28                     | 0.48              |
| 1:BB:18:PHE:HB3   | 1:BB:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:BE:44:TYR:CE1   | 1:BE:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:BT:44:TYR:CE1   | 1:BT:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:BX:98:LEU:HD13  | 1:BX:107:ARG:HD2 | 1.95                     | 0.48              |
| 1:CJ:44:TYR:CE1   | 1:CJ:68:VAL:HG13 | 2.49                     | 0.48              |
| 1:CL:18:PHE:HB3   | 1:CL:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:CL:75:THR:HB    | 1:CL:82:SER:HB3  | 1.95                     | 0.48              |
| 1:CO:18:PHE:HB3   | 1:CO:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:CP:50:VAL:HG12  | 1:CP:62:VAL:HG12 | 1.96                     | 0.48              |
| 1:CS:44:TYR:CE1   | 1:CS:68:VAL:HG13 | 2.49                     | 0.48              |
| 1:CT:41:ILE:HG23  | 1:CT:42:GLY:N    | 2.28                     | 0.48              |
| 1:CT:50:VAL:HG12  | 1:CT:62:VAL:HG12 | 1.94                     | 0.48              |
| 1:CZ:62:VAL:HG23  | 1:CZ:96:PHE:HB2  | 1.95                     | 0.48              |
| 1:DA:75:THR:HB    | 1:DA:82:SER:HB3  | 1.95                     | 0.48              |
| 1:DH:44:TYR:CE1   | 1:DH:68:VAL:HG13 | 2.49                     | 0.48              |
| 1:DH:98:LEU:HD13  | 1:DH:107:ARG:HD2 | 1.95                     | 0.48              |
| 1:DJ:18:PHE:HB3   | 1:DJ:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:AA:18:PHE:HB3   | 1:AA:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:AI:94:VAL:HG13  | 1:CB:94:VAL:HG22 | 1.96                     | 0.48              |
| 1:AP:44:TYR:CE1   | 1:AP:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:AP:132:HIS:HE1  | 1:AT:52:GLU:CG   | 2.27                     | 0.48              |
| 1:AR:41:ILE:HG23  | 1:AR:42:GLY:N    | 2.28                     | 0.48              |
| 1:AR:50:VAL:HG12  | 1:AR:62:VAL:HG12 | 1.95                     | 0.48              |
| 1:AX:123:ILE:HD11 | 1:CN:6:ILE:HD13  | 1.96                     | 0.48              |
| 1:BC:98:LEU:HD13  | 1:BC:107:ARG:HD2 | 1.95                     | 0.48              |
| 1:BE:75:THR:HB    | 1:BE:82:SER:HB3  | 1.95                     | 0.48              |
| 1:BH:18:PHE:HB3   | 1:BH:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:BO:131:GLU:CB   | 1:DG:1:PRO:HD3   | 2.43                     | 0.48              |
| 1:BR:44:TYR:CE1   | 1:BR:68:VAL:HG13 | 2.49                     | 0.48              |
| 1:BU:50:VAL:HG12  | 1:BU:62:VAL:HG12 | 1.96                     | 0.48              |
| 1:BX:44:TYR:CE1   | 1:BX:68:VAL:HG13 | 2.49                     | 0.48              |
| 1:BZ:18:PHE:HB3   | 1:BZ:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:CC:11:HIS:HB2   | 1:CG:109:ASP:HB3 | 1.95                     | 0.48              |
| 1:CC:75:THR:HB    | 1:CC:82:SER:HB3  | 1.95                     | 0.48              |
| 1:CG:21:THR:O     | 1:CP:132:HIS:HB2 | 2.14                     | 0.48              |
| 1:DD:44:TYR:CE1   | 1:DD:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:DD:44:TYR:HE1   | 1:DD:68:VAL:HG13 | 1.79                     | 0.48              |
| 1:DF:41:ILE:HG23  | 1:DF:42:GLY:N    | 2.28                     | 0.48              |
| 1:DJ:44:TYR:CE1   | 1:DJ:68:VAL:HG13 | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:DL:50:VAL:HG12 | 1:DL:62:VAL:HG12 | 1.94                     | 0.48              |
| 1:DL:62:VAL:HG23 | 1:DL:96:PHE:HB2  | 1.95                     | 0.48              |
| 1:AC:41:ILE:HG23 | 1:AC:42:GLY:N    | 2.28                     | 0.48              |
| 1:AN:44:TYR:CE1  | 1:AN:68:VAL:HG13 | 2.49                     | 0.48              |
| 1:AO:62:VAL:HG23 | 1:AO:96:PHE:HB2  | 1.95                     | 0.48              |
| 1:AS:75:THR:HB   | 1:AS:82:SER:HB3  | 1.95                     | 0.48              |
| 1:AV:74:ILE:HA   | 1:CB:78:GLY:O    | 2.14                     | 0.48              |
| 1:BE:18:PHE:HB3  | 1:BE:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:BK:18:PHE:HB3  | 1:BK:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:CF:44:TYR:CE1  | 1:CF:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:CI:18:PHE:HB3  | 1:CI:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:CQ:50:VAL:HG12 | 1:CQ:62:VAL:HG12 | 1.94                     | 0.48              |
| 1:DG:18:PHE:HB3  | 1:DG:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:DG:44:TYR:HE1  | 1:DG:68:VAL:HG13 | 1.79                     | 0.48              |
| 1:AD:44:TYR:CE1  | 1:AD:68:VAL:HG13 | 2.48                     | 0.48              |
| 1:AM:18:PHE:HB3  | 1:AM:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:AP:44:TYR:HE1  | 1:AP:68:VAL:HG13 | 1.79                     | 0.48              |
| 1:AV:44:TYR:HE1  | 1:AV:68:VAL:HG13 | 1.79                     | 0.48              |
| 1:AW:44:TYR:CE1  | 1:AW:68:VAL:HG13 | 2.49                     | 0.48              |
| 1:AY:18:PHE:HB3  | 1:AY:31:PHE:HB3  | 1.96                     | 0.48              |
| 1:BD:62:VAL:HG23 | 1:BD:96:PHE:HB2  | 1.95                     | 0.48              |
| 1:BF:50:VAL:HG12 | 1:BF:62:VAL:HG12 | 1.96                     | 0.48              |
| 1:CF:44:TYR:HE1  | 1:CF:68:VAL:HG13 | 1.79                     | 0.48              |
| 1:CG:44:TYR:CE1  | 1:CG:68:VAL:HG13 | 2.49                     | 0.48              |
| 1:CR:75:THR:HB   | 1:CR:82:SER:HB3  | 1.95                     | 0.48              |
| 1:DK:98:LEU:HD13 | 1:DK:107:ARG:HD2 | 1.95                     | 0.48              |
| 1:AA:44:TYR:HE1  | 1:AA:68:VAL:HG13 | 1.79                     | 0.47              |
| 1:AK:44:TYR:CE1  | 1:AK:68:VAL:HG13 | 2.49                     | 0.47              |
| 1:AS:1:PRO:HD3   | 1:BX:131:GLU:CB  | 2.43                     | 0.47              |
| 1:AU:41:ILE:HG23 | 1:AU:42:GLY:N    | 2.28                     | 0.47              |
| 1:AY:75:THR:HB   | 1:AY:82:SER:HB3  | 1.95                     | 0.47              |
| 1:BH:44:TYR:HE1  | 1:BH:68:VAL:HG13 | 1.79                     | 0.47              |
| 1:BK:44:TYR:HE1  | 1:BK:68:VAL:HG13 | 1.79                     | 0.47              |
| 1:BO:44:TYR:CE1  | 1:BO:68:VAL:HG13 | 2.49                     | 0.47              |
| 1:BS:90:ASN:CG   | 1:DL:99:PRO:HD2  | 2.38                     | 0.47              |
| 1:BW:134:TYR:HB2 | 1:DC:3:LEU:HD23  | 1.96                     | 0.47              |
| 1:CA:50:VAL:HG12 | 1:CA:62:VAL:HG12 | 1.96                     | 0.47              |
| 1:CH:44:TYR:CE1  | 1:CH:68:VAL:HG13 | 2.49                     | 0.47              |
| 1:CJ:50:VAL:HG12 | 1:CJ:62:VAL:HG12 | 1.96                     | 0.47              |
| 1:CK:44:TYR:CE1  | 1:CK:68:VAL:HG13 | 2.49                     | 0.47              |
| 1:CR:44:TYR:HE1  | 1:CR:68:VAL:HG13 | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CW:50:VAL:HG12  | 1:CW:62:VAL:HG12  | 1.94                     | 0.47              |
| 1:CW:62:VAL:HG23  | 1:CW:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:CX:44:TYR:CE1   | 1:CX:68:VAL:HG13  | 2.48                     | 0.47              |
| 1:DB:44:TYR:CE1   | 1:DB:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:DB:50:VAL:HG12  | 1:DB:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:AG:44:TYR:CE1   | 1:AG:68:VAL:HG13  | 2.48                     | 0.47              |
| 1:AK:99:PRO:HD2   | 1:CI:90:ASN:CG    | 2.39                     | 0.47              |
| 1:AL:108:GLU:HG3  | 1:CE:128:VAL:CG1  | 2.44                     | 0.47              |
| 1:AM:44:TYR:HE1   | 1:AM:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:AO:44:TYR:CE1   | 1:AO:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:AP:130:VAL:CG1  | 1:AT:60:PHE:CE1   | 2.92                     | 0.47              |
| 1:AT:50:VAL:HG12  | 1:AT:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:BF:44:TYR:CE1   | 1:BF:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:BJ:44:TYR:CE1   | 1:BJ:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:BM:50:VAL:HG12  | 1:BM:62:VAL:HG12  | 1.94                     | 0.47              |
| 1:BY:44:TYR:CE1   | 1:BY:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:CV:50:VAL:HG12  | 1:CV:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:CZ:44:TYR:CE1   | 1:CZ:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:AG:18:PHE:HB3   | 1:AG:31:PHE:HB3   | 1.96                     | 0.47              |
| 1:AN:6:ILE:HD13   | 1:CL:123:ILE:HD11 | 1.96                     | 0.47              |
| 1:AT:44:TYR:CE1   | 1:AT:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:AZ:98:LEU:HD13  | 1:AZ:107:ARG:HD2  | 1.95                     | 0.47              |
| 1:AZ:126:THR:HG22 | 1:AZ:127:ILE:HD13 | 1.97                     | 0.47              |
| 1:BC:126:THR:HG22 | 1:BC:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:BD:44:TYR:CE1   | 1:BD:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:BD:131:GLU:OE1  | 1:CW:1:PRO:HD3    | 2.14                     | 0.47              |
| 1:BF:3:LEU:HD23   | 1:DE:134:TYR:CD1  | 2.50                     | 0.47              |
| 1:BG:44:TYR:CE1   | 1:BG:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:BI:50:VAL:HG12  | 1:BI:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:BO:123:ILE:HD11 | 1:DG:6:ILE:HD13   | 1.96                     | 0.47              |
| 1:BW:44:TYR:HE1   | 1:BW:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:BW:132:HIS:NE2  | 1:DB:50:VAL:HG23  | 2.28                     | 0.47              |
| 1:BY:41:ILE:HG23  | 1:BY:42:GLY:N     | 2.28                     | 0.47              |
| 1:CU:18:PHE:HB3   | 1:CU:31:PHE:HB3   | 1.96                     | 0.47              |
| 1:DJ:44:TYR:HE1   | 1:DJ:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:AG:50:VAL:O     | 1:AZ:132:HIS:NE2  | 2.47                     | 0.47              |
| 1:AH:44:TYR:CE1   | 1:AH:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:AS:44:TYR:HE1   | 1:AS:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:AX:41:ILE:HG23  | 1:AX:42:GLY:N     | 2.28                     | 0.47              |
| 1:AX:44:TYR:CE1   | 1:AX:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:AX:62:VAL:HG23  | 1:AX:96:PHE:HB2   | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BF:50:VAL:HG23  | 1:BK:132:HIS:NE2  | 2.30                     | 0.47              |
| 1:BL:50:VAL:HG12  | 1:BL:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:BN:75:THR:HB    | 1:BN:82:SER:HB3   | 1.95                     | 0.47              |
| 1:BO:98:LEU:HD13  | 1:BO:107:ARG:HD2  | 1.95                     | 0.47              |
| 1:BP:62:VAL:HG23  | 1:BP:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:BV:44:TYR:CE1   | 1:BV:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:CC:18:PHE:HB3   | 1:CC:31:PHE:HB3   | 1.96                     | 0.47              |
| 1:CC:44:TYR:HE1   | 1:CC:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:CD:44:TYR:CE1   | 1:CD:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:CE:62:VAL:HG23  | 1:CE:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:CL:44:TYR:HE1   | 1:CL:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:CM:126:THR:HG22 | 1:CM:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:CV:44:TYR:CE1   | 1:CV:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:CY:50:VAL:HG12  | 1:CY:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:AE:123:ILE:O    | 1:AE:126:THR:HB   | 2.15                     | 0.47              |
| 1:AI:134:TYR:CZ   | 1:BZ:20:PRO:HB2   | 2.49                     | 0.47              |
| 1:AJ:44:TYR:HE1   | 1:AJ:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:AK:50:VAL:HG12  | 1:AK:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:AR:62:VAL:HG23  | 1:AR:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:AR:73:THR:H     | 1:CF:80:ASP:CB    | 2.28                     | 0.47              |
| 1:AS:1:PRO:CD     | 1:BX:132:HIS:O    | 2.62                     | 0.47              |
| 1:AU:130:VAL:CG1  | 1:CK:60:PHE:CE1   | 2.96                     | 0.47              |
| 1:BC:123:ILE:O    | 1:BC:126:THR:HB   | 2.15                     | 0.47              |
| 1:BM:44:TYR:CE1   | 1:BM:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:BN:44:TYR:HE1   | 1:BN:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:BO:123:ILE:O    | 1:BO:126:THR:HB   | 2.15                     | 0.47              |
| 1:BP:44:TYR:CE1   | 1:BP:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:BR:126:THR:HG22 | 1:BR:127:ILE:HD13 | 1.97                     | 0.47              |
| 1:BS:44:TYR:CE1   | 1:BS:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:BW:18:PHE:HB3   | 1:BW:31:PHE:HB3   | 1.96                     | 0.47              |
| 1:CA:126:THR:HG22 | 1:CA:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:CC:131:GLU:CB   | 1:CG:1:PRO:HD3    | 2.41                     | 0.47              |
| 1:CJ:123:ILE:O    | 1:CJ:126:THR:HB   | 2.15                     | 0.47              |
| 1:CQ:44:TYR:CE1   | 1:CQ:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:CV:126:THR:HG22 | 1:CV:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:CX:18:PHE:HB3   | 1:CX:31:PHE:HB3   | 1.96                     | 0.47              |
| 1:CX:44:TYR:HE1   | 1:CX:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:CY:1:PRO:CD     | 1:DJ:131:GLU:HB3  | 2.45                     | 0.47              |
| 1:CY:44:TYR:CE1   | 1:CY:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:DF:44:TYR:CE1   | 1:DF:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:DH:123:ILE:O    | 1:DH:126:THR:HB   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AB:44:TYR:CE1   | 1:AB:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:AB:126:THR:HG22 | 1:AB:127:ILE:HD13 | 1.97                     | 0.47              |
| 1:AF:11:HIS:H     | 1:BY:109:ASP:HB3  | 1.78                     | 0.47              |
| 1:AK:99:PRO:HD2   | 1:CI:90:ASN:OD1   | 2.15                     | 0.47              |
| 1:AK:126:THR:HG22 | 1:AK:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:AL:44:TYR:CE1   | 1:AL:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:AN:1:PRO:CD     | 1:CL:131:GLU:HB3  | 2.43                     | 0.47              |
| 1:AW:123:ILE:O    | 1:AW:126:THR:HB   | 2.15                     | 0.47              |
| 1:AX:132:HIS:CE1  | 1:CN:50:VAL:HG23  | 2.50                     | 0.47              |
| 1:BC:131:GLU:HB3  | 1:BH:1:PRO:HD3    | 1.96                     | 0.47              |
| 1:BI:44:TYR:CE1   | 1:BI:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:BO:126:THR:HG22 | 1:BO:127:ILE:HD13 | 1.97                     | 0.47              |
| 1:BR:50:VAL:HG12  | 1:BR:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:BV:41:ILE:HG23  | 1:BV:42:GLY:N     | 2.28                     | 0.47              |
| 1:CG:50:VAL:HG12  | 1:CG:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:CG:126:THR:HG22 | 1:CG:127:ILE:HD13 | 1.97                     | 0.47              |
| 1:CM:50:VAL:HG12  | 1:CM:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:CO:44:TYR:HE1   | 1:CO:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:CT:44:TYR:CE1   | 1:CT:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:CY:60:PHE:CE1   | 1:DJ:130:VAL:HG11 | 2.49                     | 0.47              |
| 1:CZ:41:ILE:HG23  | 1:CZ:42:GLY:N     | 2.28                     | 0.47              |
| 1:DE:44:TYR:CE1   | 1:DE:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:DK:50:VAL:HG12  | 1:DK:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:DK:126:THR:HG22 | 1:DK:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:AB:123:ILE:O    | 1:AB:126:THR:HB   | 2.15                     | 0.47              |
| 1:AD:44:TYR:HE1   | 1:AD:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:AH:123:ILE:O    | 1:AH:126:THR:HB   | 2.15                     | 0.47              |
| 1:AK:123:ILE:O    | 1:AK:126:THR:HB   | 2.15                     | 0.47              |
| 1:AN:50:VAL:HG23  | 1:CL:132:HIS:CE1  | 2.50                     | 0.47              |
| 1:AQ:126:THR:HG22 | 1:AQ:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:AT:123:ILE:O    | 1:AT:126:THR:HB   | 2.15                     | 0.47              |
| 1:AZ:44:TYR:CE1   | 1:AZ:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:AZ:123:ILE:O    | 1:AZ:126:THR:HB   | 2.15                     | 0.47              |
| 1:BA:41:ILE:HG23  | 1:BA:42:GLY:N     | 2.28                     | 0.47              |
| 1:BA:44:TYR:CE1   | 1:BA:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:BB:130:VAL:HG11 | 1:DH:60:PHE:CE1   | 2.49                     | 0.47              |
| 1:BF:123:ILE:O    | 1:BF:126:THR:HB   | 2.15                     | 0.47              |
| 1:BI:123:ILE:O    | 1:BI:126:THR:HB   | 2.15                     | 0.47              |
| 1:BJ:1:PRO:HD2    | 1:DC:132:HIS:O    | 2.14                     | 0.47              |
| 1:BL:44:TYR:CE1   | 1:BL:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:BP:131:GLU:CB   | 1:DF:1:PRO:HD3    | 2.43                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BS:1:PRO:HD3    | 1:DL:131:GLU:CB   | 2.40                     | 0.47              |
| 1:BS:62:VAL:HG23  | 1:BS:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:BT:132:HIS:CE1  | 1:DK:50:VAL:HG23  | 2.50                     | 0.47              |
| 1:BW:1:PRO:HD3    | 1:DB:131:GLU:HB3  | 1.96                     | 0.47              |
| 1:BW:132:HIS:CE1  | 1:DB:50:VAL:HG23  | 2.49                     | 0.47              |
| 1:BX:123:ILE:O    | 1:BX:126:THR:HB   | 2.15                     | 0.47              |
| 1:BX:126:THR:HG22 | 1:BX:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:BZ:44:TYR:HE1   | 1:BZ:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:CD:50:VAL:HG12  | 1:CD:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:CF:50:VAL:HG23  | 1:CP:132:HIS:CE1  | 2.49                     | 0.47              |
| 1:CN:44:TYR:CE1   | 1:CN:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:CP:44:TYR:CE1   | 1:CP:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:DB:123:ILE:O    | 1:DB:126:THR:HB   | 2.15                     | 0.47              |
| 1:DF:62:VAL:HG23  | 1:DF:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:DI:44:TYR:CE1   | 1:DI:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:DI:62:VAL:HG23  | 1:DI:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:AA:21:THR:O     | 1:BV:132:HIS:HB2  | 2.15                     | 0.47              |
| 1:AK:60:PHE:CD1   | 1:CI:130:VAL:HG11 | 2.49                     | 0.47              |
| 1:AL:62:VAL:HG23  | 1:AL:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:AQ:44:TYR:CE1   | 1:AQ:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:AU:44:TYR:CE1   | 1:AU:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:BC:50:VAL:HG12  | 1:BC:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:BS:6:ILE:HD13   | 1:DL:123:ILE:HD11 | 1.97                     | 0.47              |
| 1:BU:123:ILE:O    | 1:BU:126:THR:HB   | 2.15                     | 0.47              |
| 1:CM:123:ILE:O    | 1:CM:126:THR:HB   | 2.15                     | 0.47              |
| 1:CS:50:VAL:HG12  | 1:CS:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:CW:44:TYR:CE1   | 1:CW:68:VAL:HG13  | 2.50                     | 0.47              |
| 1:CY:126:THR:HG22 | 1:CY:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:DE:126:THR:HG22 | 1:DE:127:ILE:HD13 | 1.97                     | 0.47              |
| 1:AF:48:SER:OG    | 1:BY:126:THR:HG21 | 2.15                     | 0.47              |
| 1:AF:88:ARG:HD2   | 1:BY:99:PRO:CB    | 2.45                     | 0.47              |
| 1:AN:123:ILE:O    | 1:AN:126:THR:HB   | 2.15                     | 0.47              |
| 1:AQ:50:VAL:HG12  | 1:AQ:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:AW:50:VAL:HG12  | 1:AW:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:BW:50:VAL:O     | 1:DB:132:HIS:NE2  | 2.47                     | 0.47              |
| 1:CA:123:ILE:O    | 1:CA:126:THR:HB   | 2.15                     | 0.47              |
| 1:CB:44:TYR:CE1   | 1:CB:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:CI:44:TYR:HE1   | 1:CI:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:CN:62:VAL:HG23  | 1:CN:96:PHE:HB2   | 1.95                     | 0.47              |
| 1:CV:123:ILE:O    | 1:CV:126:THR:HB   | 2.15                     | 0.47              |
| 1:AB:50:VAL:HG23  | 1:DA:132:HIS:NE2  | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AE:44:TYR:CE1   | 1:AE:68:VAL:HG13  | 2.49                     | 0.47              |
| 1:AE:50:VAL:HG12  | 1:AE:62:VAL:HG12  | 1.96                     | 0.47              |
| 1:AE:126:THR:HG22 | 1:AE:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:AH:11:HIS:CB    | 1:CX:109:ASP:HB3  | 2.45                     | 0.47              |
| 1:AH:126:THR:HG22 | 1:AH:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:AI:41:ILE:HG23  | 1:AI:42:GLY:N     | 2.28                     | 0.47              |
| 1:AP:108:GLU:OE1  | 1:AT:11:HIS:NE2   | 2.48                     | 0.47              |
| 1:AU:126:THR:HG23 | 1:CK:50:VAL:HG13  | 1.97                     | 0.47              |
| 1:AW:126:THR:HG22 | 1:AW:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:BG:3:LEU:HD23   | 1:BK:134:TYR:HB2  | 1.96                     | 0.47              |
| 1:BQ:44:TYR:HE1   | 1:BQ:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:BT:44:TYR:HE1   | 1:BT:68:VAL:HG13  | 1.79                     | 0.47              |
| 1:CG:123:ILE:O    | 1:CG:126:THR:HB   | 2.15                     | 0.47              |
| 1:CK:80:ASP:HB2   | 1:CR:73:THR:N     | 2.15                     | 0.47              |
| 1:CP:123:ILE:O    | 1:CP:126:THR:HB   | 2.15                     | 0.47              |
| 1:CP:126:THR:HG22 | 1:CP:127:ILE:HD13 | 1.97                     | 0.47              |
| 1:CS:126:THR:HG22 | 1:CS:127:ILE:HD13 | 1.96                     | 0.47              |
| 1:CY:94:VAL:HG22  | 1:DJ:94:VAL:HG13  | 1.96                     | 0.47              |
| 1:AL:132:HIS:CE1  | 1:CE:50:VAL:HG23  | 2.50                     | 0.46              |
| 1:AN:50:VAL:HG12  | 1:AN:62:VAL:HG12  | 1.96                     | 0.46              |
| 1:AP:73:THR:H     | 1:AU:80:ASP:CB    | 2.27                     | 0.46              |
| 1:AT:126:THR:HG22 | 1:AT:127:ILE:HD13 | 1.96                     | 0.46              |
| 1:BC:44:TYR:CE1   | 1:BC:68:VAL:HG13  | 2.49                     | 0.46              |
| 1:BF:126:THR:HG22 | 1:BF:127:ILE:HD13 | 1.96                     | 0.46              |
| 1:BO:50:VAL:HG12  | 1:BO:62:VAL:HG12  | 1.96                     | 0.46              |
| 1:CE:44:TYR:CE1   | 1:CE:68:VAL:HG13  | 2.50                     | 0.46              |
| 1:CS:123:ILE:O    | 1:CS:126:THR:HB   | 2.15                     | 0.46              |
| 1:DB:126:THR:HG22 | 1:DB:127:ILE:HD13 | 1.96                     | 0.46              |
| 1:AC:44:TYR:CE1   | 1:AC:68:VAL:HG13  | 2.50                     | 0.46              |
| 1:AF:3:LEU:N      | 1:BY:134:TYR:O    | 2.39                     | 0.46              |
| 1:AF:44:TYR:CE1   | 1:AF:68:VAL:HG13  | 2.49                     | 0.46              |
| 1:AG:44:TYR:HE1   | 1:AG:68:VAL:HG13  | 1.79                     | 0.46              |
| 1:AG:80:ASP:HB3   | 1:CB:73:THR:H     | 1.79                     | 0.46              |
| 1:AI:44:TYR:CE1   | 1:AI:68:VAL:HG13  | 2.50                     | 0.46              |
| 1:AP:11:HIS:CE1   | 1:AT:108:GLU:OE1  | 2.67                     | 0.46              |
| 1:AS:18:PHE:HB3   | 1:AS:31:PHE:HB3   | 1.96                     | 0.46              |
| 1:AU:94:VAL:HA    | 1:CK:93:GLN:O     | 2.15                     | 0.46              |
| 1:BD:80:ASP:HB2   | 1:BH:73:THR:N     | 2.21                     | 0.46              |
| 1:BN:94:VAL:HG13  | 1:BR:94:VAL:HG22  | 1.96                     | 0.46              |
| 1:BV:53:PRO:HB3   | 1:BV:59:VAL:O     | 2.16                     | 0.46              |
| 1:CA:44:TYR:CE1   | 1:CA:68:VAL:HG13  | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CD:123:ILE:O    | 1:CD:126:THR:HB   | 2.15                     | 0.46              |
| 1:CU:44:TYR:HE1   | 1:CU:68:VAL:HG13  | 1.79                     | 0.46              |
| 1:CY:123:ILE:O    | 1:CY:126:THR:HB   | 2.15                     | 0.46              |
| 1:DG:50:VAL:HB    | 1:DG:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:DH:126:THR:HG22 | 1:DH:127:ILE:HD13 | 1.96                     | 0.46              |
| 1:DL:44:TYR:CE1   | 1:DL:68:VAL:HG13  | 2.49                     | 0.46              |
| 1:AA:132:HIS:CE1  | 1:AQ:50:VAL:HG23  | 2.50                     | 0.46              |
| 1:AC:53:PRO:HB3   | 1:AC:59:VAL:O     | 2.16                     | 0.46              |
| 1:AI:132:HIS:HB2  | 1:BZ:21:THR:O     | 2.14                     | 0.46              |
| 1:AX:53:PRO:HB3   | 1:AX:59:VAL:O     | 2.16                     | 0.46              |
| 1:BG:53:PRO:HB3   | 1:BG:59:VAL:O     | 2.16                     | 0.46              |
| 1:BI:126:THR:HG22 | 1:BI:127:ILE:HD13 | 1.96                     | 0.46              |
| 1:BL:53:PRO:HB3   | 1:BL:59:VAL:O     | 2.16                     | 0.46              |
| 1:BO:94:VAL:HG13  | 1:DG:94:VAL:HG22  | 1.97                     | 0.46              |
| 1:CK:53:PRO:HB3   | 1:CK:59:VAL:O     | 2.16                     | 0.46              |
| 1:CM:44:TYR:CE1   | 1:CM:68:VAL:HG13  | 2.49                     | 0.46              |
| 1:CQ:53:PRO:HB3   | 1:CQ:59:VAL:O     | 2.16                     | 0.46              |
| 1:DA:18:PHE:HB3   | 1:DA:31:PHE:HB3   | 1.96                     | 0.46              |
| 1:DC:44:TYR:CE1   | 1:DC:68:VAL:HG13  | 2.50                     | 0.46              |
| 1:DH:50:VAL:HG12  | 1:DH:62:VAL:HG12  | 1.96                     | 0.46              |
| 1:DK:53:PRO:HB3   | 1:DK:59:VAL:O     | 2.16                     | 0.46              |
| 1:AH:50:VAL:HG12  | 1:AH:62:VAL:HG12  | 1.96                     | 0.46              |
| 1:AO:3:LEU:HD23   | 1:CL:134:TYR:HB2  | 1.97                     | 0.46              |
| 1:AO:53:PRO:HB3   | 1:AO:59:VAL:O     | 2.16                     | 0.46              |
| 1:AZ:53:PRO:HB3   | 1:AZ:59:VAL:O     | 2.16                     | 0.46              |
| 1:BJ:53:PRO:HB3   | 1:BJ:59:VAL:O     | 2.16                     | 0.46              |
| 1:BM:53:PRO:HB3   | 1:BM:59:VAL:O     | 2.16                     | 0.46              |
| 1:BP:53:PRO:HB3   | 1:BP:59:VAL:O     | 2.16                     | 0.46              |
| 1:CS:53:PRO:HB3   | 1:CS:59:VAL:O     | 2.16                     | 0.46              |
| 1:CZ:53:PRO:HB3   | 1:CZ:59:VAL:O     | 2.16                     | 0.46              |
| 1:DE:50:VAL:HG12  | 1:DE:62:VAL:HG12  | 1.96                     | 0.46              |
| 1:DE:53:PRO:HB3   | 1:DE:59:VAL:O     | 2.16                     | 0.46              |
| 1:DH:53:PRO:HB3   | 1:DH:59:VAL:O     | 2.16                     | 0.46              |
| 1:AE:53:PRO:HB3   | 1:AE:59:VAL:O     | 2.16                     | 0.46              |
| 1:AK:3:LEU:HD13   | 1:CI:133:PHE:HB3  | 1.97                     | 0.46              |
| 1:AL:52:GLU:OE2   | 1:CE:132:HIS:NE2  | 2.42                     | 0.46              |
| 1:AL:53:PRO:HB3   | 1:AL:59:VAL:O     | 2.16                     | 0.46              |
| 1:AP:126:THR:HG23 | 1:AT:50:VAL:CG1   | 2.46                     | 0.46              |
| 1:AU:53:PRO:HB3   | 1:AU:59:VAL:O     | 2.16                     | 0.46              |
| 1:AY:44:TYR:HE1   | 1:AY:68:VAL:HG13  | 1.79                     | 0.46              |
| 1:AY:50:VAL:HB    | 1:AY:62:VAL:HG12  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BC:132:HIS:O    | 1:BH:1:PRO:HD2    | 2.16                     | 0.46              |
| 1:BE:44:TYR:HE1   | 1:BE:68:VAL:HG13  | 1.79                     | 0.46              |
| 1:BP:18:PHE:HB3   | 1:BP:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:BU:126:THR:HG22 | 1:BU:127:ILE:HD13 | 1.96                     | 0.46              |
| 1:CE:18:PHE:HB3   | 1:CE:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:CP:53:PRO:HB3   | 1:CP:59:VAL:O     | 2.16                     | 0.46              |
| 1:DE:123:ILE:O    | 1:DE:126:THR:HB   | 2.15                     | 0.46              |
| 1:AA:80:ASP:HB3   | 1:BV:73:THR:H     | 1.81                     | 0.46              |
| 1:AC:18:PHE:HB3   | 1:AC:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:AC:123:ILE:HD11 | 1:BV:6:ILE:HD13   | 1.97                     | 0.46              |
| 1:AP:80:ASP:HB2   | 1:CH:73:THR:N     | 2.29                     | 0.46              |
| 1:AR:44:TYR:CE1   | 1:AR:68:VAL:HG13  | 2.50                     | 0.46              |
| 1:AS:50:VAL:HB    | 1:AS:62:VAL:HG12  | 1.97                     | 0.46              |
| 1:AT:53:PRO:HB3   | 1:AT:59:VAL:O     | 2.16                     | 0.46              |
| 1:BB:44:TYR:HE1   | 1:BB:68:VAL:HG13  | 1.79                     | 0.46              |
| 1:BB:50:VAL:HB    | 1:BB:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:BF:53:PRO:HB3   | 1:BF:59:VAL:O     | 2.16                     | 0.46              |
| 1:BL:123:ILE:O    | 1:BL:126:THR:HB   | 2.15                     | 0.46              |
| 1:BS:94:VAL:HG22  | 1:DL:94:VAL:HG13  | 1.98                     | 0.46              |
| 1:CA:53:PRO:HB3   | 1:CA:59:VAL:O     | 2.16                     | 0.46              |
| 1:CD:126:THR:HG22 | 1:CD:127:ILE:HD13 | 1.96                     | 0.46              |
| 1:CY:53:PRO:HB3   | 1:CY:59:VAL:O     | 2.16                     | 0.46              |
| 1:CZ:18:PHE:HB3   | 1:CZ:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:DC:18:PHE:HB3   | 1:DC:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:AI:134:TYR:CD1  | 1:BZ:3:LEU:HD23   | 2.51                     | 0.46              |
| 1:AL:18:PHE:HB3   | 1:AL:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:AN:126:THR:HG22 | 1:AN:127:ILE:HD13 | 1.97                     | 0.46              |
| 1:AP:108:GLU:OE1  | 1:AT:11:HIS:CD2   | 2.69                     | 0.46              |
| 1:AP:130:VAL:CG1  | 1:AT:60:PHE:CD1   | 2.93                     | 0.46              |
| 1:AZ:50:VAL:HG12  | 1:AZ:62:VAL:HG12  | 1.96                     | 0.46              |
| 1:BC:53:PRO:HB3   | 1:BC:59:VAL:O     | 2.16                     | 0.46              |
| 1:BD:31:PHE:HZ    | 1:CW:133:PHE:CE1  | 2.33                     | 0.46              |
| 1:BD:53:PRO:HB3   | 1:BD:59:VAL:O     | 2.16                     | 0.46              |
| 1:BJ:18:PHE:HB3   | 1:BJ:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:BN:18:PHE:HB3   | 1:BN:31:PHE:HB3   | 1.96                     | 0.46              |
| 1:BN:109:ASP:HB3  | 1:BR:11:HIS:H     | 1.80                     | 0.46              |
| 1:BR:123:ILE:O    | 1:BR:126:THR:HB   | 2.15                     | 0.46              |
| 1:CC:50:VAL:HB    | 1:CC:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:DA:44:TYR:HE1   | 1:DA:68:VAL:HG13  | 1.79                     | 0.46              |
| 1:DC:62:VAL:HG23  | 1:DC:96:PHE:HB2   | 1.95                     | 0.46              |
| 1:AI:53:PRO:HB3   | 1:AI:59:VAL:O     | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AJ:50:VAL:HB    | 1:AJ:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:AQ:53:PRO:HB3   | 1:AQ:59:VAL:O     | 2.16                     | 0.46              |
| 1:BD:134:TYR:CZ   | 1:CU:20:PRO:HB2   | 2.51                     | 0.46              |
| 1:BG:18:PHE:HB3   | 1:BG:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:BL:126:THR:HG22 | 1:BL:127:ILE:HD13 | 1.97                     | 0.46              |
| 1:CQ:18:PHE:HB3   | 1:CQ:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:CT:53:PRO:HB3   | 1:CT:59:VAL:O     | 2.16                     | 0.46              |
| 1:CU:50:VAL:HB    | 1:CU:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:CY:131:GLU:CB   | 1:DJ:1:PRO:HD3    | 2.45                     | 0.46              |
| 1:DB:53:PRO:HB3   | 1:DB:59:VAL:O     | 2.16                     | 0.46              |
| 1:DC:53:PRO:HB3   | 1:DC:59:VAL:O     | 2.16                     | 0.46              |
| 1:DF:18:PHE:HB3   | 1:DF:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:DK:44:TYR:CE1   | 1:DK:68:VAL:HG13  | 2.49                     | 0.46              |
| 1:DK:123:ILE:O    | 1:DK:126:THR:HB   | 2.15                     | 0.46              |
| 1:DL:53:PRO:HB3   | 1:DL:59:VAL:O     | 2.16                     | 0.46              |
| 1:AI:47:SER:HB2   | 1:AI:65:PHE:HB2   | 1.98                     | 0.46              |
| 1:AK:53:PRO:HB3   | 1:AK:59:VAL:O     | 2.16                     | 0.46              |
| 1:AM:50:VAL:HB    | 1:AM:62:VAL:HG12  | 1.97                     | 0.46              |
| 1:AU:133:PHE:CE1  | 1:CK:31:PHE:HZ    | 2.34                     | 0.46              |
| 1:AW:53:PRO:HB3   | 1:AW:59:VAL:O     | 2.16                     | 0.46              |
| 1:AX:18:PHE:HB3   | 1:AX:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:BA:62:VAL:HG23  | 1:BA:96:PHE:HB2   | 1.95                     | 0.46              |
| 1:BA:99:PRO:HD2   | 1:CQ:90:ASN:CG    | 2.41                     | 0.46              |
| 1:BD:18:PHE:HB3   | 1:BD:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:BE:69:PRO:HB3   | 1:BE:89:THR:HG22  | 1.98                     | 0.46              |
| 1:BF:11:HIS:H     | 1:BK:109:ASP:HB3  | 1.80                     | 0.46              |
| 1:BI:53:PRO:HB3   | 1:BI:59:VAL:O     | 2.16                     | 0.46              |
| 1:BU:44:TYR:CE1   | 1:BU:68:VAL:HG13  | 2.49                     | 0.46              |
| 1:BX:50:VAL:HG12  | 1:BX:62:VAL:HG12  | 1.96                     | 0.46              |
| 1:BX:53:PRO:HB3   | 1:BX:59:VAL:O     | 2.16                     | 0.46              |
| 1:CB:18:PHE:HB3   | 1:CB:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:CB:53:PRO:HB3   | 1:CB:59:VAL:O     | 2.16                     | 0.46              |
| 1:CJ:126:THR:HG22 | 1:CJ:127:ILE:HD13 | 1.96                     | 0.46              |
| 1:CJ:134:TYR:CD1  | 1:CS:3:LEU:HD23   | 2.51                     | 0.46              |
| 1:CO:50:VAL:HB    | 1:CO:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:CR:50:VAL:HB    | 1:CR:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:CV:53:PRO:HB3   | 1:CV:59:VAL:O     | 2.16                     | 0.46              |
| 1:AA:108:GLU:OE1  | 1:AQ:11:HIS:NE2   | 2.49                     | 0.46              |
| 1:AF:3:LEU:HD12   | 1:BY:133:PHE:CD1  | 2.50                     | 0.46              |
| 1:AG:50:VAL:HB    | 1:AG:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:AI:132:HIS:CE1  | 1:CB:50:VAL:HG23  | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:48:SER:OG    | 1:CI:126:THR:HG21 | 2.14                     | 0.46              |
| 1:AQ:123:ILE:O    | 1:AQ:126:THR:HB   | 2.15                     | 0.46              |
| 1:AY:69:PRO:HB3   | 1:AY:89:THR:HG22  | 1.98                     | 0.46              |
| 1:BA:18:PHE:HB3   | 1:BA:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:BB:11:HIS:HB2   | 1:DH:109:ASP:CB   | 2.40                     | 0.46              |
| 1:BD:60:PHE:CE1   | 1:CW:130:VAL:HG11 | 2.51                     | 0.46              |
| 1:BF:123:ILE:HD11 | 1:BK:6:ILE:HD13   | 1.97                     | 0.46              |
| 1:BF:132:HIS:NE2  | 1:BK:50:VAL:O     | 2.49                     | 0.46              |
| 1:BH:21:THR:O     | 1:DC:132:HIS:HB2  | 2.16                     | 0.46              |
| 1:BH:50:VAL:HB    | 1:BH:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:BT:50:VAL:O     | 1:DK:132:HIS:NE2  | 2.49                     | 0.46              |
| 1:BT:69:PRO:HB3   | 1:BT:89:THR:HG22  | 1.98                     | 0.46              |
| 1:BV:18:PHE:HB3   | 1:BV:31:PHE:HB3   | 1.98                     | 0.46              |
| 1:BY:53:PRO:HB3   | 1:BY:59:VAL:O     | 2.16                     | 0.46              |
| 1:CE:53:PRO:HB3   | 1:CE:59:VAL:O     | 2.16                     | 0.46              |
| 1:CO:69:PRO:HB3   | 1:CO:89:THR:HG22  | 1.98                     | 0.46              |
| 1:CY:132:HIS:NE2  | 1:DJ:50:VAL:O     | 2.49                     | 0.46              |
| 1:DA:50:VAL:HB    | 1:DA:62:VAL:HG12  | 1.98                     | 0.46              |
| 1:DI:53:PRO:HB3   | 1:DI:59:VAL:O     | 2.16                     | 0.46              |
| 1:AB:53:PRO:HB3   | 1:AB:59:VAL:O     | 2.16                     | 0.45              |
| 1:AF:47:SER:HB2   | 1:AF:65:PHE:HB2   | 1.99                     | 0.45              |
| 1:AH:53:PRO:HB3   | 1:AH:59:VAL:O     | 2.16                     | 0.45              |
| 1:AS:69:PRO:HB3   | 1:AS:89:THR:HG22  | 1.98                     | 0.45              |
| 1:AU:6:ILE:HD13   | 1:CK:123:ILE:HD11 | 1.98                     | 0.45              |
| 1:AY:1:PRO:HD2    | 1:BU:132:HIS:O    | 2.16                     | 0.45              |
| 1:BC:123:ILE:HD11 | 1:BH:6:ILE:HD13   | 1.98                     | 0.45              |
| 1:BO:109:ASP:HB3  | 1:DG:11:HIS:HB2   | 1.97                     | 0.45              |
| 1:BU:53:PRO:HB3   | 1:BU:59:VAL:O     | 2.16                     | 0.45              |
| 1:CC:69:PRO:HB3   | 1:CC:89:THR:HG22  | 1.98                     | 0.45              |
| 1:CD:53:PRO:HB3   | 1:CD:59:VAL:O     | 2.16                     | 0.45              |
| 1:CM:53:PRO:HB3   | 1:CM:59:VAL:O     | 2.16                     | 0.45              |
| 1:CN:18:PHE:HB3   | 1:CN:31:PHE:HB3   | 1.98                     | 0.45              |
| 1:CT:18:PHE:HB3   | 1:CT:31:PHE:HB3   | 1.98                     | 0.45              |
| 1:CU:69:PRO:HB3   | 1:CU:89:THR:HG22  | 1.98                     | 0.45              |
| 1:DF:53:PRO:HB3   | 1:DF:59:VAL:O     | 2.16                     | 0.45              |
| 1:AF:53:PRO:HB3   | 1:AF:59:VAL:O     | 2.16                     | 0.45              |
| 1:AG:8:LEU:HB3    | 1:AZ:116:SER:OG   | 2.17                     | 0.45              |
| 1:AU:90:ASN:CG    | 1:CK:99:PRO:CD    | 2.80                     | 0.45              |
| 1:AX:94:VAL:HG22  | 1:CN:94:VAL:HG13  | 1.99                     | 0.45              |
| 1:BH:69:PRO:HB3   | 1:BH:89:THR:HG22  | 1.98                     | 0.45              |
| 1:BN:69:PRO:HB3   | 1:BN:89:THR:HG22  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:BR:53:PRO:HB3  | 1:BR:59:VAL:O    | 2.16                     | 0.45              |
| 1:BT:132:HIS:HB2 | 1:DL:21:THR:O    | 2.16                     | 0.45              |
| 1:CI:50:VAL:HB   | 1:CI:62:VAL:HG12 | 1.98                     | 0.45              |
| 1:CI:69:PRO:HB3  | 1:CI:89:THR:HG22 | 1.98                     | 0.45              |
| 1:CW:53:PRO:HB3  | 1:CW:59:VAL:O    | 2.16                     | 0.45              |
| 1:DA:69:PRO:HB3  | 1:DA:89:THR:HG22 | 1.98                     | 0.45              |
| 1:DF:47:SER:HB2  | 1:DF:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:AG:69:PRO:HB3  | 1:AG:89:THR:HG22 | 1.98                     | 0.45              |
| 1:AH:1:PRO:HD3   | 1:CX:131:GLU:CB  | 2.42                     | 0.45              |
| 1:AR:53:PRO:HB3  | 1:AR:59:VAL:O    | 2.16                     | 0.45              |
| 1:AU:47:SER:HB2  | 1:AU:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:AX:99:PRO:HD2  | 1:CN:90:ASN:CG   | 2.41                     | 0.45              |
| 1:BB:69:PRO:HB3  | 1:BB:89:THR:HG22 | 1.98                     | 0.45              |
| 1:BF:24:ASP:HB3  | 1:BF:28:VAL:H    | 1.82                     | 0.45              |
| 1:BM:18:PHE:HB3  | 1:BM:31:PHE:HB3  | 1.98                     | 0.45              |
| 1:CE:47:SER:HB2  | 1:CE:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:CJ:24:ASP:HB3  | 1:CJ:28:VAL:H    | 1.82                     | 0.45              |
| 1:CM:24:ASP:HB3  | 1:CM:28:VAL:H    | 1.82                     | 0.45              |
| 1:CP:24:ASP:HB3  | 1:CP:28:VAL:H    | 1.82                     | 0.45              |
| 1:DD:50:VAL:HB   | 1:DD:62:VAL:HG12 | 1.98                     | 0.45              |
| 1:DD:69:PRO:HB3  | 1:DD:89:THR:HG22 | 1.98                     | 0.45              |
| 1:DG:69:PRO:HB3  | 1:DG:89:THR:HG22 | 1.98                     | 0.45              |
| 1:AE:24:ASP:HB3  | 1:AE:28:VAL:H    | 1.82                     | 0.45              |
| 1:AE:134:TYR:CZ  | 1:CV:20:PRO:HB2  | 2.51                     | 0.45              |
| 1:AG:21:THR:O    | 1:CB:132:HIS:HB2 | 2.17                     | 0.45              |
| 1:AN:53:PRO:HB3  | 1:AN:59:VAL:O    | 2.16                     | 0.45              |
| 1:AQ:24:ASP:HB3  | 1:AQ:28:VAL:H    | 1.82                     | 0.45              |
| 1:BB:90:ASN:CG   | 1:DH:99:PRO:HD2  | 2.41                     | 0.45              |
| 1:BC:109:ASP:HB3 | 1:BH:11:HIS:HB2  | 1.97                     | 0.45              |
| 1:BD:47:SER:HB2  | 1:BD:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:BG:47:SER:HB2  | 1:BG:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:BS:18:PHE:HB3  | 1:BS:31:PHE:HB3  | 1.98                     | 0.45              |
| 1:BZ:50:VAL:HB   | 1:BZ:62:VAL:HG12 | 1.98                     | 0.45              |
| 1:CF:109:ASP:HB3 | 1:CP:11:HIS:H    | 1.81                     | 0.45              |
| 1:CJ:53:PRO:HB3  | 1:CJ:59:VAL:O    | 2.16                     | 0.45              |
| 1:CK:18:PHE:HB3  | 1:CK:31:PHE:HB3  | 1.98                     | 0.45              |
| 1:AD:50:VAL:HB   | 1:AD:62:VAL:HG12 | 1.97                     | 0.45              |
| 1:AM:69:PRO:HB3  | 1:AM:89:THR:HG22 | 1.98                     | 0.45              |
| 1:AP:1:PRO:HG3   | 1:AT:125:SER:CB  | 2.47                     | 0.45              |
| 1:AU:18:PHE:HB3  | 1:AU:31:PHE:HB3  | 1.98                     | 0.45              |
| 1:AV:69:PRO:HB3  | 1:AV:89:THR:HG22 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BT:134:TYR:HB2  | 1:DL:3:LEU:HD23  | 1.98                     | 0.45              |
| 1:BW:69:PRO:HB3   | 1:BW:89:THR:HG22 | 1.98                     | 0.45              |
| 1:CK:44:TYR:HE1   | 1:CK:68:VAL:HG13 | 1.82                     | 0.45              |
| 1:CK:47:SER:HB2   | 1:CK:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:CL:69:PRO:HB3   | 1:CL:89:THR:HG22 | 1.98                     | 0.45              |
| 1:CM:131:GLU:HB3  | 1:CO:1:PRO:HD3   | 1.98                     | 0.45              |
| 1:AA:69:PRO:HB3   | 1:AA:89:THR:HG22 | 1.98                     | 0.45              |
| 1:AK:24:ASP:HB3   | 1:AK:28:VAL:H    | 1.82                     | 0.45              |
| 1:AL:47:SER:HB2   | 1:AL:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:AX:50:VAL:HG23  | 1:CN:132:HIS:CE1 | 2.52                     | 0.45              |
| 1:AY:131:GLU:HB3  | 1:BU:1:PRO:HD3   | 1.99                     | 0.45              |
| 1:BF:20:PRO:HB2   | 1:DE:134:TYR:CZ  | 2.51                     | 0.45              |
| 1:BJ:47:SER:HB2   | 1:BJ:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:BN:73:THR:H     | 1:BS:80:ASP:HB2  | 1.81                     | 0.45              |
| 1:BO:53:PRO:HB3   | 1:BO:59:VAL:O    | 2.16                     | 0.45              |
| 1:BS:44:TYR:HE1   | 1:BS:68:VAL:HG13 | 1.82                     | 0.45              |
| 1:BS:53:PRO:HB3   | 1:BS:59:VAL:O    | 2.16                     | 0.45              |
| 1:BW:50:VAL:HB    | 1:BW:62:VAL:HG12 | 1.98                     | 0.45              |
| 1:BY:47:SER:HB2   | 1:BY:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:CA:24:ASP:HB3   | 1:CA:28:VAL:H    | 1.82                     | 0.45              |
| 1:CG:53:PRO:HB3   | 1:CG:59:VAL:O    | 2.16                     | 0.45              |
| 1:CH:44:TYR:HE1   | 1:CH:68:VAL:HG13 | 1.82                     | 0.45              |
| 1:CQ:47:SER:HB2   | 1:CQ:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:CZ:3:LEU:HD23   | 1:DJ:134:TYR:HB2 | 1.97                     | 0.45              |
| 1:DJ:69:PRO:HB3   | 1:DJ:89:THR:HG22 | 1.98                     | 0.45              |
| 1:DL:18:PHE:HB3   | 1:DL:31:PHE:HB3  | 1.98                     | 0.45              |
| 1:AZ:24:ASP:HB3   | 1:AZ:28:VAL:H    | 1.82                     | 0.45              |
| 1:BA:44:TYR:HE1   | 1:BA:68:VAL:HG13 | 1.82                     | 0.45              |
| 1:BA:94:VAL:HG22  | 1:CQ:94:VAL:HG13 | 1.99                     | 0.45              |
| 1:BB:99:PRO:HD2   | 1:DH:90:ASN:ND2  | 2.32                     | 0.45              |
| 1:BE:50:VAL:HB    | 1:BE:62:VAL:HG12 | 1.97                     | 0.45              |
| 1:BM:47:SER:HB2   | 1:BM:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:BN:130:VAL:HG11 | 1:BR:60:PHE:CE1  | 2.51                     | 0.45              |
| 1:BY:18:PHE:HB3   | 1:BY:31:PHE:HB3  | 1.98                     | 0.45              |
| 1:CH:18:PHE:HB3   | 1:CH:31:PHE:HB3  | 1.98                     | 0.45              |
| 1:CW:47:SER:HB2   | 1:CW:65:PHE:HB2  | 1.99                     | 0.45              |
| 1:CX:50:VAL:HB    | 1:CX:62:VAL:HG12 | 1.98                     | 0.45              |
| 1:CZ:44:TYR:HE1   | 1:CZ:68:VAL:HG13 | 1.82                     | 0.45              |
| 1:DB:24:ASP:HB3   | 1:DB:28:VAL:H    | 1.82                     | 0.45              |
| 1:DI:44:TYR:HE1   | 1:DI:68:VAL:HG13 | 1.82                     | 0.45              |
| 1:AA:22:GLN:HB2   | 1:BV:132:HIS:CD2 | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AF:18:PHE:HB3   | 1:AF:31:PHE:HB3   | 1.98                     | 0.45              |
| 1:AJ:69:PRO:HB3   | 1:AJ:89:THR:HG22  | 1.98                     | 0.45              |
| 1:AN:60:PHE:CE1   | 1:CL:130:VAL:HG11 | 2.51                     | 0.45              |
| 1:AP:50:VAL:HB    | 1:AP:62:VAL:HG12  | 1.98                     | 0.45              |
| 1:AX:44:TYR:HE1   | 1:AX:68:VAL:HG13  | 1.82                     | 0.45              |
| 1:BA:47:SER:HB2   | 1:BA:65:PHE:HB2   | 1.99                     | 0.45              |
| 1:BA:53:PRO:HB3   | 1:BA:59:VAL:O     | 2.16                     | 0.45              |
| 1:BB:6:ILE:HD13   | 1:DH:123:ILE:HD11 | 1.99                     | 0.45              |
| 1:BC:128:VAL:HG13 | 1:BH:108:GLU:HG3  | 1.98                     | 0.45              |
| 1:BL:24:ASP:HB3   | 1:BL:28:VAL:H     | 1.82                     | 0.45              |
| 1:BO:24:ASP:HB3   | 1:BO:28:VAL:H     | 1.82                     | 0.45              |
| 1:CB:44:TYR:HE1   | 1:CB:68:VAL:HG13  | 1.82                     | 0.45              |
| 1:CU:58:ASP:O     | 1:CU:99:PRO:HA    | 2.17                     | 0.45              |
| 1:CV:24:ASP:HB3   | 1:CV:28:VAL:H     | 1.82                     | 0.45              |
| 1:CW:44:TYR:HE1   | 1:CW:68:VAL:HG13  | 1.82                     | 0.45              |
| 1:CX:69:PRO:HB3   | 1:CX:89:THR:HG22  | 1.98                     | 0.45              |
| 1:DI:18:PHE:HB3   | 1:DI:31:PHE:HB3   | 1.98                     | 0.45              |
| 1:DK:24:ASP:HB3   | 1:DK:28:VAL:H     | 1.82                     | 0.45              |
| 1:AA:50:VAL:HB    | 1:AA:62:VAL:HG12  | 1.98                     | 0.45              |
| 1:AO:44:TYR:HE1   | 1:AO:68:VAL:HG13  | 1.82                     | 0.45              |
| 1:AV:94:VAL:HG22  | 1:CA:94:VAL:HG13  | 1.98                     | 0.45              |
| 1:AW:24:ASP:HB3   | 1:AW:28:VAL:H     | 1.82                     | 0.45              |
| 1:BC:24:ASP:HB3   | 1:BC:28:VAL:H     | 1.82                     | 0.45              |
| 1:BK:69:PRO:HB3   | 1:BK:89:THR:HG22  | 1.98                     | 0.45              |
| 1:BN:50:VAL:HB    | 1:BN:62:VAL:HG12  | 1.98                     | 0.45              |
| 1:BO:20:PRO:HB2   | 1:BR:134:TYR:CZ   | 2.52                     | 0.45              |
| 1:BQ:69:PRO:HB3   | 1:BQ:89:THR:HG22  | 1.98                     | 0.45              |
| 1:BT:50:VAL:HB    | 1:BT:62:VAL:HG12  | 1.98                     | 0.45              |
| 1:BU:24:ASP:HB3   | 1:BU:28:VAL:H     | 1.82                     | 0.45              |
| 1:CG:24:ASP:HB3   | 1:CG:28:VAL:H     | 1.82                     | 0.45              |
| 1:CM:11:HIS:H     | 1:CO:109:ASP:HB3  | 1.82                     | 0.45              |
| 1:DF:44:TYR:HE1   | 1:DF:68:VAL:HG13  | 1.82                     | 0.45              |
| 1:AA:58:ASP:O     | 1:AA:99:PRO:HA    | 2.17                     | 0.45              |
| 1:AD:58:ASP:O     | 1:AD:99:PRO:HA    | 2.17                     | 0.45              |
| 1:AF:94:VAL:HA    | 1:BY:93:GLN:O     | 2.16                     | 0.45              |
| 1:AR:18:PHE:HB3   | 1:AR:31:PHE:HB3   | 1.98                     | 0.45              |
| 1:AU:44:TYR:HE1   | 1:AU:68:VAL:HG13  | 1.82                     | 0.45              |
| 1:BE:11:HIS:HB2   | 1:DE:109:ASP:HB3  | 1.99                     | 0.45              |
| 1:BH:58:ASP:O     | 1:BH:99:PRO:HA    | 2.17                     | 0.45              |
| 1:BI:109:ASP:HB3  | 1:BQ:11:HIS:CB    | 2.43                     | 0.45              |
| 1:BK:50:VAL:HB    | 1:BK:62:VAL:HG12  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BN:132:HIS:HB2 | 1:BS:21:THR:O     | 2.17                     | 0.45              |
| 1:BP:47:SER:HB2  | 1:BP:65:PHE:HB2   | 1.99                     | 0.45              |
| 1:BQ:50:VAL:HB   | 1:BQ:62:VAL:HG12  | 1.98                     | 0.45              |
| 1:BW:58:ASP:O    | 1:BW:99:PRO:HA    | 2.17                     | 0.45              |
| 1:CF:50:VAL:HB   | 1:CF:62:VAL:HG12  | 1.98                     | 0.45              |
| 1:CN:53:PRO:HB3  | 1:CN:59:VAL:O     | 2.16                     | 0.45              |
| 1:CT:47:SER:HB2  | 1:CT:65:PHE:HB2   | 1.99                     | 0.45              |
| 1:AV:50:VAL:HB   | 1:AV:62:VAL:HG12  | 1.98                     | 0.44              |
| 1:AV:58:ASP:O    | 1:AV:99:PRO:HA    | 2.17                     | 0.44              |
| 1:BA:11:HIS:H    | 1:CQ:109:ASP:HB3  | 1.82                     | 0.44              |
| 1:BF:109:ASP:HB3 | 1:BK:11:HIS:CB    | 2.46                     | 0.44              |
| 1:BT:58:ASP:O    | 1:BT:99:PRO:HA    | 2.17                     | 0.44              |
| 1:CF:6:ILE:HD13  | 1:CP:123:ILE:HD11 | 1.99                     | 0.44              |
| 1:CH:53:PRO:HB3  | 1:CH:59:VAL:O     | 2.16                     | 0.44              |
| 1:CO:58:ASP:O    | 1:CO:99:PRO:HA    | 2.17                     | 0.44              |
| 1:DA:58:ASP:O    | 1:DA:99:PRO:HA    | 2.17                     | 0.44              |
| 1:DE:24:ASP:HB3  | 1:DE:28:VAL:H     | 1.82                     | 0.44              |
| 1:DG:58:ASP:O    | 1:DG:99:PRO:HA    | 2.17                     | 0.44              |
| 1:AE:132:HIS:HE1 | 1:CU:52:GLU:HG3   | 1.83                     | 0.44              |
| 1:AG:108:GLU:OE1 | 1:AZ:11:HIS:NE2   | 2.50                     | 0.44              |
| 1:AK:132:HIS:O   | 1:CI:1:PRO:HD2    | 2.17                     | 0.44              |
| 1:AO:18:PHE:HB3  | 1:AO:31:PHE:HB3   | 1.98                     | 0.44              |
| 1:AR:47:SER:HB2  | 1:AR:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:AU:68:VAL:HG23 | 1:CK:110:LEU:HD13 | 1.99                     | 0.44              |
| 1:BN:58:ASP:O    | 1:BN:99:PRO:HA    | 2.17                     | 0.44              |
| 1:BP:94:VAL:HG13 | 1:DF:94:VAL:HG22  | 1.99                     | 0.44              |
| 1:CF:1:PRO:HD3   | 1:CP:131:GLU:HB3  | 1.99                     | 0.44              |
| 1:CL:50:VAL:HB   | 1:CL:62:VAL:HG12  | 1.98                     | 0.44              |
| 1:CQ:44:TYR:HE1  | 1:CQ:68:VAL:HG13  | 1.82                     | 0.44              |
| 1:DH:24:ASP:HB3  | 1:DH:28:VAL:H     | 1.82                     | 0.44              |
| 1:AM:58:ASP:O    | 1:AM:99:PRO:HA    | 2.17                     | 0.44              |
| 1:AS:58:ASP:O    | 1:AS:99:PRO:HA    | 2.17                     | 0.44              |
| 1:AY:58:ASP:O    | 1:AY:99:PRO:HA    | 2.17                     | 0.44              |
| 1:BA:132:HIS:CE1 | 1:CQ:50:VAL:HG23  | 2.51                     | 0.44              |
| 1:BB:90:ASN:OD1  | 1:DH:99:PRO:HD2   | 2.17                     | 0.44              |
| 1:BY:44:TYR:HE1  | 1:BY:68:VAL:HG13  | 1.82                     | 0.44              |
| 1:CI:58:ASP:O    | 1:CI:99:PRO:HA    | 2.17                     | 0.44              |
| 1:CR:58:ASP:O    | 1:CR:99:PRO:HA    | 2.17                     | 0.44              |
| 1:CS:24:ASP:HB3  | 1:CS:28:VAL:H     | 1.82                     | 0.44              |
| 1:DJ:58:ASP:O    | 1:DJ:99:PRO:HA    | 2.17                     | 0.44              |
| 1:AF:44:TYR:HE1  | 1:AF:68:VAL:HG13  | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AX:47:SER:HB2   | 1:AX:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:BA:123:ILE:HD11 | 1:CQ:6:ILE:HD13   | 1.99                     | 0.44              |
| 1:BB:58:ASP:O     | 1:BB:99:PRO:HA    | 2.17                     | 0.44              |
| 1:BP:52:GLU:OE2   | 1:DF:132:HIS:NE2  | 2.50                     | 0.44              |
| 1:BT:109:ASP:HB3  | 1:DK:11:HIS:CB    | 2.48                     | 0.44              |
| 1:BW:132:HIS:CD2  | 1:DB:50:VAL:HG23  | 2.52                     | 0.44              |
| 1:CF:69:PRO:HB3   | 1:CF:89:THR:HG22  | 1.98                     | 0.44              |
| 1:AE:92:ALA:HB1   | 1:CU:114:LEU:HD22 | 1.99                     | 0.44              |
| 1:AE:109:ASP:HB3  | 1:CU:11:HIS:N     | 2.31                     | 0.44              |
| 1:AI:18:PHE:HB3   | 1:AI:31:PHE:HB3   | 1.98                     | 0.44              |
| 1:AX:94:VAL:HG13  | 1:CN:94:VAL:HG22  | 1.98                     | 0.44              |
| 1:AX:99:PRO:HD2   | 1:CN:90:ASN:ND2   | 2.31                     | 0.44              |
| 1:AY:11:HIS:CB    | 1:BU:109:ASP:HB3  | 2.48                     | 0.44              |
| 1:BD:48:SER:OG    | 1:CW:126:THR:HG21 | 2.18                     | 0.44              |
| 1:BZ:69:PRO:HB3   | 1:BZ:89:THR:HG22  | 1.98                     | 0.44              |
| 1:CR:69:PRO:HB3   | 1:CR:89:THR:HG22  | 1.98                     | 0.44              |
| 1:DJ:50:VAL:HB    | 1:DJ:62:VAL:HG12  | 1.98                     | 0.44              |
| 1:AA:130:VAL:HG11 | 1:AQ:60:PHE:CE1   | 2.53                     | 0.44              |
| 1:AC:47:SER:HB2   | 1:AC:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:AD:69:PRO:HB3   | 1:AD:89:THR:HG22  | 1.98                     | 0.44              |
| 1:AE:60:PHE:CD1   | 1:CU:130:VAL:CG1  | 2.98                     | 0.44              |
| 1:AE:116:SER:OG   | 1:CU:8:LEU:HB3    | 2.18                     | 0.44              |
| 1:AH:24:ASP:HB3   | 1:AH:28:VAL:H     | 1.82                     | 0.44              |
| 1:AL:134:TYR:CZ   | 1:CC:20:PRO:HB2   | 2.53                     | 0.44              |
| 1:AO:47:SER:HB2   | 1:AO:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:BB:132:HIS:CE1  | 1:DH:50:VAL:HG23  | 2.53                     | 0.44              |
| 1:BQ:58:ASP:O     | 1:BQ:99:PRO:HA    | 2.17                     | 0.44              |
| 1:BS:132:HIS:CE1  | 1:DL:50:VAL:HG23  | 2.52                     | 0.44              |
| 1:CB:47:SER:HB2   | 1:CB:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:CH:47:SER:HB2   | 1:CH:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:CY:24:ASP:HB3   | 1:CY:28:VAL:H     | 1.82                     | 0.44              |
| 1:CZ:47:SER:HB2   | 1:CZ:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:DC:47:SER:HB2   | 1:DC:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:AF:109:ASP:HB3  | 1:BY:11:HIS:CB    | 2.47                     | 0.44              |
| 1:BI:24:ASP:HB3   | 1:BI:28:VAL:H     | 1.82                     | 0.44              |
| 1:BT:109:ASP:HB3  | 1:DK:11:HIS:H     | 1.82                     | 0.44              |
| 1:CC:58:ASP:O     | 1:CC:99:PRO:HA    | 2.17                     | 0.44              |
| 1:CW:18:PHE:HB3   | 1:CW:31:PHE:HB3   | 1.98                     | 0.44              |
| 1:DG:3:LEU:HD12   | 1:DG:3:LEU:HA     | 1.88                     | 0.44              |
| 1:AA:6:ILE:HD13   | 1:AQ:123:ILE:HD11 | 2.00                     | 0.44              |
| 1:AF:109:ASP:HB3  | 1:BY:11:HIS:HB3   | 1.99                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BF:131:GLU:CB  | 1:BK:1:PRO:HD3    | 2.48                     | 0.44              |
| 1:BG:44:TYR:HE1  | 1:BG:68:VAL:HG13  | 1.82                     | 0.44              |
| 1:BK:3:LEU:HD12  | 1:BK:3:LEU:HA     | 1.88                     | 0.44              |
| 1:BP:134:TYR:CD1 | 1:DD:3:LEU:HD23   | 2.53                     | 0.44              |
| 1:BR:24:ASP:HB3  | 1:BR:28:VAL:H     | 1.82                     | 0.44              |
| 1:BT:132:HIS:CD2 | 1:DK:50:VAL:HG23  | 2.53                     | 0.44              |
| 1:BX:24:ASP:HB3  | 1:BX:28:VAL:H     | 1.82                     | 0.44              |
| 1:AE:50:VAL:HG13 | 1:CU:126:THR:HG23 | 2.00                     | 0.44              |
| 1:AF:131:GLU:OE1 | 1:BY:1:PRO:HD3    | 2.17                     | 0.44              |
| 1:AG:58:ASP:O    | 1:AG:99:PRO:HA    | 2.17                     | 0.44              |
| 1:AN:131:GLU:CB  | 1:CL:1:PRO:HD3    | 2.48                     | 0.44              |
| 1:AO:35:GLN:HG3  | 1:AO:71:VAL:HG21  | 2.00                     | 0.44              |
| 1:AP:69:PRO:HB3  | 1:AP:89:THR:HG22  | 1.98                     | 0.44              |
| 1:BD:99:PRO:HD2  | 1:CW:90:ASN:CG    | 2.43                     | 0.44              |
| 1:BK:58:ASP:O    | 1:BK:99:PRO:HA    | 2.17                     | 0.44              |
| 1:BS:94:VAL:HG13 | 1:DL:94:VAL:HG22  | 2.00                     | 0.44              |
| 1:BZ:58:ASP:O    | 1:BZ:99:PRO:HA    | 2.17                     | 0.44              |
| 1:CN:47:SER:HB2  | 1:CN:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:CX:58:ASP:O    | 1:CX:99:PRO:HA    | 2.17                     | 0.44              |
| 1:DD:58:ASP:O    | 1:DD:99:PRO:HA    | 2.17                     | 0.44              |
| 1:DI:47:SER:HB2  | 1:DI:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:DL:47:SER:HB2  | 1:DL:65:PHE:HB2   | 1.99                     | 0.44              |
| 1:AB:24:ASP:HB3  | 1:AB:28:VAL:H     | 1.82                     | 0.43              |
| 1:AU:99:PRO:HD2  | 1:CK:90:ASN:CG    | 2.43                     | 0.43              |
| 1:BA:11:HIS:CB   | 1:CQ:109:ASP:HB3  | 2.48                     | 0.43              |
| 1:BA:94:VAL:HG13 | 1:CQ:94:VAL:HG22  | 2.00                     | 0.43              |
| 1:BJ:3:LEU:N     | 1:DC:134:TYR:O    | 2.44                     | 0.43              |
| 1:BS:47:SER:HB2  | 1:BS:65:PHE:HB2   | 1.99                     | 0.43              |
| 1:CE:44:TYR:HE1  | 1:CE:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:AK:11:HIS:H    | 1:CI:109:ASP:HB3  | 1.83                     | 0.43              |
| 1:BD:35:GLN:HG3  | 1:BD:71:VAL:HG21  | 2.00                     | 0.43              |
| 1:BE:58:ASP:O    | 1:BE:99:PRO:HA    | 2.17                     | 0.43              |
| 1:DL:44:TYR:HE1  | 1:DL:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:AP:79:SER:CB   | 1:CH:74:ILE:HG12  | 2.48                     | 0.43              |
| 1:AP:134:TYR:CG  | 1:AU:3:LEU:HD23   | 2.47                     | 0.43              |
| 1:AR:44:TYR:HE1  | 1:AR:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:BJ:44:TYR:HE1  | 1:BJ:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:BV:44:TYR:HE1  | 1:BV:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:CD:24:ASP:HB3  | 1:CD:28:VAL:H     | 1.82                     | 0.43              |
| 1:CF:58:ASP:O    | 1:CF:99:PRO:HA    | 2.17                     | 0.43              |
| 1:CT:35:GLN:HG3  | 1:CT:71:VAL:HG21  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:DC:44:TYR:HE1  | 1:DC:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:AP:58:ASP:O    | 1:AP:99:PRO:HA    | 2.17                     | 0.43              |
| 1:BU:3:LEU:HG    | 1:BU:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:CT:44:TYR:HE1  | 1:CT:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:AF:35:GLN:HG3  | 1:AF:71:VAL:HG21  | 2.00                     | 0.43              |
| 1:AF:99:PRO:CB   | 1:BY:88:ARG:HD2   | 2.48                     | 0.43              |
| 1:AL:44:TYR:HE1  | 1:AL:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:AN:132:HIS:HE1 | 1:CL:52:GLU:HG3   | 1.83                     | 0.43              |
| 1:AT:24:ASP:HB3  | 1:AT:28:VAL:H     | 1.82                     | 0.43              |
| 1:AU:11:HIS:HB2  | 1:CK:109:ASP:N    | 2.33                     | 0.43              |
| 1:BD:44:TYR:HE1  | 1:BD:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:BE:80:ASP:CB   | 1:CZ:73:THR:H     | 2.32                     | 0.43              |
| 1:BI:1:PRO:HD3   | 1:BQ:131:GLU:CB   | 2.46                     | 0.43              |
| 1:BV:47:SER:HB2  | 1:BV:65:PHE:HB2   | 1.99                     | 0.43              |
| 1:AB:132:HIS:NE2 | 1:DA:50:VAL:O     | 2.51                     | 0.43              |
| 1:AG:3:LEU:HD12  | 1:AG:3:LEU:HA     | 1.88                     | 0.43              |
| 1:AL:108:GLU:HG3 | 1:CE:128:VAL:HG11 | 1.99                     | 0.43              |
| 1:AP:3:LEU:HD12  | 1:AP:3:LEU:HA     | 1.88                     | 0.43              |
| 1:BB:11:HIS:H    | 1:DH:109:ASP:HB3  | 1.84                     | 0.43              |
| 1:BI:50:VAL:HG23 | 1:BQ:132:HIS:NE2  | 2.33                     | 0.43              |
| 1:BR:3:LEU:HG    | 1:BR:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:CA:3:LEU:HG    | 1:CA:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:CM:3:LEU:HG    | 1:CM:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:DB:3:LEU:HG    | 1:DB:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:DB:45:THR:OG1  | 1:DB:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:DK:45:THR:OG1  | 1:DK:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:AC:3:LEU:N     | 1:BV:134:TYR:O    | 2.42                     | 0.43              |
| 1:AI:44:TYR:HE1  | 1:AI:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:AK:45:THR:OG1  | 1:AK:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:AN:24:ASP:HB3  | 1:AN:28:VAL:H     | 1.82                     | 0.43              |
| 1:AP:116:SER:C   | 1:AT:8:LEU:HD22   | 2.43                     | 0.43              |
| 1:AQ:45:THR:OG1  | 1:AQ:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:AT:22:GLN:HB2  | 1:BX:132:HIS:ND1  | 2.33                     | 0.43              |
| 1:AU:11:HIS:N    | 1:CK:109:ASP:HB3  | 2.21                     | 0.43              |
| 1:AU:130:VAL:CG1 | 1:CK:60:PHE:CD1   | 3.01                     | 0.43              |
| 1:AY:21:THR:O    | 1:CQ:132:HIS:HB2  | 2.18                     | 0.43              |
| 1:BJ:80:ASP:HB2  | 1:BQ:73:THR:H     | 1.84                     | 0.43              |
| 1:BZ:130:VAL:O   | 1:BZ:130:VAL:HG12 | 2.19                     | 0.43              |
| 1:CN:35:GLN:HG3  | 1:CN:71:VAL:HG21  | 2.00                     | 0.43              |
| 1:DC:35:GLN:HG3  | 1:DC:71:VAL:HG21  | 2.00                     | 0.43              |
| 1:AK:131:GLU:HB2 | 1:CI:1:PRO:HD3    | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AM:109:ASP:HB3  | 1:CD:11:HIS:H     | 1.83                     | 0.43              |
| 1:AN:3:LEU:HG     | 1:AN:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:AQ:3:LEU:HG     | 1:AQ:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:AY:94:VAL:HG22  | 1:BU:94:VAL:HG13  | 1.99                     | 0.43              |
| 1:AZ:3:LEU:HG     | 1:AZ:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:BI:1:PRO:HD2    | 1:BQ:132:HIS:O    | 2.18                     | 0.43              |
| 1:BL:45:THR:OG1   | 1:BL:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:BM:44:TYR:HE1   | 1:BM:68:VAL:HG13  | 1.82                     | 0.43              |
| 1:BT:130:VAL:O    | 1:BT:130:VAL:HG12 | 2.19                     | 0.43              |
| 1:CD:45:THR:OG1   | 1:CD:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:CF:52:GLU:HG3   | 1:CP:132:HIS:HE1  | 1.83                     | 0.43              |
| 1:CG:3:LEU:HG     | 1:CG:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:CI:130:VAL:HG12 | 1:CI:130:VAL:O    | 2.19                     | 0.43              |
| 1:CY:45:THR:OG1   | 1:CY:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:AA:50:VAL:HG23  | 1:AQ:132:HIS:CE1  | 2.54                     | 0.43              |
| 1:AA:80:ASP:CB    | 1:BV:73:THR:H     | 2.32                     | 0.43              |
| 1:AC:132:HIS:CD2  | 1:BT:22:GLN:HB2   | 2.54                     | 0.43              |
| 1:AE:50:VAL:CG1   | 1:CU:126:THR:HG23 | 2.49                     | 0.43              |
| 1:AM:1:PRO:HD3    | 1:CD:131:GLU:HB3  | 2.00                     | 0.43              |
| 1:AU:11:HIS:CE1   | 1:CK:108:GLU:CD   | 2.97                     | 0.43              |
| 1:BD:3:LEU:HD12   | 1:CW:133:PHE:CD1  | 2.53                     | 0.43              |
| 1:BJ:130:VAL:HG12 | 1:BJ:130:VAL:O    | 2.19                     | 0.43              |
| 1:BL:3:LEU:HG     | 1:BL:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:BM:35:GLN:HG3   | 1:BM:71:VAL:HG21  | 2.00                     | 0.43              |
| 1:BO:3:LEU:HD23   | 1:BR:134:TYR:CD1  | 2.54                     | 0.43              |
| 1:BU:45:THR:OG1   | 1:BU:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:CB:35:GLN:HG3   | 1:CB:71:VAL:HG21  | 2.00                     | 0.43              |
| 1:CC:130:VAL:O    | 1:CC:130:VAL:HG12 | 2.19                     | 0.43              |
| 1:CM:50:VAL:HG23  | 1:CO:132:HIS:NE2  | 2.34                     | 0.43              |
| 1:CS:45:THR:OG1   | 1:CS:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:CV:3:LEU:HG     | 1:CV:20:PRO:HB3   | 2.01                     | 0.43              |
| 1:AH:11:HIS:NE2   | 1:CX:108:GLU:OE1  | 2.52                     | 0.43              |
| 1:AJ:58:ASP:O     | 1:AJ:99:PRO:HA    | 2.17                     | 0.43              |
| 1:AO:80:ASP:HB2   | 1:CL:73:THR:H     | 1.83                     | 0.43              |
| 1:BD:94:VAL:HG13  | 1:CW:94:VAL:HG22  | 2.00                     | 0.43              |
| 1:BJ:108:GLU:HG3  | 1:DC:128:VAL:CG1  | 2.48                     | 0.43              |
| 1:BK:130:VAL:O    | 1:BK:130:VAL:HG12 | 2.19                     | 0.43              |
| 1:BV:35:GLN:HG3   | 1:BV:71:VAL:HG21  | 2.00                     | 0.43              |
| 1:CC:1:PRO:HD3    | 1:CG:131:GLU:HB3  | 2.01                     | 0.43              |
| 1:CU:130:VAL:O    | 1:CU:130:VAL:HG12 | 2.19                     | 0.43              |
| 1:CW:35:GLN:HG3   | 1:CW:71:VAL:HG21  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CZ:35:GLN:HG3   | 1:CZ:71:VAL:HG21  | 2.00                     | 0.43              |
| 1:DC:130:VAL:O    | 1:DC:130:VAL:HG12 | 2.19                     | 0.43              |
| 1:DE:45:THR:OG1   | 1:DE:67:ASN:HB2   | 2.19                     | 0.43              |
| 1:DL:130:VAL:O    | 1:DL:130:VAL:HG12 | 2.19                     | 0.43              |
| 1:AH:3:LEU:HG     | 1:AH:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:AI:80:ASP:CB    | 1:CX:73:THR:H     | 2.31                     | 0.42              |
| 1:AO:130:VAL:O    | 1:AO:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AP:79:SER:CA    | 1:CH:74:ILE:HG12  | 2.48                     | 0.42              |
| 1:AR:130:VAL:O    | 1:AR:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AU:123:ILE:O    | 1:AU:126:THR:HB   | 2.19                     | 0.42              |
| 1:AW:45:THR:OG1   | 1:AW:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:BG:35:GLN:HG3   | 1:BG:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:BG:130:VAL:HG12 | 1:BG:130:VAL:O    | 2.19                     | 0.42              |
| 1:BM:123:ILE:O    | 1:BM:126:THR:HB   | 2.19                     | 0.42              |
| 1:BO:45:THR:OG1   | 1:BO:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:BQ:21:THR:O     | 1:DL:132:HIS:HB2  | 2.18                     | 0.42              |
| 1:CE:130:VAL:O    | 1:CE:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:CF:130:VAL:HG12 | 1:CF:130:VAL:O    | 2.19                     | 0.42              |
| 1:CH:35:GLN:HG3   | 1:CH:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:DH:3:LEU:HG     | 1:DH:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:DI:35:GLN:HG3   | 1:DI:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:DK:3:LEU:HG     | 1:DK:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:AC:44:TYR:HE1   | 1:AC:68:VAL:HG13  | 1.82                     | 0.42              |
| 1:AE:132:HIS:NE2  | 1:CU:50:VAL:O     | 2.52                     | 0.42              |
| 1:AP:50:VAL:HG22  | 1:AT:132:HIS:HA   | 2.02                     | 0.42              |
| 1:BD:130:VAL:O    | 1:BD:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BF:132:HIS:HE1  | 1:BK:52:GLU:HG3   | 1.84                     | 0.42              |
| 1:BX:45:THR:OG1   | 1:BX:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:CE:123:ILE:O    | 1:CE:126:THR:HB   | 2.19                     | 0.42              |
| 1:CJ:45:THR:OG1   | 1:CJ:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:CK:123:ILE:O    | 1:CK:126:THR:HB   | 2.20                     | 0.42              |
| 1:CL:58:ASP:O     | 1:CL:99:PRO:HA    | 2.17                     | 0.42              |
| 1:CQ:130:VAL:O    | 1:CQ:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:CS:3:LEU:HG     | 1:CS:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:CX:130:VAL:O    | 1:CX:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:DC:58:ASP:O     | 1:DC:99:PRO:HA    | 2.20                     | 0.42              |
| 1:DC:123:ILE:O    | 1:DC:126:THR:HB   | 2.19                     | 0.42              |
| 1:DF:123:ILE:O    | 1:DF:126:THR:HB   | 2.20                     | 0.42              |
| 1:DJ:3:LEU:HD12   | 1:DJ:3:LEU:HA     | 1.88                     | 0.42              |
| 1:AB:3:LEU:HD23   | 1:AQ:134:TYR:CD1  | 2.53                     | 0.42              |
| 1:AI:35:GLN:HG3   | 1:AI:71:VAL:HG21  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AJ:130:VAL:O    | 1:AJ:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AN:45:THR:OG1   | 1:AN:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:AR:58:ASP:O     | 1:AR:99:PRO:HA    | 2.20                     | 0.42              |
| 1:AS:130:VAL:O    | 1:AS:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AU:130:VAL:O    | 1:AU:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AZ:45:THR:OG1   | 1:AZ:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:BG:128:VAL:HG11 | 1:CZ:108:GLU:HG3  | 2.01                     | 0.42              |
| 1:BJ:35:GLN:HG3   | 1:BJ:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:BJ:123:ILE:O    | 1:BJ:126:THR:HB   | 2.20                     | 0.42              |
| 1:CA:45:THR:OG1   | 1:CA:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:CB:123:ILE:O    | 1:CB:126:THR:HB   | 2.20                     | 0.42              |
| 1:CJ:109:ASP:HB3  | 1:CR:11:HIS:HB2   | 2.01                     | 0.42              |
| 1:CL:130:VAL:O    | 1:CL:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:CT:123:ILE:O    | 1:CT:126:THR:HB   | 2.19                     | 0.42              |
| 1:CW:130:VAL:HG12 | 1:CW:130:VAL:O    | 2.19                     | 0.42              |
| 1:DF:58:ASP:O     | 1:DF:99:PRO:HA    | 2.20                     | 0.42              |
| 1:DI:58:ASP:O     | 1:DI:99:PRO:HA    | 2.20                     | 0.42              |
| 1:DL:58:ASP:O     | 1:DL:99:PRO:HA    | 2.20                     | 0.42              |
| 1:AC:35:GLN:HG3   | 1:AC:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:AF:123:ILE:O    | 1:AF:126:THR:HB   | 2.19                     | 0.42              |
| 1:AG:11:HIS:CE1   | 1:AZ:108:GLU:OE1  | 2.72                     | 0.42              |
| 1:AI:58:ASP:O     | 1:AI:99:PRO:HA    | 2.20                     | 0.42              |
| 1:AM:6:ILE:HD13   | 1:CD:123:ILE:HD11 | 2.02                     | 0.42              |
| 1:AM:130:VAL:O    | 1:AM:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AO:58:ASP:O     | 1:AO:99:PRO:HA    | 2.20                     | 0.42              |
| 1:AR:116:SER:OG   | 1:CH:8:LEU:HB3    | 2.18                     | 0.42              |
| 1:AU:116:SER:OG   | 1:CK:8:LEU:HB3    | 2.19                     | 0.42              |
| 1:AW:3:LEU:HG     | 1:AW:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:BA:58:ASP:O     | 1:BA:99:PRO:HA    | 2.20                     | 0.42              |
| 1:BA:123:ILE:O    | 1:BA:126:THR:HB   | 2.20                     | 0.42              |
| 1:BD:123:ILE:O    | 1:BD:126:THR:HB   | 2.19                     | 0.42              |
| 1:BD:132:HIS:CE1  | 1:CW:50:VAL:HG23  | 2.54                     | 0.42              |
| 1:BE:3:LEU:HD12   | 1:BE:3:LEU:HA     | 1.88                     | 0.42              |
| 1:BG:73:THR:H     | 1:CX:80:ASP:CB    | 2.31                     | 0.42              |
| 1:BM:130:VAL:O    | 1:BM:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BP:44:TYR:HE1   | 1:BP:68:VAL:HG13  | 1.82                     | 0.42              |
| 1:BP:50:VAL:HG23  | 1:DF:132:HIS:CE1  | 2.54                     | 0.42              |
| 1:BT:1:PRO:HD3    | 1:DK:131:GLU:HB3  | 2.02                     | 0.42              |
| 1:CE:35:GLN:HG3   | 1:CE:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:CE:58:ASP:O     | 1:CE:99:PRO:HA    | 2.20                     | 0.42              |
| 1:CR:130:VAL:O    | 1:CR:130:VAL:HG12 | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CY:50:VAL:HG23  | 1:DJ:132:HIS:NE2  | 2.35                     | 0.42              |
| 1:AB:3:LEU:HG     | 1:AB:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:AE:45:THR:OG1   | 1:AE:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:AE:94:VAL:HG13  | 1:CU:94:VAL:HG22  | 2.01                     | 0.42              |
| 1:AL:35:GLN:HG3   | 1:AL:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:AL:130:VAL:O    | 1:AL:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AN:132:HIS:O    | 1:CL:1:PRO:HD2    | 2.20                     | 0.42              |
| 1:AP:79:SER:OG    | 1:CH:74:ILE:HG12  | 2.20                     | 0.42              |
| 1:AP:130:VAL:O    | 1:AP:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AR:35:GLN:HG3   | 1:AR:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:AV:130:VAL:HG12 | 1:AV:130:VAL:O    | 2.19                     | 0.42              |
| 1:AX:58:ASP:O     | 1:AX:99:PRO:HA    | 2.20                     | 0.42              |
| 1:AX:90:ASN:CG    | 1:CN:99:PRO:HD2   | 2.44                     | 0.42              |
| 1:BA:130:VAL:O    | 1:BA:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BC:45:THR:OG1   | 1:BC:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:BD:99:PRO:HD2   | 1:CW:90:ASN:ND2   | 2.34                     | 0.42              |
| 1:BJ:58:ASP:O     | 1:BJ:99:PRO:HA    | 2.20                     | 0.42              |
| 1:BO:3:LEU:HG     | 1:BO:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:BY:35:GLN:HG3   | 1:BY:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:CB:58:ASP:O     | 1:CB:99:PRO:HA    | 2.20                     | 0.42              |
| 1:CH:130:VAL:O    | 1:CH:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:CI:3:LEU:HD12   | 1:CI:3:LEU:HA     | 1.88                     | 0.42              |
| 1:CK:35:GLN:HG3   | 1:CK:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:CK:130:VAL:O    | 1:CK:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:CQ:58:ASP:O     | 1:CQ:99:PRO:HA    | 2.20                     | 0.42              |
| 1:CZ:123:ILE:O    | 1:CZ:126:THR:HB   | 2.19                     | 0.42              |
| 1:DI:130:VAL:O    | 1:DI:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:DL:35:GLN:HG3   | 1:DL:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:AC:130:VAL:O    | 1:AC:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AG:130:VAL:O    | 1:AG:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AI:123:ILE:O    | 1:AI:126:THR:HB   | 2.19                     | 0.42              |
| 1:AV:123:ILE:HD11 | 1:CA:6:ILE:HD13   | 2.01                     | 0.42              |
| 1:BC:94:VAL:HG13  | 1:BH:94:VAL:HG22  | 2.00                     | 0.42              |
| 1:BG:58:ASP:O     | 1:BG:99:PRO:HA    | 2.20                     | 0.42              |
| 1:BJ:94:VAL:HG22  | 1:DC:94:VAL:HG13  | 2.01                     | 0.42              |
| 1:BS:130:VAL:O    | 1:BS:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BW:130:VAL:O    | 1:BW:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BY:123:ILE:O    | 1:BY:126:THR:HB   | 2.19                     | 0.42              |
| 1:CH:58:ASP:O     | 1:CH:99:PRO:HA    | 2.20                     | 0.42              |
| 1:CJ:3:LEU:HG     | 1:CJ:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:CM:123:ILE:HD11 | 1:CO:6:ILE:HD13   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CN:123:ILE:O    | 1:CN:126:THR:HB   | 2.20                     | 0.42              |
| 1:CQ:35:GLN:HG3   | 1:CQ:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:CT:130:VAL:O    | 1:CT:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:DF:35:GLN:HG3   | 1:DF:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:DF:130:VAL:O    | 1:DF:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AA:109:ASP:HB3  | 1:AQ:11:HIS:HB3   | 2.01                     | 0.42              |
| 1:AB:94:VAL:HG22  | 1:DA:94:VAL:HG22  | 2.02                     | 0.42              |
| 1:AD:123:ILE:O    | 1:AD:126:THR:HB   | 2.20                     | 0.42              |
| 1:AE:60:PHE:CE1   | 1:CU:130:VAL:CG1  | 2.94                     | 0.42              |
| 1:AF:3:LEU:HD23   | 1:CU:134:TYR:CG   | 2.53                     | 0.42              |
| 1:AG:94:VAL:HG22  | 1:AZ:94:VAL:HG13  | 2.01                     | 0.42              |
| 1:AJ:123:ILE:O    | 1:AJ:126:THR:HB   | 2.20                     | 0.42              |
| 1:AL:58:ASP:O     | 1:AL:99:PRO:HA    | 2.20                     | 0.42              |
| 1:AP:126:THR:HG23 | 1:AT:50:VAL:HG13  | 2.01                     | 0.42              |
| 1:AU:58:ASP:O     | 1:AU:99:PRO:HA    | 2.20                     | 0.42              |
| 1:BA:35:GLN:HG3   | 1:BA:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:BQ:123:ILE:O    | 1:BQ:126:THR:HB   | 2.20                     | 0.42              |
| 1:BQ:130:VAL:O    | 1:BQ:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:CO:130:VAL:O    | 1:CO:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:CQ:123:ILE:O    | 1:CQ:126:THR:HB   | 2.20                     | 0.42              |
| 1:CY:3:LEU:HG     | 1:CY:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:DH:45:THR:OG1   | 1:DH:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:DJ:130:VAL:O    | 1:DJ:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AB:1:PRO:HD3    | 1:DA:131:GLU:CB   | 2.45                     | 0.42              |
| 1:AF:80:ASP:HB2   | 1:CU:73:THR:H     | 1.84                     | 0.42              |
| 1:AN:50:VAL:HG23  | 1:CL:132:HIS:NE2  | 2.35                     | 0.42              |
| 1:AY:3:LEU:HD12   | 1:AY:3:LEU:HA     | 1.88                     | 0.42              |
| 1:BE:123:ILE:O    | 1:BE:126:THR:HB   | 2.20                     | 0.42              |
| 1:BH:130:VAL:O    | 1:BH:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BJ:108:GLU:HG3  | 1:DC:128:VAL:HG11 | 2.02                     | 0.42              |
| 1:BJ:132:HIS:HB2  | 1:DA:21:THR:O     | 2.19                     | 0.42              |
| 1:BN:123:ILE:O    | 1:BN:126:THR:HB   | 2.20                     | 0.42              |
| 1:BV:123:ILE:O    | 1:BV:126:THR:HB   | 2.19                     | 0.42              |
| 1:BW:6:ILE:HD13   | 1:DB:123:ILE:HD11 | 2.01                     | 0.42              |
| 1:CI:123:ILE:O    | 1:CI:126:THR:HB   | 2.20                     | 0.42              |
| 1:CK:58:ASP:O     | 1:CK:99:PRO:HA    | 2.20                     | 0.42              |
| 1:CM:50:VAL:HG23  | 1:CO:132:HIS:CE1  | 2.55                     | 0.42              |
| 1:CN:44:TYR:HE1   | 1:CN:68:VAL:HG13  | 1.82                     | 0.42              |
| 1:DA:130:VAL:O    | 1:DA:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:DI:123:ILE:O    | 1:DI:126:THR:HB   | 2.19                     | 0.42              |
| 1:AC:131:GLU:CB   | 1:BV:1:PRO:HD3    | 2.37                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AI:6:ILE:HD13  | 1:CB:123:ILE:HD11 | 2.01                     | 0.42              |
| 1:AR:123:ILE:O   | 1:AR:126:THR:HB   | 2.20                     | 0.42              |
| 1:AS:123:ILE:O   | 1:AS:126:THR:HB   | 2.20                     | 0.42              |
| 1:AS:134:TYR:HB2 | 1:BY:3:LEU:CD2    | 2.41                     | 0.42              |
| 1:AU:35:GLN:HG3  | 1:AU:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:AX:35:GLN:HG3  | 1:AX:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:AX:123:ILE:O   | 1:AX:126:THR:HB   | 2.19                     | 0.42              |
| 1:BF:3:LEU:HG    | 1:BF:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:BI:3:LEU:HG    | 1:BI:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:BM:58:ASP:O    | 1:BM:99:PRO:HA    | 2.20                     | 0.42              |
| 1:BN:130:VAL:O   | 1:BN:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BS:11:HIS:CB   | 1:DL:109:ASP:HB3  | 2.49                     | 0.42              |
| 1:BS:35:GLN:HG3  | 1:BS:71:VAL:HG21  | 2.00                     | 0.42              |
| 1:BY:58:ASP:O    | 1:BY:99:PRO:HA    | 2.20                     | 0.42              |
| 1:CH:123:ILE:O   | 1:CH:126:THR:HB   | 2.19                     | 0.42              |
| 1:CM:45:THR:OG1  | 1:CM:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:CO:123:ILE:O   | 1:CO:126:THR:HB   | 2.20                     | 0.42              |
| 1:CP:45:THR:OG1  | 1:CP:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:CZ:130:VAL:O   | 1:CZ:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AA:130:VAL:O   | 1:AA:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:AB:11:HIS:H    | 1:DA:109:ASP:HB3  | 1.84                     | 0.42              |
| 1:AB:45:THR:OG1  | 1:AB:67:ASN:HB2   | 2.19                     | 0.42              |
| 1:AK:3:LEU:HG    | 1:AK:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:AL:6:ILE:HD13  | 1:CE:123:ILE:HD11 | 2.02                     | 0.42              |
| 1:AL:123:ILE:O   | 1:AL:126:THR:HB   | 2.20                     | 0.42              |
| 1:AO:123:ILE:O   | 1:AO:126:THR:HB   | 2.19                     | 0.42              |
| 1:AT:3:LEU:HD23  | 1:BX:134:TYR:HB2  | 2.02                     | 0.42              |
| 1:AV:123:ILE:O   | 1:AV:126:THR:HB   | 2.20                     | 0.42              |
| 1:AX:130:VAL:O   | 1:AX:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BC:3:LEU:HG    | 1:BC:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:BE:130:VAL:O   | 1:BE:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:BP:94:VAL:HG22 | 1:DF:94:VAL:HG13  | 2.01                     | 0.42              |
| 1:BX:3:LEU:HG    | 1:BX:20:PRO:HB3   | 2.01                     | 0.42              |
| 1:BZ:123:ILE:O   | 1:BZ:126:THR:HB   | 2.20                     | 0.42              |
| 1:CC:123:ILE:O   | 1:CC:126:THR:HB   | 2.20                     | 0.42              |
| 1:CN:130:VAL:O   | 1:CN:130:VAL:HG12 | 2.19                     | 0.42              |
| 1:CW:58:ASP:O    | 1:CW:99:PRO:HA    | 2.20                     | 0.42              |
| 1:CY:60:PHE:CD1  | 1:DJ:130:VAL:HG11 | 2.55                     | 0.42              |
| 1:DG:123:ILE:O   | 1:DG:126:THR:HB   | 2.20                     | 0.42              |
| 1:AE:3:LEU:HG    | 1:AE:20:PRO:HB3   | 2.01                     | 0.41              |
| 1:AK:109:ASP:HB3 | 1:CI:11:HIS:H     | 1.85                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AV:108:GLU:HG3 | 1:CA:128:VAL:HG13 | 2.01                     | 0.41              |
| 1:AX:1:PRO:HD3   | 1:CN:131:GLU:CB   | 2.45                     | 0.41              |
| 1:BD:58:ASP:O    | 1:BD:99:PRO:HA    | 2.20                     | 0.41              |
| 1:BG:123:ILE:O   | 1:BG:126:THR:HB   | 2.20                     | 0.41              |
| 1:BH:123:ILE:O   | 1:BH:126:THR:HB   | 2.20                     | 0.41              |
| 1:BI:45:THR:OG1  | 1:BI:67:ASN:HB2   | 2.19                     | 0.41              |
| 1:BN:132:HIS:NE2 | 1:BR:50:VAL:HG23  | 2.35                     | 0.41              |
| 1:BP:123:ILE:O   | 1:BP:126:THR:HB   | 2.19                     | 0.41              |
| 1:BS:58:ASP:O    | 1:BS:99:PRO:HA    | 2.20                     | 0.41              |
| 1:BS:123:ILE:O   | 1:BS:126:THR:HB   | 2.19                     | 0.41              |
| 1:BV:130:VAL:O   | 1:BV:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:CV:45:THR:OG1  | 1:CV:67:ASN:HB2   | 2.19                     | 0.41              |
| 1:CW:123:ILE:O   | 1:CW:126:THR:HB   | 2.19                     | 0.41              |
| 1:AD:130:VAL:O   | 1:AD:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:AF:130:VAL:O   | 1:AF:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:AG:11:HIS:HB2  | 1:AZ:109:ASP:HB3  | 2.02                     | 0.41              |
| 1:AL:73:THR:H    | 1:CC:80:ASP:CB    | 2.33                     | 0.41              |
| 1:AP:3:LEU:HD13  | 1:AT:133:PHE:CD1  | 2.56                     | 0.41              |
| 1:AU:134:TYR:CZ  | 1:CI:20:PRO:HB2   | 2.54                     | 0.41              |
| 1:BE:50:VAL:HG23 | 1:DE:132:HIS:CE1  | 2.55                     | 0.41              |
| 1:BF:45:THR:OG1  | 1:BF:67:ASN:HB2   | 2.19                     | 0.41              |
| 1:BP:35:GLN:HG3  | 1:BP:71:VAL:HG21  | 2.00                     | 0.41              |
| 1:BT:123:ILE:O   | 1:BT:126:THR:HB   | 2.20                     | 0.41              |
| 1:BT:131:GLU:CB  | 1:DK:1:PRO:HD3    | 2.43                     | 0.41              |
| 1:CQ:55:THR:O    | 1:CQ:55:THR:HG22  | 2.21                     | 0.41              |
| 1:CT:58:ASP:O    | 1:CT:99:PRO:HA    | 2.20                     | 0.41              |
| 1:CU:123:ILE:O   | 1:CU:126:THR:HB   | 2.20                     | 0.41              |
| 1:AC:55:THR:O    | 1:AC:55:THR:HG22  | 2.21                     | 0.41              |
| 1:AF:1:PRO:HD2   | 1:BY:132:HIS:O    | 2.20                     | 0.41              |
| 1:AG:123:ILE:O   | 1:AG:126:THR:HB   | 2.20                     | 0.41              |
| 1:AH:45:THR:OG1  | 1:AH:67:ASN:HB2   | 2.19                     | 0.41              |
| 1:AL:55:THR:O    | 1:AL:55:THR:HG22  | 2.21                     | 0.41              |
| 1:AP:123:ILE:O   | 1:AP:126:THR:HB   | 2.20                     | 0.41              |
| 1:AT:3:LEU:HG    | 1:AT:20:PRO:HB3   | 2.01                     | 0.41              |
| 1:AT:45:THR:OG1  | 1:AT:67:ASN:HB2   | 2.19                     | 0.41              |
| 1:AU:91:ARG:O    | 1:CK:97:ILE:N     | 2.47                     | 0.41              |
| 1:AX:55:THR:HG22 | 1:AX:55:THR:O     | 2.21                     | 0.41              |
| 1:BD:94:VAL:HG22 | 1:CW:94:VAL:HG13  | 2.02                     | 0.41              |
| 1:BJ:55:THR:O    | 1:BJ:55:THR:HG22  | 2.21                     | 0.41              |
| 1:CB:130:VAL:O   | 1:CB:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:CD:3:LEU:HG    | 1:CD:20:PRO:HB3   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CO:3:LEU:HD12   | 1:CO:3:LEU:HA     | 1.88                     | 0.41              |
| 1:CS:24:ASP:HB2   | 1:CS:28:VAL:HB    | 2.03                     | 0.41              |
| 1:DD:3:LEU:HD12   | 1:DD:3:LEU:HA     | 1.88                     | 0.41              |
| 1:AF:55:THR:O     | 1:AF:55:THR:HG22  | 2.21                     | 0.41              |
| 1:AF:58:ASP:O     | 1:AF:99:PRO:HA    | 2.20                     | 0.41              |
| 1:AF:133:PHE:CE1  | 1:BY:31:PHE:HZ    | 2.38                     | 0.41              |
| 1:AH:50:VAL:HG23  | 1:CX:132:HIS:NE2  | 2.35                     | 0.41              |
| 1:AI:1:PRO:CD     | 1:CB:131:GLU:HB3  | 2.40                     | 0.41              |
| 1:AM:123:ILE:O    | 1:AM:126:THR:HB   | 2.20                     | 0.41              |
| 1:AV:11:HIS:CB    | 1:CA:109:ASP:HB3  | 2.50                     | 0.41              |
| 1:AY:130:VAL:HG12 | 1:AY:130:VAL:O    | 2.19                     | 0.41              |
| 1:BB:1:PRO:HD3    | 1:DH:131:GLU:HB3  | 2.01                     | 0.41              |
| 1:BB:52:GLU:HG3   | 1:DH:132:HIS:HE1  | 1.85                     | 0.41              |
| 1:BB:130:VAL:O    | 1:BB:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:BP:55:THR:O     | 1:BP:55:THR:HG22  | 2.20                     | 0.41              |
| 1:DD:130:VAL:O    | 1:DD:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:DG:130:VAL:O    | 1:DG:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:DL:123:ILE:O    | 1:DL:126:THR:HB   | 2.20                     | 0.41              |
| 1:AC:3:LEU:HD23   | 1:DA:134:TYR:HB2  | 2.02                     | 0.41              |
| 1:AF:93:GLN:O     | 1:BY:94:VAL:HA    | 2.20                     | 0.41              |
| 1:AF:94:VAL:HG22  | 1:BY:94:VAL:HG13  | 2.03                     | 0.41              |
| 1:AF:132:HIS:CD2  | 1:BW:22:GLN:HB2   | 2.56                     | 0.41              |
| 1:AN:24:ASP:HB2   | 1:AN:28:VAL:HB    | 2.03                     | 0.41              |
| 1:AS:131:GLU:HB3  | 1:BX:1:PRO:CD     | 2.50                     | 0.41              |
| 1:AU:55:THR:HG22  | 1:AU:55:THR:O     | 2.21                     | 0.41              |
| 1:AY:123:ILE:O    | 1:AY:126:THR:HB   | 2.20                     | 0.41              |
| 1:BC:24:ASP:HB2   | 1:BC:28:VAL:HB    | 2.03                     | 0.41              |
| 1:BF:24:ASP:HB2   | 1:BF:28:VAL:HB    | 2.03                     | 0.41              |
| 1:BG:132:HIS:CD2  | 1:CX:22:GLN:HB2   | 2.56                     | 0.41              |
| 1:BL:24:ASP:HB2   | 1:BL:28:VAL:HB    | 2.03                     | 0.41              |
| 1:BP:130:VAL:O    | 1:BP:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:BP:131:GLU:OE1  | 1:DF:1:PRO:HD3    | 2.20                     | 0.41              |
| 1:BR:24:ASP:HB2   | 1:BR:28:VAL:HB    | 2.03                     | 0.41              |
| 1:CD:24:ASP:HB2   | 1:CD:28:VAL:HB    | 2.03                     | 0.41              |
| 1:CG:45:THR:OG1   | 1:CG:67:ASN:HB2   | 2.19                     | 0.41              |
| 1:CJ:24:ASP:HB2   | 1:CJ:28:VAL:HB    | 2.03                     | 0.41              |
| 1:CR:123:ILE:O    | 1:CR:126:THR:HB   | 2.20                     | 0.41              |
| 1:DA:123:ILE:O    | 1:DA:126:THR:HB   | 2.20                     | 0.41              |
| 1:DE:3:LEU:HG     | 1:DE:20:PRO:HB3   | 2.01                     | 0.41              |
| 1:DF:55:THR:O     | 1:DF:55:THR:HG22  | 2.20                     | 0.41              |
| 1:AB:94:VAL:HG22  | 1:DA:94:VAL:HG13  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:58:ASP:O     | 1:AC:99:PRO:HA    | 2.20                     | 0.41              |
| 1:AE:62:VAL:HG23  | 1:CU:127:ILE:HD12 | 2.02                     | 0.41              |
| 1:AE:94:VAL:HG22  | 1:CU:94:VAL:HG22  | 2.02                     | 0.41              |
| 1:AO:55:THR:O     | 1:AO:55:THR:HG22  | 2.21                     | 0.41              |
| 1:AU:88:ARG:HD2   | 1:CK:99:PRO:CB    | 2.50                     | 0.41              |
| 1:BV:58:ASP:O     | 1:BV:99:PRO:HA    | 2.20                     | 0.41              |
| 1:CY:24:ASP:HB2   | 1:CY:28:VAL:HB    | 2.03                     | 0.41              |
| 1:AB:109:ASP:CB   | 1:DA:11:HIS:HB2   | 2.48                     | 0.41              |
| 1:AB:110:LEU:HD22 | 1:DA:90:ASN:HB3   | 2.01                     | 0.41              |
| 1:AC:123:ILE:O    | 1:AC:126:THR:HB   | 2.19                     | 0.41              |
| 1:AK:96:PHE:HA    | 1:CI:91:ARG:O     | 2.21                     | 0.41              |
| 1:AK:113:LEU:HD23 | 1:CI:9:THR:O      | 2.21                     | 0.41              |
| 1:AN:132:HIS:NE2  | 1:CL:50:VAL:O     | 2.54                     | 0.41              |
| 1:AS:102:SER:HA   | 1:BX:70:GLU:OE2   | 2.20                     | 0.41              |
| 1:AT:24:ASP:HB2   | 1:AT:28:VAL:HB    | 2.03                     | 0.41              |
| 1:BO:24:ASP:HB2   | 1:BO:28:VAL:HB    | 2.03                     | 0.41              |
| 1:BR:45:THR:OG1   | 1:BR:67:ASN:HB2   | 2.19                     | 0.41              |
| 1:BS:1:PRO:HD2    | 1:DL:132:HIS:O    | 2.20                     | 0.41              |
| 1:BS:55:THR:O     | 1:BS:55:THR:HG22  | 2.21                     | 0.41              |
| 1:BW:1:PRO:HD3    | 1:DB:131:GLU:CB   | 2.51                     | 0.41              |
| 1:CF:94:VAL:HG22  | 1:CP:94:VAL:HG13  | 2.03                     | 0.41              |
| 1:CP:3:LEU:HG     | 1:CP:20:PRO:HB3   | 2.01                     | 0.41              |
| 1:CZ:58:ASP:O     | 1:CZ:99:PRO:HA    | 2.20                     | 0.41              |
| 1:DC:55:THR:HG22  | 1:DC:55:THR:O     | 2.20                     | 0.41              |
| 1:DD:123:ILE:O    | 1:DD:126:THR:HB   | 2.20                     | 0.41              |
| 1:AA:50:VAL:O     | 1:AQ:132:HIS:NE2  | 2.54                     | 0.41              |
| 1:BB:123:ILE:O    | 1:BB:126:THR:HB   | 2.20                     | 0.41              |
| 1:BD:55:THR:O     | 1:BD:55:THR:HG22  | 2.21                     | 0.41              |
| 1:BG:132:HIS:O    | 1:CZ:1:PRO:HD2    | 2.21                     | 0.41              |
| 1:BP:58:ASP:O     | 1:BP:99:PRO:HA    | 2.20                     | 0.41              |
| 1:BS:11:HIS:H     | 1:DL:109:ASP:HB3  | 1.86                     | 0.41              |
| 1:CF:123:ILE:O    | 1:CF:126:THR:HB   | 2.20                     | 0.41              |
| 1:CG:24:ASP:HB2   | 1:CG:28:VAL:HB    | 2.03                     | 0.41              |
| 1:CL:123:ILE:O    | 1:CL:126:THR:HB   | 2.20                     | 0.41              |
| 1:CM:24:ASP:HB2   | 1:CM:28:VAL:HB    | 2.03                     | 0.41              |
| 1:AF:94:VAL:HG22  | 1:BY:94:VAL:HG22  | 2.03                     | 0.41              |
| 1:AF:134:TYR:O    | 1:BY:3:LEU:N      | 2.43                     | 0.41              |
| 1:AG:134:TYR:HB2  | 1:BA:3:LEU:CD2    | 2.51                     | 0.41              |
| 1:AI:130:VAL:O    | 1:AI:130:VAL:HG12 | 2.19                     | 0.41              |
| 1:AU:131:GLU:CB   | 1:CK:1:PRO:HD3    | 2.50                     | 0.41              |
| 1:AW:24:ASP:HB2   | 1:AW:28:VAL:HB    | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AY:116:SER:OG   | 1:BU:8:LEU:HB3    | 2.21                     | 0.41              |
| 1:BK:123:ILE:O    | 1:BK:126:THR:HB   | 2.20                     | 0.41              |
| 1:BO:132:HIS:CE1  | 1:DG:50:VAL:HG23  | 2.56                     | 0.41              |
| 1:BT:65:PHE:HD1   | 1:BT:93:GLN:HG2   | 1.86                     | 0.41              |
| 1:BW:123:ILE:O    | 1:BW:126:THR:HB   | 2.20                     | 0.41              |
| 1:CJ:134:TYR:CE2  | 1:CS:20:PRO:HB2   | 2.56                     | 0.41              |
| 1:CW:55:THR:O     | 1:CW:55:THR:HG22  | 2.21                     | 0.41              |
| 1:CX:123:ILE:O    | 1:CX:126:THR:HB   | 2.20                     | 0.41              |
| 1:CY:132:HIS:HE1  | 1:DJ:52:GLU:HG3   | 1.86                     | 0.41              |
| 1:DB:24:ASP:HB2   | 1:DB:28:VAL:HB    | 2.03                     | 0.41              |
| 1:DJ:123:ILE:O    | 1:DJ:126:THR:HB   | 2.20                     | 0.41              |
| 1:AA:123:ILE:O    | 1:AA:126:THR:HB   | 2.20                     | 0.41              |
| 1:AA:132:HIS:NE2  | 1:AQ:50:VAL:HG23  | 2.36                     | 0.41              |
| 1:AD:65:PHE:HD1   | 1:AD:93:GLN:HG2   | 1.86                     | 0.41              |
| 1:AF:50:VAL:HG23  | 1:BY:132:HIS:CE1  | 2.56                     | 0.41              |
| 1:AJ:22:GLN:HB2   | 1:CE:132:HIS:CD2  | 2.56                     | 0.41              |
| 1:AK:1:PRO:HD3    | 1:CI:131:GLU:CB   | 2.51                     | 0.41              |
| 1:AK:108:GLU:OE1  | 1:CI:11:HIS:NE2   | 2.53                     | 0.41              |
| 1:AX:131:GLU:HB3  | 1:CN:1:PRO:CD     | 2.39                     | 0.41              |
| 1:BN:109:ASP:HB3  | 1:BR:11:HIS:CB    | 2.51                     | 0.41              |
| 1:BZ:65:PHE:HD1   | 1:BZ:93:GLN:HG2   | 1.86                     | 0.41              |
| 1:CF:1:PRO:HD2    | 1:CP:132:HIS:O    | 2.21                     | 0.41              |
| 1:CN:55:THR:HG22  | 1:CN:55:THR:O     | 2.21                     | 0.41              |
| 1:AA:109:ASP:CA   | 1:AQ:11:HIS:HB2   | 2.51                     | 0.40              |
| 1:AC:128:VAL:HG11 | 1:BV:108:GLU:HG3  | 2.01                     | 0.40              |
| 1:AH:11:HIS:HB3   | 1:CX:109:ASP:HB3  | 2.03                     | 0.40              |
| 1:AK:24:ASP:HB2   | 1:AK:28:VAL:HB    | 2.03                     | 0.40              |
| 1:BA:109:ASP:HB3  | 1:CQ:11:HIS:H     | 1.86                     | 0.40              |
| 1:BG:80:ASP:HB2   | 1:BK:73:THR:H     | 1.84                     | 0.40              |
| 1:BM:55:THR:O     | 1:BM:55:THR:HG22  | 2.20                     | 0.40              |
| 1:BN:134:TYR:HB2  | 1:BS:3:LEU:HD23   | 2.03                     | 0.40              |
| 1:BV:55:THR:O     | 1:BV:55:THR:HG22  | 2.20                     | 0.40              |
| 1:BY:130:VAL:O    | 1:BY:130:VAL:HG12 | 2.19                     | 0.40              |
| 1:CL:3:LEU:HD12   | 1:CL:3:LEU:HA     | 1.88                     | 0.40              |
| 1:CN:58:ASP:O     | 1:CN:99:PRO:HA    | 2.20                     | 0.40              |
| 1:DA:65:PHE:HD1   | 1:DA:93:GLN:HG2   | 1.87                     | 0.40              |
| 1:DD:65:PHE:HD1   | 1:DD:93:GLN:HG2   | 1.86                     | 0.40              |
| 1:AA:65:PHE:HD1   | 1:AA:93:GLN:HG2   | 1.86                     | 0.40              |
| 1:AE:109:ASP:CA   | 1:CU:11:HIS:HB2   | 2.51                     | 0.40              |
| 1:AJ:80:ASP:HB3   | 1:CE:73:THR:H     | 1.86                     | 0.40              |
| 1:AL:132:HIS:CD2  | 1:CC:22:GLN:HB2   | 2.56                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AU:133:PHE:CD1 | 1:CK:3:LEU:CD1    | 3.05                     | 0.40              |
| 1:BO:47:SER:HB2  | 1:BO:65:PHE:HB2   | 2.04                     | 0.40              |
| 1:BP:8:LEU:HB3   | 1:DF:116:SER:OG   | 2.21                     | 0.40              |
| 1:CB:55:THR:O    | 1:CB:55:THR:HG22  | 2.21                     | 0.40              |
| 1:CC:3:LEU:HD12  | 1:CC:3:LEU:HA     | 1.88                     | 0.40              |
| 1:CT:55:THR:HG22 | 1:CT:55:THR:O     | 2.21                     | 0.40              |
| 1:DJ:65:PHE:HD1  | 1:DJ:93:GLN:HG2   | 1.87                     | 0.40              |
| 1:AA:96:PHE:HA   | 1:AQ:91:ARG:O     | 2.20                     | 0.40              |
| 1:AA:109:ASP:HB3 | 1:AQ:11:HIS:N     | 2.29                     | 0.40              |
| 1:AG:53:PRO:HB3  | 1:AG:59:VAL:O     | 2.22                     | 0.40              |
| 1:AI:55:THR:HG22 | 1:AI:55:THR:O     | 2.21                     | 0.40              |
| 1:AL:1:PRO:HD3   | 1:CE:131:GLU:CB   | 2.40                     | 0.40              |
| 1:AQ:24:ASP:HB2  | 1:AQ:28:VAL:HB    | 2.03                     | 0.40              |
| 1:AR:55:THR:O    | 1:AR:55:THR:HG22  | 2.20                     | 0.40              |
| 1:AS:1:PRO:HB2   | 1:BX:133:PHE:CE1  | 2.57                     | 0.40              |
| 1:AS:53:PRO:HB3  | 1:AS:59:VAL:O     | 2.22                     | 0.40              |
| 1:AZ:24:ASP:HB2  | 1:AZ:28:VAL:HB    | 2.03                     | 0.40              |
| 1:BA:55:THR:HG22 | 1:BA:55:THR:O     | 2.21                     | 0.40              |
| 1:BB:20:PRO:HB2  | 1:CW:134:TYR:CZ   | 2.56                     | 0.40              |
| 1:BH:53:PRO:HB3  | 1:BH:59:VAL:O     | 2.22                     | 0.40              |
| 1:BK:65:PHE:HD1  | 1:BK:93:GLN:HG2   | 1.87                     | 0.40              |
| 1:BQ:53:PRO:HB3  | 1:BQ:59:VAL:O     | 2.22                     | 0.40              |
| 1:BX:47:SER:HB2  | 1:BX:65:PHE:HB2   | 2.04                     | 0.40              |
| 1:CK:55:THR:HG22 | 1:CK:55:THR:O     | 2.21                     | 0.40              |
| 1:DI:55:THR:HG22 | 1:DI:55:THR:O     | 2.21                     | 0.40              |
| 1:DK:24:ASP:HB2  | 1:DK:28:VAL:HB    | 2.03                     | 0.40              |
| 1:AB:91:ARG:O    | 1:DA:96:PHE:HA    | 2.21                     | 0.40              |
| 1:AD:22:GLN:HB2  | 1:BY:132:HIS:CD2  | 2.56                     | 0.40              |
| 1:AF:109:ASP:HB3 | 1:BY:11:HIS:H     | 1.86                     | 0.40              |
| 1:AH:47:SER:HB2  | 1:AH:65:PHE:HB2   | 2.04                     | 0.40              |
| 1:AP:11:HIS:CD2  | 1:AT:108:GLU:OE1  | 2.74                     | 0.40              |
| 1:AW:47:SER:HB2  | 1:AW:65:PHE:HB2   | 2.04                     | 0.40              |
| 1:AY:73:THR:H    | 1:BV:80:ASP:CB    | 2.32                     | 0.40              |
| 1:BC:47:SER:HB2  | 1:BC:65:PHE:HB2   | 2.04                     | 0.40              |
| 1:BG:2:ALA:HA    | 1:CZ:134:TYR:O    | 2.21                     | 0.40              |
| 1:BT:73:THR:H    | 1:DL:80:ASP:CB    | 2.34                     | 0.40              |
| 1:BT:90:ASN:HB3  | 1:DK:110:LEU:HD22 | 2.03                     | 0.40              |
| 1:BY:55:THR:O    | 1:BY:55:THR:HG22  | 2.20                     | 0.40              |
| 1:CH:55:THR:HG22 | 1:CH:55:THR:O     | 2.21                     | 0.40              |
| 1:CO:65:PHE:HD1  | 1:CO:93:GLN:HG2   | 1.86                     | 0.40              |
| 1:CR:65:PHE:HD1  | 1:CR:93:GLN:HG2   | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:CY:47:SER:HB2  | 1:CY:65:PHE:HB2  | 2.04                     | 0.40              |
| 1:AB:3:LEU:HD13  | 1:DA:133:PHE:HB3 | 2.04                     | 0.40              |
| 1:AB:3:LEU:N     | 1:DA:134:TYR:O   | 2.27                     | 0.40              |
| 1:AC:21:THR:O    | 1:DA:132:HIS:HB2 | 2.21                     | 0.40              |
| 1:AV:65:PHE:HD1  | 1:AV:93:GLN:HG2  | 1.86                     | 0.40              |
| 1:BE:74:ILE:HA   | 1:DF:78:GLY:O    | 2.21                     | 0.40              |
| 1:BG:55:THR:O    | 1:BG:55:THR:HG22 | 2.21                     | 0.40              |
| 1:BO:132:HIS:HE1 | 1:DG:52:GLU:HG3  | 1.86                     | 0.40              |
| 1:BW:53:PRO:HB3  | 1:BW:59:VAL:O    | 2.22                     | 0.40              |
| 1:BX:24:ASP:HB2  | 1:BX:28:VAL:HB   | 2.03                     | 0.40              |
| 1:CA:24:ASP:HB2  | 1:CA:28:VAL:HB   | 2.03                     | 0.40              |
| 1:CC:132:HIS:NE2 | 1:CG:50:VAL:HG23 | 2.36                     | 0.40              |
| 1:CG:47:SER:HB2  | 1:CG:65:PHE:HB2  | 2.04                     | 0.40              |
| 1:CM:47:SER:HB2  | 1:CM:65:PHE:HB2  | 2.04                     | 0.40              |
| 1:CP:47:SER:HB2  | 1:CP:65:PHE:HB2  | 2.04                     | 0.40              |
| 1:DL:46:VAL:HA   | 1:DL:65:PHE:O    | 2.22                     | 0.40              |
| 1:DL:55:THR:HG22 | 1:DL:55:THR:O    | 2.21                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------------|--------------------------|-------------------|
| 1:AW:121:THR:OG1 | 1:AZ:12:SER:O[4_565] | 1.95                     | 0.25              |
| 1:AJ:121:THR:OG1 | 1:AT:12:SER:O[4_566] | 2.10                     | 0.10              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AA    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AB    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AC    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AD    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AE    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AF    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AG    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AH    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AI    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AJ    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AK    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AL    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AM    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AN    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AO    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AP    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AQ    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AR    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AS    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AT    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AU    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AV    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AW    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AX    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AY    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AZ    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BA    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BB    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BC    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BD    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BE    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BF    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BG    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | BH    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BI    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BJ    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BK    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BL    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BM    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BN    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BO    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BP    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BQ    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BR    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BS    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BT    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BU    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BV    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BW    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BX    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BY    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BZ    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CA    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CB    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CC    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CD    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CE    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CF    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CG    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CH    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CI    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CJ    | 119/134 (89%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CK    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CL    | 132/134 (98%) | 130 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | CM    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CN    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CO    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CP    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CQ    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CR    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CS    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CT    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CU    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CV    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CW    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CX    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CY    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | CZ    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DA    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DB    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DC    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DD    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DE    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DF    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DG    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DH    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DI    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DJ    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DK    | 119/134 (89%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | DL    | 132/134 (98%)     | 130 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| All | All   | 11490/12060 (95%) | 11310 (98%) | 180 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | AA    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AB    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | AC    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AD    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AE    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | AF    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AG    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AH    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | AI    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AJ    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AK    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | AL    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AM    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AN    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | AO    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AP    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AQ    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | AR    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AS    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AT    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | AU    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AV    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AW    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | AX    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AY    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | AZ    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | BA    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BB    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BC    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | BD    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BE    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BF    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | BG    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BH    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BI    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | BJ    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BK    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BL    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | BM    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BN    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BO    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | BP    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BQ    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BR    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | BS    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BT    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BU    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | BV    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BW    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BX    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | BY    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | BZ    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CA    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CB    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CC    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CD    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CE    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | CF    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CG    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CH    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CI    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CJ    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CK    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CL    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CM    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CN    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CO    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CP    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CQ    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CR    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CS    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CT    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CU    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CV    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CW    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CX    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | CY    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | CZ    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | DA    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | DB    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | DC    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | DD    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | DE    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | DF    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | DG    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | DH    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 1   | DI    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 1   | DJ    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | DK    | 102/112 (91%)    | 102 (100%)  | 0        | 100         | 100 |
| 1   | DL    | 112/112 (100%)   | 112 (100%)  | 0        | 100         | 100 |
| All | All   | 9780/10080 (97%) | 9780 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 67  | ASN  |
| 1   | AB    | 35  | GLN  |
| 1   | AC    | 11  | HIS  |
| 1   | AC    | 77  | ASN  |
| 1   | AD    | 67  | ASN  |
| 1   | AF    | 67  | ASN  |
| 1   | AF    | 77  | ASN  |
| 1   | AG    | 67  | ASN  |
| 1   | AH    | 132 | HIS  |
| 1   | AI    | 77  | ASN  |
| 1   | AJ    | 67  | ASN  |
| 1   | AK    | 35  | GLN  |
| 1   | AL    | 11  | HIS  |
| 1   | AL    | 77  | ASN  |
| 1   | AL    | 90  | ASN  |
| 1   | AM    | 67  | ASN  |
| 1   | AN    | 35  | GLN  |
| 1   | AO    | 67  | ASN  |
| 1   | AP    | 67  | ASN  |
| 1   | AP    | 132 | HIS  |
| 1   | AQ    | 35  | GLN  |
| 1   | AR    | 11  | HIS  |
| 1   | AR    | 67  | ASN  |
| 1   | AR    | 90  | ASN  |
| 1   | AS    | 67  | ASN  |
| 1   | AT    | 35  | GLN  |
| 1   | AU    | 67  | ASN  |
| 1   | AU    | 77  | ASN  |
| 1   | AV    | 67  | ASN  |
| 1   | AX    | 67  | ASN  |
| 1   | AX    | 77  | ASN  |
| 1   | AY    | 67  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AZ    | 132 | HIS  |
| 1   | BA    | 77  | ASN  |
| 1   | BB    | 67  | ASN  |
| 1   | BC    | 11  | HIS  |
| 1   | BD    | 77  | ASN  |
| 1   | BE    | 67  | ASN  |
| 1   | BE    | 90  | ASN  |
| 1   | BG    | 11  | HIS  |
| 1   | BG    | 67  | ASN  |
| 1   | BG    | 77  | ASN  |
| 1   | BG    | 90  | ASN  |
| 1   | BH    | 67  | ASN  |
| 1   | BI    | 35  | GLN  |
| 1   | BJ    | 11  | HIS  |
| 1   | BJ    | 67  | ASN  |
| 1   | BJ    | 77  | ASN  |
| 1   | BK    | 67  | ASN  |
| 1   | BL    | 35  | GLN  |
| 1   | BM    | 67  | ASN  |
| 1   | BN    | 67  | ASN  |
| 1   | BO    | 35  | GLN  |
| 1   | BO    | 132 | HIS  |
| 1   | BQ    | 67  | ASN  |
| 1   | BR    | 35  | GLN  |
| 1   | BS    | 77  | ASN  |
| 1   | BT    | 67  | ASN  |
| 1   | BU    | 11  | HIS  |
| 1   | BU    | 35  | GLN  |
| 1   | BV    | 11  | HIS  |
| 1   | BV    | 67  | ASN  |
| 1   | BV    | 90  | ASN  |
| 1   | BW    | 67  | ASN  |
| 1   | BX    | 11  | HIS  |
| 1   | BX    | 35  | GLN  |
| 1   | BY    | 77  | ASN  |
| 1   | BZ    | 67  | ASN  |
| 1   | CA    | 11  | HIS  |
| 1   | CA    | 35  | GLN  |
| 1   | CB    | 11  | HIS  |
| 1   | CB    | 67  | ASN  |
| 1   | CC    | 67  | ASN  |
| 1   | CD    | 35  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CD    | 132 | HIS  |
| 1   | CE    | 11  | HIS  |
| 1   | CF    | 67  | ASN  |
| 1   | CG    | 35  | GLN  |
| 1   | CG    | 132 | HIS  |
| 1   | CH    | 67  | ASN  |
| 1   | CI    | 67  | ASN  |
| 1   | CJ    | 35  | GLN  |
| 1   | CJ    | 132 | HIS  |
| 1   | CK    | 67  | ASN  |
| 1   | CK    | 77  | ASN  |
| 1   | CL    | 67  | ASN  |
| 1   | CM    | 35  | GLN  |
| 1   | CN    | 67  | ASN  |
| 1   | CN    | 77  | ASN  |
| 1   | CO    | 67  | ASN  |
| 1   | CP    | 35  | GLN  |
| 1   | CP    | 132 | HIS  |
| 1   | CQ    | 67  | ASN  |
| 1   | CR    | 67  | ASN  |
| 1   | CR    | 90  | ASN  |
| 1   | CS    | 35  | GLN  |
| 1   | CT    | 67  | ASN  |
| 1   | CU    | 67  | ASN  |
| 1   | CW    | 67  | ASN  |
| 1   | CW    | 77  | ASN  |
| 1   | CX    | 67  | ASN  |
| 1   | CZ    | 11  | HIS  |
| 1   | CZ    | 67  | ASN  |
| 1   | CZ    | 77  | ASN  |
| 1   | DA    | 67  | ASN  |
| 1   | DC    | 11  | HIS  |
| 1   | DC    | 67  | ASN  |
| 1   | DD    | 67  | ASN  |
| 1   | DE    | 35  | GLN  |
| 1   | DE    | 132 | HIS  |
| 1   | DF    | 67  | ASN  |
| 1   | DF    | 77  | ASN  |
| 1   | DG    | 67  | ASN  |
| 1   | DG    | 90  | ASN  |
| 1   | DH    | 35  | GLN  |
| 1   | DJ    | 67  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DK    | 35  | GLN  |
| 1   | DK    | 132 | HIS  |
| 1   | DL    | 11  | HIS  |
| 1   | DL    | 67  | ASN  |
| 1   | DL    | 77  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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   | AA    | 134/134 (100%) | 0.43   | 4 (2%) 52 36  | 64, 102, 139, 208     | 0     |
| 1   | AB    | 123/134 (91%)  | 0.69   | 9 (7%) 21 19  | 67, 109, 164, 214     | 0     |
| 1   | AC    | 134/134 (100%) | 0.55   | 10 (7%) 20 18 | 66, 105, 140, 217     | 0     |
| 1   | AD    | 134/134 (100%) | 0.82   | 12 (8%) 15 16 | 64, 102, 139, 208     | 0     |
| 1   | AE    | 123/134 (91%)  | 0.64   | 8 (6%) 25 21  | 67, 109, 164, 214     | 0     |
| 1   | AF    | 134/134 (100%) | 0.71   | 9 (6%) 24 20  | 66, 105, 140, 217     | 0     |
| 1   | AG    | 134/134 (100%) | 0.75   | 7 (5%) 33 25  | 64, 102, 139, 208     | 0     |
| 1   | AH    | 123/134 (91%)  | 0.45   | 4 (3%) 49 34  | 67, 109, 164, 214     | 0     |
| 1   | AI    | 134/134 (100%) | 0.68   | 8 (5%) 27 22  | 66, 105, 140, 217     | 0     |
| 1   | AJ    | 134/134 (100%) | 0.62   | 11 (8%) 17 17 | 64, 102, 139, 208     | 0     |
| 1   | AK    | 123/134 (91%)  | 0.63   | 8 (6%) 25 21  | 67, 109, 164, 214     | 0     |
| 1   | AL    | 134/134 (100%) | 0.61   | 11 (8%) 17 17 | 66, 105, 140, 217     | 0     |
| 1   | AM    | 134/134 (100%) | 0.34   | 4 (2%) 52 36  | 64, 102, 139, 208     | 0     |
| 1   | AN    | 123/134 (91%)  | 0.41   | 5 (4%) 41 30  | 67, 109, 164, 214     | 0     |
| 1   | AO    | 134/134 (100%) | 0.43   | 5 (3%) 45 31  | 66, 105, 140, 217     | 0     |
| 1   | AP    | 134/134 (100%) | 0.74   | 13 (9%) 13 15 | 64, 102, 139, 208     | 0     |
| 1   | AQ    | 123/134 (91%)  | 0.59   | 8 (6%) 25 21  | 67, 109, 164, 214     | 0     |
| 1   | AR    | 134/134 (100%) | 0.53   | 4 (2%) 52 36  | 66, 105, 140, 217     | 0     |
| 1   | AS    | 134/134 (100%) | 0.68   | 7 (5%) 33 25  | 64, 102, 139, 208     | 0     |
| 1   | AT    | 123/134 (91%)  | 0.79   | 10 (8%) 18 17 | 67, 109, 164, 214     | 0     |
| 1   | AU    | 134/134 (100%) | 0.66   | 11 (8%) 17 17 | 66, 105, 140, 217     | 0     |
| 1   | AV    | 134/134 (100%) | 0.77   | 12 (8%) 15 16 | 64, 102, 139, 208     | 0     |
| 1   | AW    | 123/134 (91%)  | 0.63   | 6 (4%) 35 26  | 67, 109, 164, 214     | 0     |
| 1   | AX    | 134/134 (100%) | 0.62   | 12 (8%) 15 16 | 66, 105, 140, 217     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 1   | AY    | 134/134 (100%) | 0.33   | 8 (5%) 27 22   | 64, 102, 139, 208     | 0     |
| 1   | AZ    | 123/134 (91%)  | 0.65   | 10 (8%) 18 17  | 67, 109, 164, 214     | 0     |
| 1   | BA    | 134/134 (100%) | 0.54   | 9 (6%) 24 20   | 66, 105, 140, 217     | 0     |
| 1   | BB    | 134/134 (100%) | 0.46   | 7 (5%) 33 25   | 64, 102, 139, 208     | 0     |
| 1   | BC    | 123/134 (91%)  | 0.55   | 6 (4%) 35 26   | 67, 109, 164, 214     | 0     |
| 1   | BD    | 134/134 (100%) | 0.63   | 7 (5%) 33 25   | 66, 105, 140, 217     | 0     |
| 1   | BE    | 134/134 (100%) | 0.51   | 5 (3%) 45 31   | 64, 102, 139, 208     | 0     |
| 1   | BF    | 123/134 (91%)  | 0.73   | 9 (7%) 21 19   | 67, 109, 164, 214     | 0     |
| 1   | BG    | 134/134 (100%) | 0.72   | 15 (11%) 10 13 | 66, 105, 140, 217     | 0     |
| 1   | BH    | 134/134 (100%) | 0.52   | 11 (8%) 17 17  | 64, 102, 139, 208     | 0     |
| 1   | BI    | 123/134 (91%)  | 0.44   | 6 (4%) 35 26   | 67, 109, 164, 214     | 0     |
| 1   | BJ    | 134/134 (100%) | 0.56   | 5 (3%) 45 31   | 66, 105, 140, 217     | 0     |
| 1   | BK    | 134/134 (100%) | 0.76   | 12 (8%) 15 16  | 64, 102, 139, 208     | 0     |
| 1   | BL    | 123/134 (91%)  | 0.62   | 4 (3%) 49 34   | 67, 109, 164, 214     | 0     |
| 1   | BM    | 134/134 (100%) | 0.65   | 4 (2%) 52 36   | 66, 105, 140, 217     | 0     |
| 1   | BN    | 134/134 (100%) | 0.49   | 3 (2%) 62 44   | 64, 102, 139, 208     | 0     |
| 1   | BO    | 123/134 (91%)  | 0.43   | 5 (4%) 41 30   | 67, 109, 164, 214     | 0     |
| 1   | BP    | 134/134 (100%) | 0.58   | 8 (5%) 27 22   | 66, 105, 140, 217     | 0     |
| 1   | BQ    | 134/134 (100%) | 0.49   | 5 (3%) 45 31   | 64, 102, 139, 208     | 0     |
| 1   | BR    | 123/134 (91%)  | 0.56   | 8 (6%) 25 21   | 67, 109, 164, 214     | 0     |
| 1   | BS    | 134/134 (100%) | 0.62   | 8 (5%) 27 22   | 66, 105, 140, 217     | 0     |
| 1   | BT    | 134/134 (100%) | 0.63   | 9 (6%) 24 20   | 64, 102, 139, 208     | 0     |
| 1   | BU    | 123/134 (91%)  | 0.43   | 8 (6%) 25 21   | 67, 109, 164, 214     | 0     |
| 1   | BV    | 134/134 (100%) | 0.63   | 13 (9%) 13 15  | 66, 105, 140, 217     | 0     |
| 1   | BW    | 134/134 (100%) | 0.76   | 10 (7%) 20 18  | 64, 102, 139, 208     | 0     |
| 1   | BX    | 123/134 (91%)  | 0.60   | 5 (4%) 41 30   | 67, 109, 164, 214     | 0     |
| 1   | BY    | 134/134 (100%) | 0.47   | 5 (3%) 45 31   | 66, 105, 140, 217     | 0     |
| 1   | BZ    | 134/134 (100%) | 0.52   | 6 (4%) 38 27   | 64, 102, 139, 208     | 0     |
| 1   | CA    | 123/134 (91%)  | 0.62   | 9 (7%) 21 19   | 67, 109, 164, 214     | 0     |
| 1   | CB    | 134/134 (100%) | 0.68   | 9 (6%) 24 20   | 66, 105, 140, 217     | 0     |
| 1   | CC    | 134/134 (100%) | 0.38   | 2 (1%) 72 50   | 64, 102, 139, 208     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|-------|-----------------------|-------|
| 1   | CD    | 123/134 (91%)  | 0.52   | 10 (8%)  | 18 17 | 67, 109, 164, 214     | 0     |
| 1   | CE    | 134/134 (100%) | 0.51   | 7 (5%)   | 33 25 | 66, 105, 140, 217     | 0     |
| 1   | CF    | 134/134 (100%) | 0.40   | 7 (5%)   | 33 25 | 64, 102, 139, 208     | 0     |
| 1   | CG    | 123/134 (91%)  | 0.50   | 6 (4%)   | 35 26 | 67, 109, 164, 214     | 0     |
| 1   | CH    | 134/134 (100%) | 0.61   | 8 (5%)   | 27 22 | 66, 105, 140, 217     | 0     |
| 1   | CI    | 134/134 (100%) | 0.61   | 9 (6%)   | 24 20 | 64, 102, 139, 208     | 0     |
| 1   | CJ    | 123/134 (91%)  | 0.65   | 11 (8%)  | 15 16 | 67, 109, 164, 214     | 0     |
| 1   | CK    | 134/134 (100%) | 0.76   | 11 (8%)  | 17 17 | 66, 105, 140, 217     | 0     |
| 1   | CL    | 134/134 (100%) | 0.48   | 5 (3%)   | 45 31 | 64, 102, 139, 208     | 0     |
| 1   | CM    | 123/134 (91%)  | 0.34   | 5 (4%)   | 41 30 | 67, 109, 164, 214     | 0     |
| 1   | CN    | 134/134 (100%) | 0.69   | 16 (11%) | 9 12  | 66, 105, 140, 217     | 0     |
| 1   | CO    | 134/134 (100%) | 0.42   | 10 (7%)  | 20 18 | 64, 102, 139, 208     | 0     |
| 1   | CP    | 123/134 (91%)  | 0.33   | 5 (4%)   | 41 30 | 67, 109, 164, 214     | 0     |
| 1   | CQ    | 134/134 (100%) | 0.50   | 8 (5%)   | 27 22 | 66, 105, 140, 217     | 0     |
| 1   | CR    | 134/134 (100%) | 0.57   | 4 (2%)   | 52 36 | 64, 102, 139, 208     | 0     |
| 1   | CS    | 123/134 (91%)  | 0.73   | 10 (8%)  | 18 17 | 67, 109, 164, 214     | 0     |
| 1   | CT    | 134/134 (100%) | 0.79   | 9 (6%)   | 24 20 | 66, 105, 140, 217     | 0     |
| 1   | CU    | 134/134 (100%) | 0.72   | 12 (8%)  | 15 16 | 64, 102, 139, 208     | 0     |
| 1   | CV    | 123/134 (91%)  | 0.63   | 9 (7%)   | 21 19 | 67, 109, 164, 214     | 0     |
| 1   | CW    | 134/134 (100%) | 0.69   | 11 (8%)  | 17 17 | 66, 105, 140, 217     | 0     |
| 1   | CX    | 134/134 (100%) | 0.43   | 6 (4%)   | 38 27 | 64, 102, 139, 208     | 0     |
| 1   | CY    | 123/134 (91%)  | 0.58   | 12 (9%)  | 13 15 | 67, 109, 164, 214     | 0     |
| 1   | CZ    | 134/134 (100%) | 0.62   | 9 (6%)   | 24 20 | 66, 105, 140, 217     | 0     |
| 1   | DA    | 134/134 (100%) | 0.60   | 10 (7%)  | 20 18 | 64, 102, 139, 208     | 0     |
| 1   | DB    | 123/134 (91%)  | 0.70   | 11 (8%)  | 15 16 | 67, 109, 164, 214     | 0     |
| 1   | DC    | 134/134 (100%) | 0.60   | 5 (3%)   | 45 31 | 66, 105, 140, 217     | 0     |
| 1   | DD    | 134/134 (100%) | 0.59   | 6 (4%)   | 38 27 | 64, 102, 139, 208     | 0     |
| 1   | DE    | 123/134 (91%)  | 0.68   | 12 (9%)  | 13 15 | 67, 109, 164, 214     | 0     |
| 1   | DF    | 134/134 (100%) | 0.65   | 9 (6%)   | 24 20 | 66, 105, 140, 217     | 0     |
| 1   | DG    | 134/134 (100%) | 0.32   | 5 (3%)   | 45 31 | 64, 102, 139, 208     | 0     |
| 1   | DH    | 123/134 (91%)  | 0.68   | 11 (8%)  | 15 16 | 67, 109, 164, 214     | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 1   | DI    | 134/134 (100%)    | 0.48   | 5 (3%) 45 31   | 66, 105, 140, 217     | 0     |
| 1   | DJ    | 134/134 (100%)    | 0.44   | 7 (5%) 33 25   | 64, 102, 139, 208     | 0     |
| 1   | DK    | 123/134 (91%)     | 0.61   | 10 (8%) 18 17  | 67, 109, 164, 214     | 0     |
| 1   | DL    | 134/134 (100%)    | 0.60   | 11 (8%) 17 17  | 66, 105, 140, 217     | 0     |
| All | All   | 11730/12060 (97%) | 0.58   | 731 (6%) 26 22 | 64, 104, 154, 217     | 0     |

All (731) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CZ    | 56  | ASN  | 8.2  |
| 1   | AW    | 56  | ASN  | 6.5  |
| 1   | BG    | 56  | ASN  | 6.5  |
| 1   | BW    | 26  | ASN  | 6.4  |
| 1   | CT    | 23  | ILE  | 6.2  |
| 1   | DL    | 26  | ASN  | 5.6  |
| 1   | AZ    | 56  | ASN  | 5.4  |
| 1   | BF    | 85  | GLU  | 5.4  |
| 1   | BF    | 56  | ASN  | 5.4  |
| 1   | CS    | 71  | VAL  | 5.2  |
| 1   | AO    | 56  | ASN  | 5.2  |
| 1   | BV    | 56  | ASN  | 5.1  |
| 1   | AV    | 23  | ILE  | 5.1  |
| 1   | AG    | 56  | ASN  | 4.9  |
| 1   | BT    | 58  | ASP  | 4.9  |
| 1   | BF    | 26  | ASN  | 4.9  |
| 1   | AD    | 23  | ILE  | 4.8  |
| 1   | AM    | 56  | ASN  | 4.8  |
| 1   | BR    | 56  | ASN  | 4.8  |
| 1   | BO    | 26  | ASN  | 4.8  |
| 1   | CP    | 85  | GLU  | 4.7  |
| 1   | CU    | 26  | ASN  | 4.6  |
| 1   | AJ    | 23  | ILE  | 4.6  |
| 1   | BG    | 58  | ASP  | 4.6  |
| 1   | CH    | 42  | GLY  | 4.6  |
| 1   | CJ    | 71  | VAL  | 4.5  |
| 1   | DC    | 23  | ILE  | 4.5  |
| 1   | BI    | 23  | ILE  | 4.5  |
| 1   | AA    | 25  | LYS  | 4.4  |
| 1   | CG    | 23  | ILE  | 4.4  |
| 1   | DH    | 72  | ALA  | 4.4  |
| 1   | AC    | 26  | ASN  | 4.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AF    | 23  | ILE  | 4.3  |
| 1   | BU    | 4   | LYS  | 4.3  |
| 1   | DG    | 26  | ASN  | 4.3  |
| 1   | CB    | 27  | GLY  | 4.3  |
| 1   | AD    | 26  | ASN  | 4.3  |
| 1   | CU    | 119 | ALA  | 4.3  |
| 1   | AX    | 61  | ARG  | 4.3  |
| 1   | CX    | 26  | ASN  | 4.2  |
| 1   | AX    | 51  | LYS  | 4.2  |
| 1   | CN    | 27  | GLY  | 4.2  |
| 1   | CO    | 58  | ASP  | 4.2  |
| 1   | BA    | 56  | ASN  | 4.2  |
| 1   | DB    | 58  | ASP  | 4.2  |
| 1   | BG    | 38  | GLY  | 4.2  |
| 1   | BH    | 23  | ILE  | 4.1  |
| 1   | AV    | 93  | GLN  | 4.1  |
| 1   | CE    | 23  | ILE  | 4.1  |
| 1   | DB    | 85  | GLU  | 4.1  |
| 1   | AF    | 26  | ASN  | 4.1  |
| 1   | AT    | 119 | ALA  | 4.1  |
| 1   | DE    | 26  | ASN  | 4.1  |
| 1   | CD    | 4   | LYS  | 4.1  |
| 1   | CK    | 42  | GLY  | 4.1  |
| 1   | BC    | 26  | ASN  | 4.1  |
| 1   | DD    | 56  | ASN  | 4.0  |
| 1   | AS    | 23  | ILE  | 4.0  |
| 1   | BV    | 103 | ALA  | 4.0  |
| 1   | CG    | 63  | LYS  | 4.0  |
| 1   | AN    | 85  | GLU  | 4.0  |
| 1   | CK    | 23  | ILE  | 4.0  |
| 1   | BL    | 85  | GLU  | 4.0  |
| 1   | DB    | 73  | THR  | 4.0  |
| 1   | BQ    | 23  | ILE  | 3.9  |
| 1   | BA    | 27  | GLY  | 3.9  |
| 1   | CK    | 34  | LEU  | 3.9  |
| 1   | AL    | 42  | GLY  | 3.9  |
| 1   | BS    | 42  | GLY  | 3.9  |
| 1   | BA    | 42  | GLY  | 3.9  |
| 1   | CN    | 42  | GLY  | 3.9  |
| 1   | BE    | 58  | ASP  | 3.8  |
| 1   | DA    | 95  | GLU  | 3.8  |
| 1   | BZ    | 26  | ASN  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AY    | 58  | ASP  | 3.8  |
| 1   | AW    | 85  | GLU  | 3.8  |
| 1   | AT    | 1   | PRO  | 3.8  |
| 1   | DD    | 26  | ASN  | 3.8  |
| 1   | CV    | 58  | ASP  | 3.8  |
| 1   | AK    | 71  | VAL  | 3.8  |
| 1   | CS    | 23  | ILE  | 3.8  |
| 1   | AX    | 38  | GLY  | 3.8  |
| 1   | BP    | 42  | GLY  | 3.8  |
| 1   | CK    | 38  | GLY  | 3.8  |
| 1   | CW    | 4   | LYS  | 3.7  |
| 1   | BE    | 56  | ASN  | 3.7  |
| 1   | AL    | 23  | ILE  | 3.7  |
| 1   | BG    | 26  | ASN  | 3.7  |
| 1   | BP    | 26  | ASN  | 3.6  |
| 1   | CG    | 26  | ASN  | 3.6  |
| 1   | AV    | 67  | ASN  | 3.6  |
| 1   | CZ    | 58  | ASP  | 3.6  |
| 1   | BL    | 56  | ASN  | 3.6  |
| 1   | BU    | 88  | ARG  | 3.6  |
| 1   | BE    | 55  | THR  | 3.6  |
| 1   | DJ    | 23  | ILE  | 3.5  |
| 1   | CL    | 119 | ALA  | 3.5  |
| 1   | CT    | 119 | ALA  | 3.5  |
| 1   | CN    | 26  | ASN  | 3.5  |
| 1   | AT    | 48  | SER  | 3.5  |
| 1   | AU    | 23  | ILE  | 3.5  |
| 1   | DB    | 23  | ILE  | 3.5  |
| 1   | DH    | 26  | ASN  | 3.5  |
| 1   | AU    | 58  | ASP  | 3.5  |
| 1   | BK    | 58  | ASP  | 3.5  |
| 1   | AT    | 85  | GLU  | 3.5  |
| 1   | BB    | 26  | ASN  | 3.5  |
| 1   | BS    | 26  | ASN  | 3.5  |
| 1   | AY    | 56  | ASN  | 3.5  |
| 1   | CM    | 85  | GLU  | 3.4  |
| 1   | BG    | 119 | ALA  | 3.4  |
| 1   | BY    | 59  | VAL  | 3.4  |
| 1   | DH    | 71  | VAL  | 3.4  |
| 1   | AH    | 119 | ALA  | 3.4  |
| 1   | AE    | 71  | VAL  | 3.4  |
| 1   | BJ    | 23  | ILE  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CO    | 26  | ASN  | 3.4  |
| 1   | DJ    | 56  | ASN  | 3.4  |
| 1   | CV    | 71  | VAL  | 3.4  |
| 1   | AC    | 80  | ASP  | 3.4  |
| 1   | DH    | 119 | ALA  | 3.4  |
| 1   | AL    | 26  | ASN  | 3.4  |
| 1   | AZ    | 26  | ASN  | 3.4  |
| 1   | BQ    | 26  | ASN  | 3.4  |
| 1   | BG    | 25  | LYS  | 3.4  |
| 1   | CU    | 4   | LYS  | 3.4  |
| 1   | CF    | 26  | ASN  | 3.3  |
| 1   | DD    | 25  | LYS  | 3.3  |
| 1   | AB    | 56  | ASN  | 3.3  |
| 1   | DB    | 56  | ASN  | 3.3  |
| 1   | BW    | 30  | TYR  | 3.3  |
| 1   | AH    | 85  | GLU  | 3.3  |
| 1   | BA    | 38  | GLY  | 3.3  |
| 1   | DJ    | 133 | PHE  | 3.3  |
| 1   | BT    | 23  | ILE  | 3.3  |
| 1   | DE    | 73  | THR  | 3.3  |
| 1   | AE    | 23  | ILE  | 3.3  |
| 1   | CL    | 30  | TYR  | 3.3  |
| 1   | AK    | 95  | GLU  | 3.3  |
| 1   | AD    | 38  | GLY  | 3.2  |
| 1   | AU    | 67  | ASN  | 3.2  |
| 1   | AE    | 39  | LYS  | 3.2  |
| 1   | AS    | 39  | LYS  | 3.2  |
| 1   | DL    | 25  | LYS  | 3.2  |
| 1   | DK    | 85  | GLU  | 3.2  |
| 1   | BR    | 23  | ILE  | 3.2  |
| 1   | AL    | 56  | ASN  | 3.2  |
| 1   | CG    | 56  | ASN  | 3.2  |
| 1   | AN    | 133 | PHE  | 3.2  |
| 1   | BM    | 23  | ILE  | 3.2  |
| 1   | CK    | 41  | ILE  | 3.2  |
| 1   | DI    | 131 | GLU  | 3.2  |
| 1   | DL    | 127 | ILE  | 3.2  |
| 1   | DA    | 48  | SER  | 3.2  |
| 1   | CZ    | 25  | LYS  | 3.2  |
| 1   | BB    | 38  | GLY  | 3.2  |
| 1   | BX    | 56  | ASN  | 3.2  |
| 1   | DF    | 24  | ASP  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | DG    | 24  | ASP  | 3.2  |
| 1   | BW    | 22  | GLN  | 3.2  |
| 1   | AK    | 73  | THR  | 3.2  |
| 1   | BW    | 23  | ILE  | 3.2  |
| 1   | BG    | 22  | GLN  | 3.2  |
| 1   | AU    | 59  | VAL  | 3.2  |
| 1   | CA    | 68  | VAL  | 3.2  |
| 1   | AU    | 38  | GLY  | 3.2  |
| 1   | CJ    | 56  | ASN  | 3.2  |
| 1   | BA    | 39  | LYS  | 3.2  |
| 1   | BC    | 85  | GLU  | 3.2  |
| 1   | CY    | 85  | GLU  | 3.2  |
| 1   | BJ    | 119 | ALA  | 3.2  |
| 1   | CS    | 59  | VAL  | 3.2  |
| 1   | DL    | 42  | GLY  | 3.1  |
| 1   | DI    | 22  | GLN  | 3.1  |
| 1   | BS    | 51  | LYS  | 3.1  |
| 1   | AF    | 59  | VAL  | 3.1  |
| 1   | CW    | 59  | VAL  | 3.1  |
| 1   | AE    | 85  | GLU  | 3.1  |
| 1   | CQ    | 59  | VAL  | 3.1  |
| 1   | AE    | 1   | PRO  | 3.1  |
| 1   | CB    | 42  | GLY  | 3.1  |
| 1   | AB    | 95  | GLU  | 3.1  |
| 1   | CF    | 131 | GLU  | 3.1  |
| 1   | CO    | 61  | ARG  | 3.1  |
| 1   | AP    | 131 | GLU  | 3.1  |
| 1   | BK    | 23  | ILE  | 3.1  |
| 1   | CW    | 23  | ILE  | 3.1  |
| 1   | CW    | 39  | LYS  | 3.1  |
| 1   | DA    | 42  | GLY  | 3.1  |
| 1   | AD    | 41  | ILE  | 3.1  |
| 1   | BU    | 85  | GLU  | 3.1  |
| 1   | CR    | 23  | ILE  | 3.0  |
| 1   | BR    | 58  | ASP  | 3.0  |
| 1   | BJ    | 42  | GLY  | 3.0  |
| 1   | AC    | 70  | GLU  | 3.0  |
| 1   | BH    | 58  | ASP  | 3.0  |
| 1   | CV    | 23  | ILE  | 3.0  |
| 1   | AA    | 23  | ILE  | 3.0  |
| 1   | AI    | 42  | GLY  | 3.0  |
| 1   | AK    | 23  | ILE  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AP    | 17  | ILE  | 3.0  |
| 1   | DC    | 41  | ILE  | 3.0  |
| 1   | CK    | 59  | VAL  | 3.0  |
| 1   | CB    | 56  | ASN  | 3.0  |
| 1   | BN    | 119 | ALA  | 3.0  |
| 1   | AK    | 85  | GLU  | 3.0  |
| 1   | AJ    | 25  | LYS  | 3.0  |
| 1   | BS    | 23  | ILE  | 3.0  |
| 1   | CI    | 34  | LEU  | 3.0  |
| 1   | BH    | 119 | ALA  | 3.0  |
| 1   | CU    | 115 | ALA  | 3.0  |
| 1   | AG    | 23  | ILE  | 2.9  |
| 1   | AR    | 23  | ILE  | 2.9  |
| 1   | AX    | 52  | GLU  | 2.9  |
| 1   | BA    | 23  | ILE  | 2.9  |
| 1   | BY    | 23  | ILE  | 2.9  |
| 1   | CB    | 4   | LYS  | 2.9  |
| 1   | CQ    | 23  | ILE  | 2.9  |
| 1   | DB    | 86  | ILE  | 2.9  |
| 1   | AG    | 38  | GLY  | 2.9  |
| 1   | CH    | 59  | VAL  | 2.9  |
| 1   | CL    | 22  | GLN  | 2.9  |
| 1   | DB    | 71  | VAL  | 2.9  |
| 1   | AL    | 25  | LYS  | 2.9  |
| 1   | AP    | 134 | TYR  | 2.9  |
| 1   | CT    | 38  | GLY  | 2.9  |
| 1   | CW    | 42  | GLY  | 2.9  |
| 1   | CG    | 59  | VAL  | 2.9  |
| 1   | DH    | 73  | THR  | 2.9  |
| 1   | DL    | 58  | ASP  | 2.9  |
| 1   | BK    | 30  | TYR  | 2.9  |
| 1   | AT    | 129 | ASN  | 2.9  |
| 1   | BR    | 85  | GLU  | 2.9  |
| 1   | BD    | 59  | VAL  | 2.9  |
| 1   | BO    | 71  | VAL  | 2.9  |
| 1   | BZ    | 128 | VAL  | 2.9  |
| 1   | BN    | 25  | LYS  | 2.9  |
| 1   | CG    | 73  | THR  | 2.9  |
| 1   | BJ    | 70  | GLU  | 2.9  |
| 1   | BM    | 56  | ASN  | 2.9  |
| 1   | CV    | 56  | ASN  | 2.9  |
| 1   | AK    | 54  | GLY  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BW    | 25  | LYS  | 2.9  |
| 1   | BY    | 103 | ALA  | 2.9  |
| 1   | BH    | 44  | TYR  | 2.9  |
| 1   | AP    | 26  | ASN  | 2.9  |
| 1   | CA    | 90  | ASN  | 2.9  |
| 1   | DK    | 95  | GLU  | 2.9  |
| 1   | AR    | 38  | GLY  | 2.8  |
| 1   | DF    | 29  | ALA  | 2.8  |
| 1   | BQ    | 30  | TYR  | 2.8  |
| 1   | CU    | 5   | PRO  | 2.8  |
| 1   | AW    | 71  | VAL  | 2.8  |
| 1   | CD    | 85  | GLU  | 2.8  |
| 1   | CS    | 85  | GLU  | 2.8  |
| 1   | CA    | 58  | ASP  | 2.8  |
| 1   | CB    | 23  | ILE  | 2.8  |
| 1   | CN    | 22  | GLN  | 2.8  |
| 1   | CN    | 41  | ILE  | 2.8  |
| 1   | DK    | 71  | VAL  | 2.8  |
| 1   | AD    | 27  | GLY  | 2.8  |
| 1   | DE    | 119 | ALA  | 2.8  |
| 1   | AP    | 23  | ILE  | 2.8  |
| 1   | BA    | 40  | PRO  | 2.8  |
| 1   | BD    | 23  | ILE  | 2.8  |
| 1   | BG    | 30  | TYR  | 2.8  |
| 1   | DL    | 38  | GLY  | 2.8  |
| 1   | CS    | 73  | THR  | 2.8  |
| 1   | BV    | 58  | ASP  | 2.8  |
| 1   | AC    | 4   | LYS  | 2.8  |
| 1   | AF    | 34  | LEU  | 2.8  |
| 1   | DH    | 85  | GLU  | 2.8  |
| 1   | CT    | 39  | LYS  | 2.8  |
| 1   | DF    | 30  | TYR  | 2.8  |
| 1   | AN    | 73  | THR  | 2.8  |
| 1   | DL    | 34  | LEU  | 2.7  |
| 1   | AQ    | 23  | ILE  | 2.7  |
| 1   | BC    | 59  | VAL  | 2.7  |
| 1   | CO    | 39  | LYS  | 2.7  |
| 1   | AI    | 103 | ALA  | 2.7  |
| 1   | BV    | 26  | ASN  | 2.7  |
| 1   | CD    | 56  | ASN  | 2.7  |
| 1   | DL    | 56  | ASN  | 2.7  |
| 1   | AY    | 23  | ILE  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BX    | 23  | ILE  | 2.7  |
| 1   | BV    | 102 | SER  | 2.7  |
| 1   | BB    | 25  | LYS  | 2.7  |
| 1   | CS    | 99  | PRO  | 2.7  |
| 1   | CZ    | 22  | GLN  | 2.7  |
| 1   | BF    | 72  | ALA  | 2.7  |
| 1   | BI    | 32  | ARG  | 2.7  |
| 1   | CO    | 67  | ASN  | 2.7  |
| 1   | BB    | 24  | ASP  | 2.7  |
| 1   | DI    | 59  | VAL  | 2.7  |
| 1   | DF    | 22  | GLN  | 2.7  |
| 1   | AP    | 2   | ALA  | 2.7  |
| 1   | AZ    | 2   | ALA  | 2.7  |
| 1   | BD    | 119 | ALA  | 2.7  |
| 1   | AV    | 56  | ASN  | 2.7  |
| 1   | DK    | 26  | ASN  | 2.7  |
| 1   | BF    | 71  | VAL  | 2.7  |
| 1   | BD    | 27  | GLY  | 2.7  |
| 1   | AX    | 39  | LYS  | 2.7  |
| 1   | AB    | 61  | ARG  | 2.7  |
| 1   | BS    | 61  | ARG  | 2.7  |
| 1   | AJ    | 42  | GLY  | 2.7  |
| 1   | AM    | 42  | GLY  | 2.7  |
| 1   | AU    | 119 | ALA  | 2.7  |
| 1   | CJ    | 86  | ILE  | 2.7  |
| 1   | DK    | 119 | ALA  | 2.7  |
| 1   | CU    | 131 | GLU  | 2.7  |
| 1   | DF    | 55  | THR  | 2.7  |
| 1   | BP    | 25  | LYS  | 2.7  |
| 1   | DD    | 77  | ASN  | 2.7  |
| 1   | BD    | 22  | GLN  | 2.6  |
| 1   | CC    | 23  | ILE  | 2.6  |
| 1   | AO    | 42  | GLY  | 2.6  |
| 1   | CB    | 38  | GLY  | 2.6  |
| 1   | BF    | 25  | LYS  | 2.6  |
| 1   | CQ    | 81  | THR  | 2.6  |
| 1   | CX    | 25  | LYS  | 2.6  |
| 1   | AY    | 131 | GLU  | 2.6  |
| 1   | BW    | 131 | GLU  | 2.6  |
| 1   | AX    | 56  | ASN  | 2.6  |
| 1   | BK    | 56  | ASN  | 2.6  |
| 1   | BG    | 23  | ILE  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AP    | 30  | TYR  | 2.6  |
| 1   | CT    | 7   | THR  | 2.6  |
| 1   | AV    | 95  | GLU  | 2.6  |
| 1   | CX    | 85  | GLU  | 2.6  |
| 1   | BN    | 26  | ASN  | 2.6  |
| 1   | CK    | 26  | ASN  | 2.6  |
| 1   | AF    | 41  | ILE  | 2.6  |
| 1   | BM    | 61  | ARG  | 2.6  |
| 1   | CH    | 41  | ILE  | 2.6  |
| 1   | CV    | 86  | ILE  | 2.6  |
| 1   | AS    | 53  | PRO  | 2.6  |
| 1   | AF    | 119 | ALA  | 2.6  |
| 1   | AG    | 119 | ALA  | 2.6  |
| 1   | AJ    | 2   | ALA  | 2.6  |
| 1   | AJ    | 112 | ALA  | 2.6  |
| 1   | AT    | 2   | ALA  | 2.6  |
| 1   | BT    | 22  | GLN  | 2.6  |
| 1   | CT    | 42  | GLY  | 2.6  |
| 1   | DH    | 27  | GLY  | 2.6  |
| 1   | DH    | 131 | GLU  | 2.6  |
| 1   | CH    | 13  | SER  | 2.6  |
| 1   | AW    | 86  | ILE  | 2.6  |
| 1   | BB    | 23  | ILE  | 2.6  |
| 1   | DL    | 23  | ILE  | 2.6  |
| 1   | CF    | 25  | LYS  | 2.6  |
| 1   | AO    | 119 | ALA  | 2.6  |
| 1   | CI    | 119 | ALA  | 2.6  |
| 1   | AB    | 4   | LYS  | 2.6  |
| 1   | DC    | 103 | ALA  | 2.6  |
| 1   | CI    | 42  | GLY  | 2.6  |
| 1   | AB    | 85  | GLU  | 2.6  |
| 1   | CD    | 119 | ALA  | 2.6  |
| 1   | CE    | 22  | GLN  | 2.6  |
| 1   | CU    | 2   | ALA  | 2.6  |
| 1   | CV    | 53  | PRO  | 2.6  |
| 1   | CY    | 53  | PRO  | 2.6  |
| 1   | AV    | 42  | GLY  | 2.6  |
| 1   | CD    | 73  | THR  | 2.5  |
| 1   | AT    | 131 | GLU  | 2.5  |
| 1   | AZ    | 85  | GLU  | 2.5  |
| 1   | CW    | 48  | SER  | 2.5  |
| 1   | CE    | 68  | VAL  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BD    | 26  | ASN  | 2.5  |
| 1   | CW    | 38  | GLY  | 2.5  |
| 1   | BG    | 55  | THR  | 2.5  |
| 1   | CT    | 41  | ILE  | 2.5  |
| 1   | DK    | 73  | THR  | 2.5  |
| 1   | AR    | 59  | VAL  | 2.5  |
| 1   | CD    | 52  | GLU  | 2.5  |
| 1   | DH    | 129 | ASN  | 2.5  |
| 1   | AD    | 103 | ALA  | 2.5  |
| 1   | AP    | 119 | ALA  | 2.5  |
| 1   | BE    | 42  | GLY  | 2.5  |
| 1   | BY    | 4   | LYS  | 2.5  |
| 1   | CY    | 59  | VAL  | 2.5  |
| 1   | AP    | 24  | ASP  | 2.5  |
| 1   | AI    | 87  | ALA  | 2.5  |
| 1   | AL    | 93  | GLN  | 2.5  |
| 1   | AC    | 42  | GLY  | 2.5  |
| 1   | AL    | 38  | GLY  | 2.5  |
| 1   | AP    | 4   | LYS  | 2.5  |
| 1   | AX    | 42  | GLY  | 2.5  |
| 1   | AX    | 54  | GLY  | 2.5  |
| 1   | CE    | 38  | GLY  | 2.5  |
| 1   | DK    | 23  | ILE  | 2.5  |
| 1   | CN    | 89  | THR  | 2.5  |
| 1   | BC    | 34  | LEU  | 2.5  |
| 1   | CW    | 110 | LEU  | 2.5  |
| 1   | CA    | 71  | VAL  | 2.5  |
| 1   | AJ    | 131 | GLU  | 2.5  |
| 1   | CA    | 85  | GLU  | 2.5  |
| 1   | BI    | 26  | ASN  | 2.5  |
| 1   | AS    | 119 | ALA  | 2.5  |
| 1   | BG    | 39  | LYS  | 2.5  |
| 1   | CD    | 2   | ALA  | 2.5  |
| 1   | CQ    | 25  | LYS  | 2.5  |
| 1   | BW    | 54  | GLY  | 2.5  |
| 1   | DB    | 54  | GLY  | 2.5  |
| 1   | AG    | 55  | THR  | 2.5  |
| 1   | AN    | 87  | ALA  | 2.5  |
| 1   | CF    | 23  | ILE  | 2.5  |
| 1   | CU    | 23  | ILE  | 2.5  |
| 1   | BJ    | 58  | ASP  | 2.5  |
| 1   | CM    | 73  | THR  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BT    | 39  | LYS  | 2.4  |
| 1   | BW    | 39  | LYS  | 2.4  |
| 1   | DA    | 39  | LYS  | 2.4  |
| 1   | DE    | 25  | LYS  | 2.4  |
| 1   | CQ    | 26  | ASN  | 2.4  |
| 1   | CN    | 53  | PRO  | 2.4  |
| 1   | BB    | 42  | GLY  | 2.4  |
| 1   | DE    | 71  | VAL  | 2.4  |
| 1   | BT    | 30  | TYR  | 2.4  |
| 1   | BC    | 23  | ILE  | 2.4  |
| 1   | BA    | 26  | ASN  | 2.4  |
| 1   | BT    | 2   | ALA  | 2.4  |
| 1   | BT    | 101 | GLN  | 2.4  |
| 1   | BV    | 104 | ALA  | 2.4  |
| 1   | CN    | 67  | ASN  | 2.4  |
| 1   | CN    | 91  | ARG  | 2.4  |
| 1   | CZ    | 42  | GLY  | 2.4  |
| 1   | CS    | 102 | SER  | 2.4  |
| 1   | CJ    | 59  | VAL  | 2.4  |
| 1   | AO    | 23  | ILE  | 2.4  |
| 1   | AW    | 23  | ILE  | 2.4  |
| 1   | CJ    | 85  | GLU  | 2.4  |
| 1   | CD    | 103 | ALA  | 2.4  |
| 1   | CV    | 103 | ALA  | 2.4  |
| 1   | DB    | 119 | ALA  | 2.4  |
| 1   | AU    | 26  | ASN  | 2.4  |
| 1   | BQ    | 42  | GLY  | 2.4  |
| 1   | AQ    | 73  | THR  | 2.4  |
| 1   | AU    | 102 | SER  | 2.4  |
| 1   | BH    | 4   | LYS  | 2.4  |
| 1   | BZ    | 25  | LYS  | 2.4  |
| 1   | AL    | 59  | VAL  | 2.4  |
| 1   | AZ    | 58  | ASP  | 2.4  |
| 1   | AO    | 41  | ILE  | 2.4  |
| 1   | AL    | 30  | TYR  | 2.4  |
| 1   | CF    | 22  | GLN  | 2.4  |
| 1   | CR    | 119 | ALA  | 2.4  |
| 1   | AZ    | 55  | THR  | 2.4  |
| 1   | BX    | 73  | THR  | 2.4  |
| 1   | BV    | 23  | ILE  | 2.4  |
| 1   | CA    | 95  | GLU  | 2.4  |
| 1   | BF    | 103 | ALA  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CR    | 63  | LYS  | 2.4  |
| 1   | AJ    | 56  | ASN  | 2.4  |
| 1   | CX    | 42  | GLY  | 2.4  |
| 1   | DE    | 38  | GLY  | 2.4  |
| 1   | AB    | 73  | THR  | 2.4  |
| 1   | BR    | 55  | THR  | 2.4  |
| 1   | BZ    | 127 | ILE  | 2.4  |
| 1   | CM    | 71  | VAL  | 2.4  |
| 1   | CR    | 71  | VAL  | 2.4  |
| 1   | DI    | 105 | THR  | 2.4  |
| 1   | DJ    | 126 | THR  | 2.4  |
| 1   | BZ    | 58  | ASP  | 2.4  |
| 1   | CI    | 4   | LYS  | 2.4  |
| 1   | BX    | 132 | HIS  | 2.3  |
| 1   | AA    | 26  | ASN  | 2.3  |
| 1   | AP    | 56  | ASN  | 2.3  |
| 1   | BZ    | 38  | GLY  | 2.3  |
| 1   | CI    | 41  | ILE  | 2.3  |
| 1   | AW    | 73  | THR  | 2.3  |
| 1   | AY    | 55  | THR  | 2.3  |
| 1   | CH    | 39  | LYS  | 2.3  |
| 1   | AA    | 119 | ALA  | 2.3  |
| 1   | AK    | 72  | ALA  | 2.3  |
| 1   | BV    | 87  | ALA  | 2.3  |
| 1   | AJ    | 11  | HIS  | 2.3  |
| 1   | BK    | 41  | ILE  | 2.3  |
| 1   | DE    | 86  | ILE  | 2.3  |
| 1   | DH    | 86  | ILE  | 2.3  |
| 1   | DJ    | 26  | ASN  | 2.3  |
| 1   | AI    | 101 | GLN  | 2.3  |
| 1   | AQ    | 85  | GLU  | 2.3  |
| 1   | AZ    | 109 | ASP  | 2.3  |
| 1   | CA    | 131 | GLU  | 2.3  |
| 1   | CQ    | 109 | ASP  | 2.3  |
| 1   | DG    | 41  | ILE  | 2.3  |
| 1   | CL    | 38  | GLY  | 2.3  |
| 1   | DF    | 38  | GLY  | 2.3  |
| 1   | BU    | 55  | THR  | 2.3  |
| 1   | CY    | 55  | THR  | 2.3  |
| 1   | AV    | 25  | LYS  | 2.3  |
| 1   | DA    | 61  | ARG  | 2.3  |
| 1   | CS    | 119 | ALA  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AT    | 23  | ILE  | 2.3  |
| 1   | AT    | 96  | PHE  | 2.3  |
| 1   | AV    | 22  | GLN  | 2.3  |
| 1   | AV    | 65  | PHE  | 2.3  |
| 1   | CI    | 17  | ILE  | 2.3  |
| 1   | BQ    | 58  | ASP  | 2.3  |
| 1   | CP    | 58  | ASP  | 2.3  |
| 1   | AF    | 38  | GLY  | 2.3  |
| 1   | BD    | 38  | GLY  | 2.3  |
| 1   | CU    | 78  | GLY  | 2.3  |
| 1   | DD    | 42  | GLY  | 2.3  |
| 1   | BR    | 26  | ASN  | 2.3  |
| 1   | BT    | 56  | ASN  | 2.3  |
| 1   | CE    | 56  | ASN  | 2.3  |
| 1   | AG    | 39  | LYS  | 2.3  |
| 1   | BV    | 4   | LYS  | 2.3  |
| 1   | AZ    | 86  | ILE  | 2.3  |
| 1   | BF    | 86  | ILE  | 2.3  |
| 1   | AE    | 59  | VAL  | 2.3  |
| 1   | AJ    | 27  | GLY  | 2.3  |
| 1   | BK    | 42  | GLY  | 2.3  |
| 1   | CQ    | 38  | GLY  | 2.3  |
| 1   | CZ    | 38  | GLY  | 2.3  |
| 1   | DE    | 109 | ASP  | 2.3  |
| 1   | DH    | 24  | ASP  | 2.3  |
| 1   | BK    | 55  | THR  | 2.3  |
| 1   | CN    | 56  | ASN  | 2.3  |
| 1   | CY    | 26  | ASN  | 2.3  |
| 1   | AE    | 86  | ILE  | 2.3  |
| 1   | AH    | 23  | ILE  | 2.3  |
| 1   | AP    | 41  | ILE  | 2.3  |
| 1   | AG    | 2   | ALA  | 2.3  |
| 1   | CK    | 119 | ALA  | 2.3  |
| 1   | AX    | 22  | GLN  | 2.3  |
| 1   | DD    | 131 | GLU  | 2.3  |
| 1   | BG    | 40  | PRO  | 2.3  |
| 1   | CH    | 38  | GLY  | 2.3  |
| 1   | CY    | 54  | GLY  | 2.3  |
| 1   | CY    | 66  | VAL  | 2.3  |
| 1   | BP    | 58  | ASP  | 2.3  |
| 1   | CB    | 24  | ASP  | 2.3  |
| 1   | BP    | 56  | ASN  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BU    | 26  | ASN  | 2.2  |
| 1   | CY    | 73  | THR  | 2.2  |
| 1   | AY    | 119 | ALA  | 2.2  |
| 1   | CE    | 39  | LYS  | 2.2  |
| 1   | DL    | 39  | LYS  | 2.2  |
| 1   | DE    | 85  | GLU  | 2.2  |
| 1   | DI    | 52  | GLU  | 2.2  |
| 1   | AD    | 42  | GLY  | 2.2  |
| 1   | BG    | 27  | GLY  | 2.2  |
| 1   | BK    | 61  | ARG  | 2.2  |
| 1   | CJ    | 88  | ARG  | 2.2  |
| 1   | AQ    | 105 | THR  | 2.2  |
| 1   | CN    | 24  | ASP  | 2.2  |
| 1   | CN    | 109 | ASP  | 2.2  |
| 1   | BB    | 56  | ASN  | 2.2  |
| 1   | CM    | 56  | ASN  | 2.2  |
| 1   | DK    | 132 | HIS  | 2.2  |
| 1   | AD    | 65  | PHE  | 2.2  |
| 1   | DG    | 23  | ILE  | 2.2  |
| 1   | AL    | 95  | GLU  | 2.2  |
| 1   | BE    | 131 | GLU  | 2.2  |
| 1   | CV    | 85  | GLU  | 2.2  |
| 1   | AQ    | 55  | THR  | 2.2  |
| 1   | CS    | 55  | THR  | 2.2  |
| 1   | AS    | 41  | ILE  | 2.2  |
| 1   | BP    | 109 | ASP  | 2.2  |
| 1   | BU    | 86  | ILE  | 2.2  |
| 1   | BV    | 24  | ASP  | 2.2  |
| 1   | CD    | 23  | ILE  | 2.2  |
| 1   | AD    | 25  | LYS  | 2.2  |
| 1   | CO    | 63  | LYS  | 2.2  |
| 1   | DC    | 4   | LYS  | 2.2  |
| 1   | AY    | 22  | GLN  | 2.2  |
| 1   | BS    | 22  | GLN  | 2.2  |
| 1   | DF    | 48  | SER  | 2.2  |
| 1   | AS    | 61  | ARG  | 2.2  |
| 1   | AV    | 106 | VAL  | 2.2  |
| 1   | CA    | 69  | PRO  | 2.2  |
| 1   | AE    | 73  | THR  | 2.2  |
| 1   | CW    | 133 | PHE  | 2.2  |
| 1   | AN    | 56  | ASN  | 2.2  |
| 1   | CW    | 58  | ASP  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CX    | 56  | ASN  | 2.2  |
| 1   | AK    | 63  | LYS  | 2.2  |
| 1   | BO    | 49  | HIS  | 2.2  |
| 1   | BM    | 119 | ALA  | 2.2  |
| 1   | AV    | 131 | GLU  | 2.2  |
| 1   | AX    | 57  | GLY  | 2.2  |
| 1   | CN    | 38  | GLY  | 2.2  |
| 1   | CO    | 42  | GLY  | 2.2  |
| 1   | CT    | 40  | PRO  | 2.2  |
| 1   | CZ    | 54  | GLY  | 2.2  |
| 1   | DA    | 60  | PHE  | 2.2  |
| 1   | BT    | 4   | LYS  | 2.2  |
| 1   | AM    | 11  | HIS  | 2.2  |
| 1   | BO    | 24  | ASP  | 2.2  |
| 1   | BS    | 80  | ASP  | 2.2  |
| 1   | CK    | 2   | ALA  | 2.2  |
| 1   | CD    | 32  | ARG  | 2.2  |
| 1   | BU    | 44  | TYR  | 2.2  |
| 1   | BV    | 59  | VAL  | 2.2  |
| 1   | BI    | 27  | GLY  | 2.2  |
| 1   | AB    | 133 | PHE  | 2.2  |
| 1   | AI    | 31  | PHE  | 2.2  |
| 1   | AC    | 39  | LYS  | 2.2  |
| 1   | AF    | 25  | LYS  | 2.2  |
| 1   | CZ    | 39  | LYS  | 2.2  |
| 1   | DC    | 39  | LYS  | 2.2  |
| 1   | AB    | 32  | ARG  | 2.1  |
| 1   | AH    | 120 | ASP  | 2.1  |
| 1   | CI    | 132 | HIS  | 2.1  |
| 1   | AT    | 62  | VAL  | 2.1  |
| 1   | AZ    | 23  | ILE  | 2.1  |
| 1   | CO    | 41  | ILE  | 2.1  |
| 1   | DL    | 41  | ILE  | 2.1  |
| 1   | BR    | 39  | LYS  | 2.1  |
| 1   | DA    | 57  | GLY  | 2.1  |
| 1   | CA    | 70  | GLU  | 2.1  |
| 1   | CH    | 70  | GLU  | 2.1  |
| 1   | DJ    | 4   | LYS  | 2.1  |
| 1   | CN    | 90  | ASN  | 2.1  |
| 1   | DA    | 26  | ASN  | 2.1  |
| 1   | DE    | 72  | ALA  | 2.1  |
| 1   | AX    | 23  | ILE  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BU    | 23  | ILE  | 2.1  |
| 1   | CP    | 86  | ILE  | 2.1  |
| 1   | DF    | 68  | VAL  | 2.1  |
| 1   | AR    | 39  | LYS  | 2.1  |
| 1   | AZ    | 4   | LYS  | 2.1  |
| 1   | BH    | 25  | LYS  | 2.1  |
| 1   | CU    | 39  | LYS  | 2.1  |
| 1   | AU    | 70  | GLU  | 2.1  |
| 1   | BO    | 85  | GLU  | 2.1  |
| 1   | BX    | 85  | GLU  | 2.1  |
| 1   | CJ    | 131 | GLU  | 2.1  |
| 1   | CZ    | 75  | THR  | 2.1  |
| 1   | AD    | 37  | ASN  | 2.1  |
| 1   | AJ    | 26  | ASN  | 2.1  |
| 1   | CP    | 26  | ASN  | 2.1  |
| 1   | DA    | 37  | ASN  | 2.1  |
| 1   | AI    | 39  | LYS  | 2.1  |
| 1   | CK    | 71  | VAL  | 2.1  |
| 1   | CL    | 11  | HIS  | 2.1  |
| 1   | DE    | 49  | HIS  | 2.1  |
| 1   | DF    | 25  | LYS  | 2.1  |
| 1   | BH    | 27  | GLY  | 2.1  |
| 1   | BH    | 131 | GLU  | 2.1  |
| 1   | AM    | 55  | THR  | 2.1  |
| 1   | BI    | 73  | THR  | 2.1  |
| 1   | AC    | 41  | ILE  | 2.1  |
| 1   | AY    | 26  | ASN  | 2.1  |
| 1   | BC    | 56  | ASN  | 2.1  |
| 1   | BW    | 37  | ASN  | 2.1  |
| 1   | CJ    | 23  | ILE  | 2.1  |
| 1   | CW    | 37  | ASN  | 2.1  |
| 1   | CY    | 86  | ILE  | 2.1  |
| 1   | DE    | 56  | ASN  | 2.1  |
| 1   | AD    | 39  | LYS  | 2.1  |
| 1   | AU    | 39  | LYS  | 2.1  |
| 1   | CB    | 39  | LYS  | 2.1  |
| 1   | DG    | 25  | LYS  | 2.1  |
| 1   | AQ    | 71  | VAL  | 2.1  |
| 1   | BG    | 49  | HIS  | 2.1  |
| 1   | CQ    | 11  | HIS  | 2.1  |
| 1   | CY    | 30  | TYR  | 2.1  |
| 1   | DK    | 44  | TYR  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AC    | 95  | GLU  | 2.1  |
| 1   | BH    | 41  | ILE  | 2.1  |
| 1   | BK    | 2   | ALA  | 2.1  |
| 1   | CX    | 41  | ILE  | 2.1  |
| 1   | BL    | 47  | SER  | 2.1  |
| 1   | CH    | 12  | SER  | 2.1  |
| 1   | CF    | 31  | PHE  | 2.1  |
| 1   | CT    | 96  | PHE  | 2.1  |
| 1   | DA    | 93  | GLN  | 2.1  |
| 1   | BW    | 24  | ASP  | 2.1  |
| 1   | CJ    | 58  | ASP  | 2.1  |
| 1   | CK    | 54  | GLY  | 2.1  |
| 1   | CI    | 131 | GLU  | 2.1  |
| 1   | AX    | 41  | ILE  | 2.1  |
| 1   | AJ    | 119 | ALA  | 2.1  |
| 1   | BV    | 106 | VAL  | 2.1  |
| 1   | CM    | 26  | ASN  | 2.1  |
| 1   | CO    | 101 | GLN  | 2.1  |
| 1   | BH    | 106 | VAL  | 2.1  |
| 1   | BK    | 62  | VAL  | 2.1  |
| 1   | CU    | 67  | ASN  | 2.1  |
| 1   | AS    | 54  | GLY  | 2.0  |
| 1   | BF    | 69  | PRO  | 2.0  |
| 1   | AF    | 58  | ASP  | 2.0  |
| 1   | CB    | 58  | ASP  | 2.0  |
| 1   | CN    | 58  | ASP  | 2.0  |
| 1   | DJ    | 58  | ASP  | 2.0  |
| 1   | AQ    | 51  | LYS  | 2.0  |
| 1   | CE    | 95  | GLU  | 2.0  |
| 1   | DB    | 25  | LYS  | 2.0  |
| 1   | AB    | 117 | ALA  | 2.0  |
| 1   | CJ    | 119 | ALA  | 2.0  |
| 1   | DB    | 65  | PHE  | 2.0  |
| 1   | AD    | 84  | VAL  | 2.0  |
| 1   | AI    | 59  | VAL  | 2.0  |
| 1   | AV    | 59  | VAL  | 2.0  |
| 1   | AQ    | 56  | ASN  | 2.0  |
| 1   | BH    | 56  | ASN  | 2.0  |
| 1   | CO    | 56  | ASN  | 2.0  |
| 1   | CU    | 129 | ASN  | 2.0  |
| 1   | AC    | 30  | TYR  | 2.0  |
| 1   | BR    | 40  | PRO  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AU    | 41  | ILE  | 2.0  |
| 1   | BY    | 105 | THR  | 2.0  |
| 1   | CI    | 23  | ILE  | 2.0  |
| 1   | CY    | 4   | LYS  | 2.0  |
| 1   | BP    | 81  | THR  | 2.0  |
| 1   | CP    | 73  | THR  | 2.0  |
| 1   | DK    | 17  | ILE  | 2.0  |
| 1   | AC    | 109 | ASP  | 2.0  |
| 1   | AI    | 24  | ASP  | 2.0  |
| 1   | BI    | 24  | ASP  | 2.0  |
| 1   | BK    | 131 | GLU  | 2.0  |
| 1   | BS    | 52  | GLU  | 2.0  |
| 1   | CC    | 95  | GLU  | 2.0  |
| 1   | CF    | 24  | ASP  | 2.0  |
| 1   | CN    | 52  | GLU  | 2.0  |
| 1   | AL    | 119 | ALA  | 2.0  |
| 1   | BP    | 22  | GLN  | 2.0  |
| 1   | AP    | 77  | ASN  | 2.0  |
| 1   | BK    | 63  | LYS  | 2.0  |
| 1   | BV    | 38  | GLY  | 2.0  |
| 1   | BA    | 41  | ILE  | 2.0  |
| 1   | CV    | 105 | THR  | 2.0  |
| 1   | CY    | 7   | THR  | 2.0  |
| 1   | CS    | 131 | GLU  | 2.0  |
| 1   | BG    | 24  | ASP  | 2.0  |
| 1   | CJ    | 87  | ALA  | 2.0  |
| 1   | BL    | 128 | VAL  | 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | CA   | AA    | 201 | 1/1   | 0.60 | 0.14 | 64,64,64,64                | 0     |
| 2   | CA   | CV    | 201 | 1/1   | 0.74 | 0.10 | 64,64,64,64                | 0     |
| 2   | CA   | BH    | 201 | 1/1   | 0.83 | 0.09 | 64,64,64,64                | 0     |
| 2   | CA   | BX    | 201 | 1/1   | 0.84 | 0.09 | 64,64,64,64                | 0     |
| 2   | CA   | AZ    | 201 | 1/1   | 0.86 | 0.09 | 64,64,64,64                | 0     |
| 2   | CA   | BB    | 201 | 1/1   | 0.87 | 0.08 | 64,64,64,64                | 0     |
| 2   | CA   | CS    | 201 | 1/1   | 0.88 | 0.07 | 64,64,64,64                | 0     |
| 2   | CA   | AE    | 201 | 1/1   | 0.88 | 0.08 | 64,64,64,64                | 0     |
| 2   | CA   | BT    | 201 | 1/1   | 0.90 | 0.11 | 64,64,64,64                | 0     |
| 2   | CA   | BI    | 201 | 1/1   | 0.90 | 0.10 | 64,64,64,64                | 0     |
| 2   | CA   | BL    | 201 | 1/1   | 0.91 | 0.10 | 64,64,64,64                | 0     |
| 2   | CA   | AB    | 201 | 1/1   | 0.91 | 0.08 | 64,64,64,64                | 0     |
| 2   | CA   | AF    | 201 | 1/1   | 0.91 | 0.07 | 64,64,64,64                | 0     |
| 2   | CA   | CD    | 201 | 1/1   | 0.91 | 0.08 | 64,64,64,64                | 0     |
| 2   | CA   | AH    | 201 | 1/1   | 0.91 | 0.09 | 64,64,64,64                | 0     |
| 2   | CA   | AK    | 201 | 1/1   | 0.91 | 0.08 | 64,64,64,64                | 0     |
| 2   | CA   | CF    | 201 | 1/1   | 0.92 | 0.06 | 64,64,64,64                | 0     |
| 2   | CA   | AG    | 201 | 1/1   | 0.92 | 0.09 | 64,64,64,64                | 0     |
| 2   | CA   | BC    | 201 | 1/1   | 0.92 | 0.06 | 64,64,64,64                | 0     |
| 2   | CA   | BR    | 201 | 1/1   | 0.93 | 0.10 | 64,64,64,64                | 0     |
| 2   | CA   | CC    | 201 | 1/1   | 0.93 | 0.09 | 64,64,64,64                | 0     |
| 2   | CA   | AN    | 201 | 1/1   | 0.93 | 0.12 | 64,64,64,64                | 0     |
| 2   | CA   | AW    | 201 | 1/1   | 0.94 | 0.08 | 64,64,64,64                | 0     |
| 2   | CA   | CJ    | 201 | 1/1   | 0.94 | 0.05 | 64,64,64,64                | 0     |
| 2   | CA   | AM    | 201 | 1/1   | 0.96 | 0.05 | 64,64,64,64                | 0     |
| 2   | CA   | CA    | 201 | 1/1   | 0.96 | 0.13 | 64,64,64,64                | 0     |
| 2   | CA   | AC    | 201 | 1/1   | 0.96 | 0.05 | 64,64,64,64                | 0     |
| 2   | CA   | AQ    | 201 | 1/1   | 0.96 | 0.04 | 64,64,64,64                | 0     |
| 2   | CA   | BF    | 201 | 1/1   | 0.97 | 0.15 | 64,64,64,64                | 0     |
| 2   | CA   | BK    | 201 | 1/1   | 0.98 | 0.09 | 64,64,64,64                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.