



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:34 AM UTC

PDB ID : 4RFT / pdb\_00004rft  
Title : T=1 subviral particle of Grouper nervous necrosis virus capsid protein deletion mutant (delta 1-34 & 218-338)  
Authors : Chen, N.C.; Chen, C.J.; Yoshimura, M.; Guan, H.H.; Chen, T.Y.  
Deposited on : 2014-09-27  
Resolution : 3.10 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                                                             |

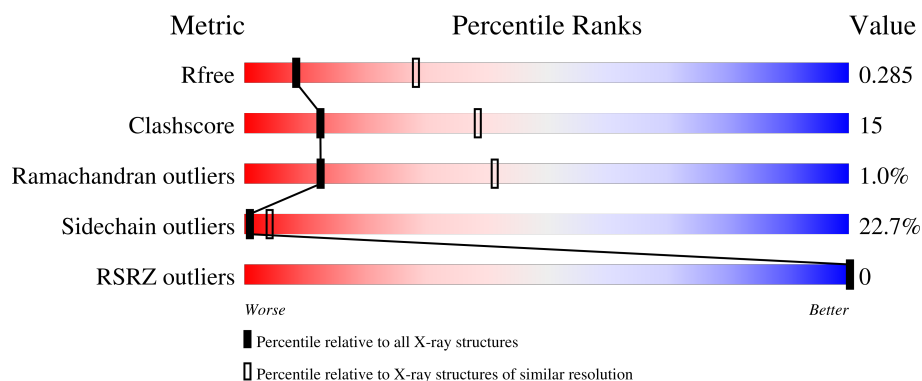
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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   | 0     | 183    |                  |
| 1   | 1     | 183    |                  |
| 1   | 2     | 183    |                  |
| 1   | 3     | 183    |                  |
| 1   | 4     | 183    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 5     | 183    |                  |
| 1   | 6     | 183    |                  |
| 1   | 7     | 183    |                  |
| 1   | 8     | 183    |                  |
| 1   | 9     | 183    |                  |
| 1   | A     | 183    |                  |
| 1   | B     | 183    |                  |
| 1   | C     | 183    |                  |
| 1   | D     | 183    |                  |
| 1   | E     | 183    |                  |
| 1   | F     | 183    |                  |
| 1   | G     | 183    |                  |
| 1   | H     | 183    |                  |
| 1   | I     | 183    |                  |
| 1   | J     | 183    |                  |
| 1   | K     | 183    |                  |
| 1   | L     | 183    |                  |
| 1   | M     | 183    |                  |
| 1   | N     | 183    |                  |
| 1   | O     | 183    |                  |
| 1   | P     | 183    |                  |
| 1   | Q     | 183    |                  |
| 1   | R     | 183    |                  |
| 1   | S     | 183    |                  |
| 1   | T     | 183    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | U     | 183    |                  |
| 1   | V     | 183    |                  |
| 1   | W     | 183    |                  |
| 1   | X     | 183    |                  |
| 1   | Y     | 183    |                  |
| 1   | Z     | 183    |                  |
| 1   | a     | 183    |                  |
| 1   | b     | 183    |                  |
| 1   | c     | 183    |                  |
| 1   | d     | 183    |                  |
| 1   | e     | 183    |                  |
| 1   | f     | 183    |                  |
| 1   | g     | 183    |                  |
| 1   | h     | 183    |                  |
| 1   | i     | 183    |                  |
| 1   | j     | 183    |                  |
| 1   | k     | 183    |                  |
| 1   | l     | 183    |                  |
| 1   | m     | 183    |                  |
| 1   | n     | 183    |                  |
| 1   | o     | 183    |                  |
| 1   | p     | 183    |                  |
| 1   | q     | 183    |                  |
| 1   | r     | 183    |                  |
| 1   | s     | 183    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | t     | 183    |  |
| 1   | u     | 183    |  |
| 1   | v     | 183    |  |
| 1   | w     | 183    |  |
| 1   | x     | 183    |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 75180 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   | A     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | B     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | C     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | D     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | E     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | F     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | G     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | H     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | I     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | J     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | K     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | L     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | M     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | N     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | O     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | P     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | Q     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | R     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | S     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | T     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | U     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | V     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | W     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | X     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | Y     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | Z     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 0     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 1     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 2     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 3     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 4     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 5     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 6     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 7     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 8     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | 9     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | a     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | b     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | c     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | d     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | e     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | f     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | g     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | h     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | i     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | j     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | k     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | l     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | m     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | n     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | o     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | p     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | q     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | r     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | s     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | t     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | u     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | v     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | w     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |
| 1   | x     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1253  | 788 | 224 | 236 | 5 |         |         |       |

There are 60 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| B     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| C     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| D     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| E     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| F     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| G     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| H     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| I     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| J     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| K     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| L     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| M     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| N     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| O     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| P     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| Q     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| R     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| S     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| T     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| U     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| V     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| W     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| X     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| Y     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| Z     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 0     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 1     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 2     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 3     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 4     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 5     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 6     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 7     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |

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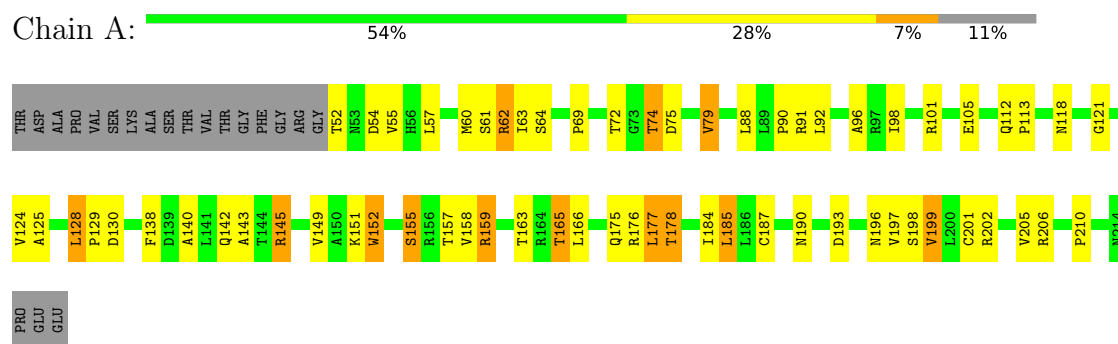
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 8     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| 9     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| a     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| b     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| c     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| d     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| e     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| f     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| g     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| h     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| i     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| j     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| k     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| l     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| m     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| n     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| o     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| p     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| q     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| r     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| s     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| t     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| u     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| v     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| w     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |
| x     | 214     | ASN      | THR    | SEE REMARK 999 | UNP Q8JNX5 |

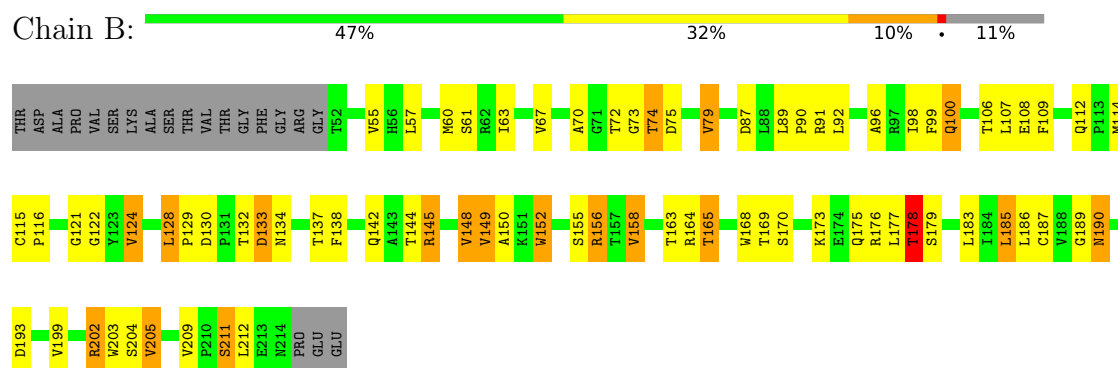
### 3 Residue-property plots

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

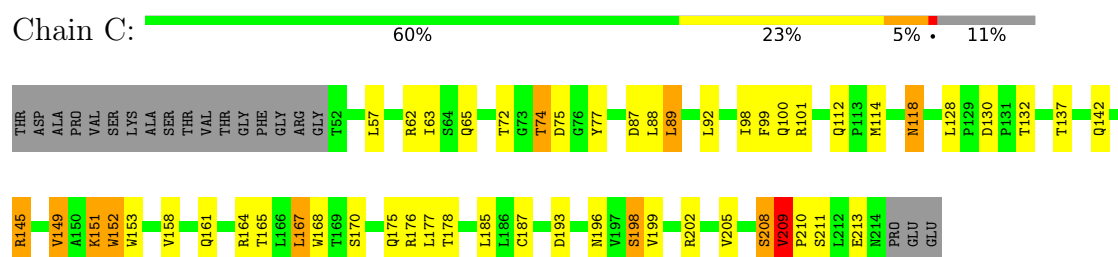
#### • Molecule 1: Coat protein



#### • Molecule 1: Coat protein

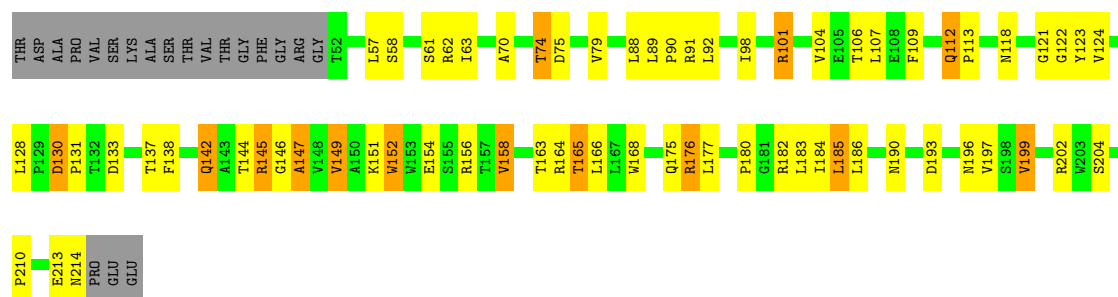


#### • Molecule 1: Coat protein



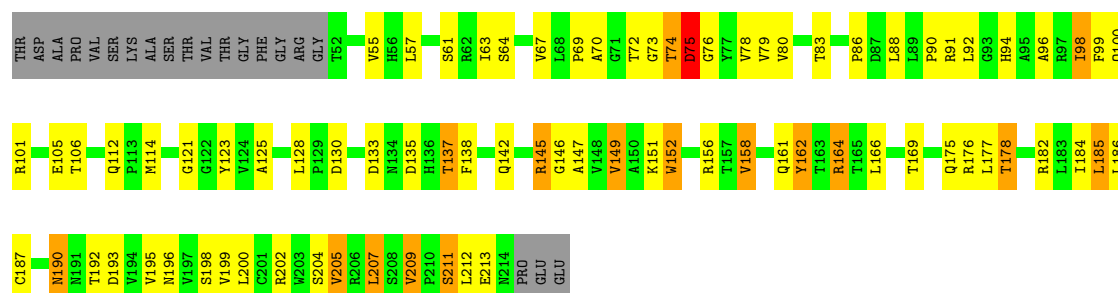
#### • Molecule 1: Coat protein

Chain D: 



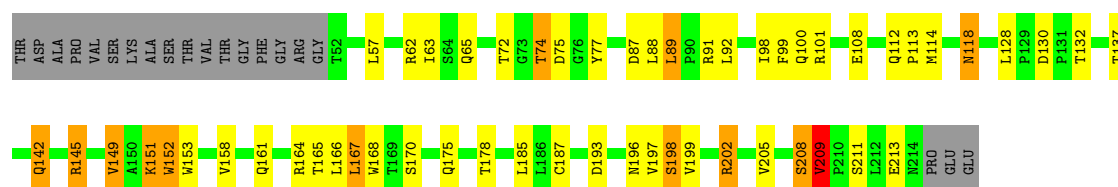
• Molecule 1: Coat protein

Chain E: 



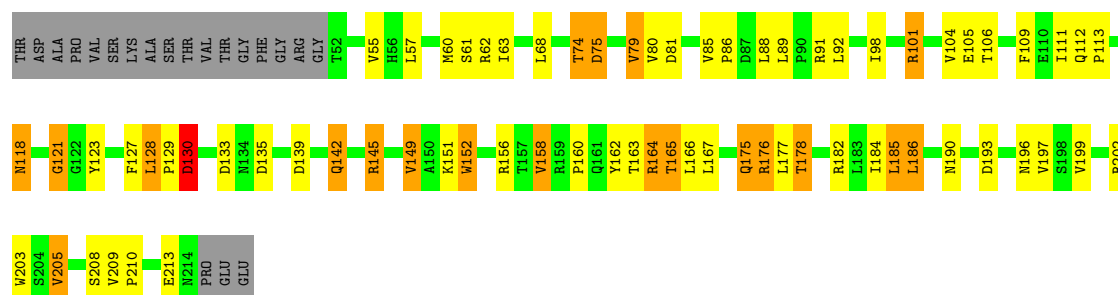
• Molecule 1: Coat protein

Chain F: 

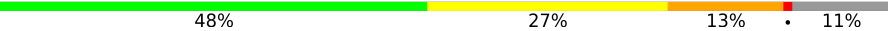


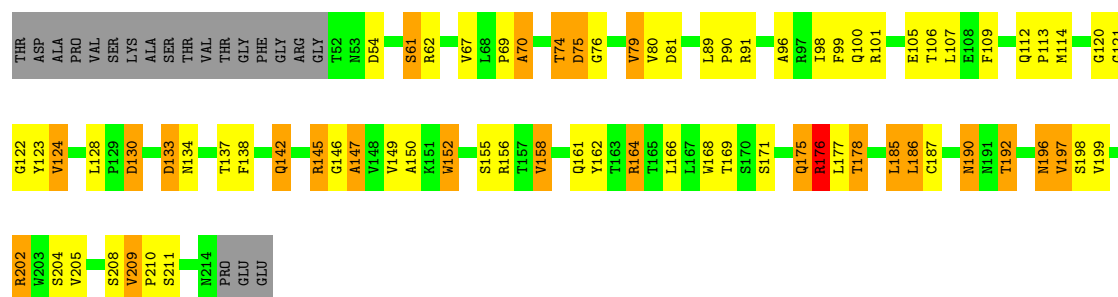
• Molecule 1: Coat protein

Chain G: 



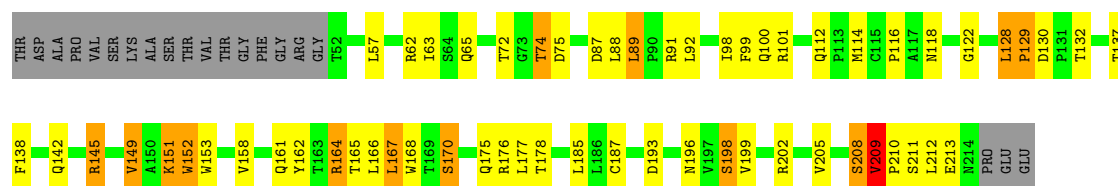
• Molecule 1: Coat protein

Chain H: 



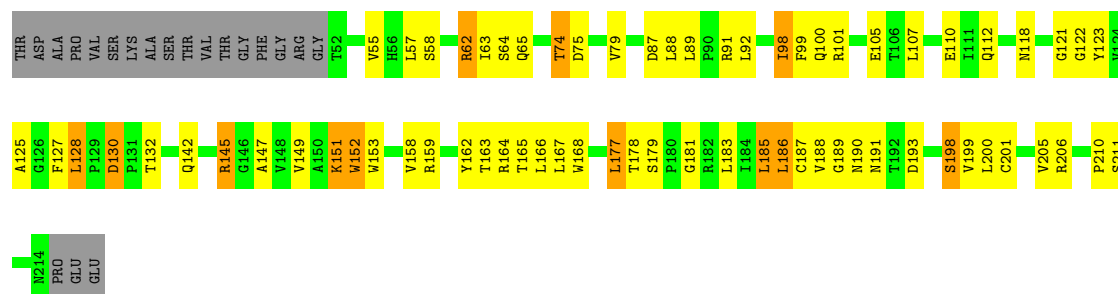
• Molecule 1: Coat protein

Chain I: 



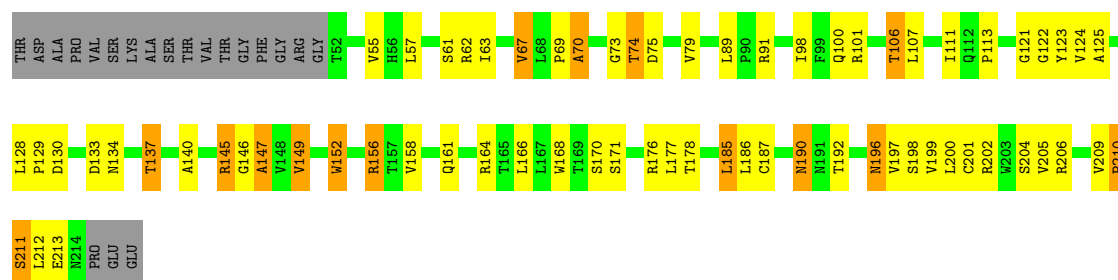
• Molecule 1: Coat protein

Chain J: 



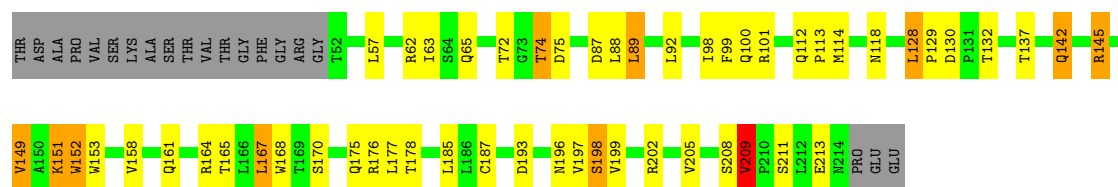
• Molecule 1: Coat protein

Chain K: 



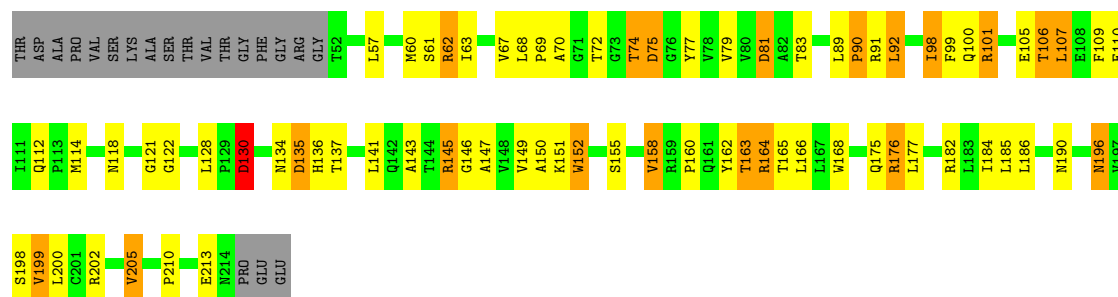
• Molecule 1: Coat protein

Chain L: 



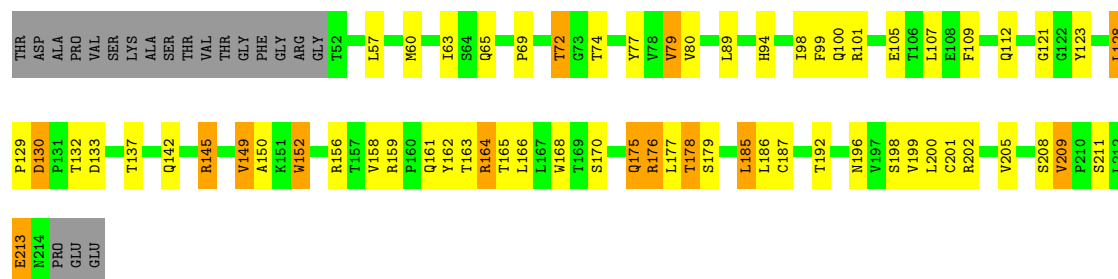
• Molecule 1: Coat protein

Chain M: 



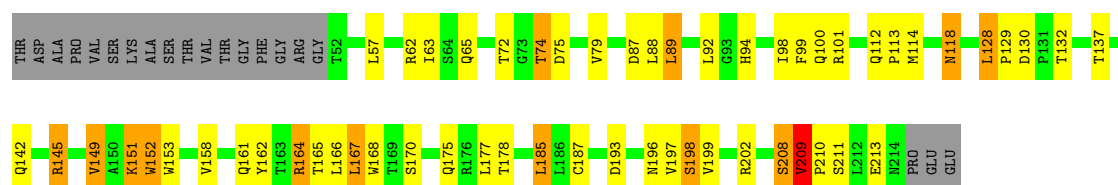
• Molecule 1: Coat protein

Chain N: 



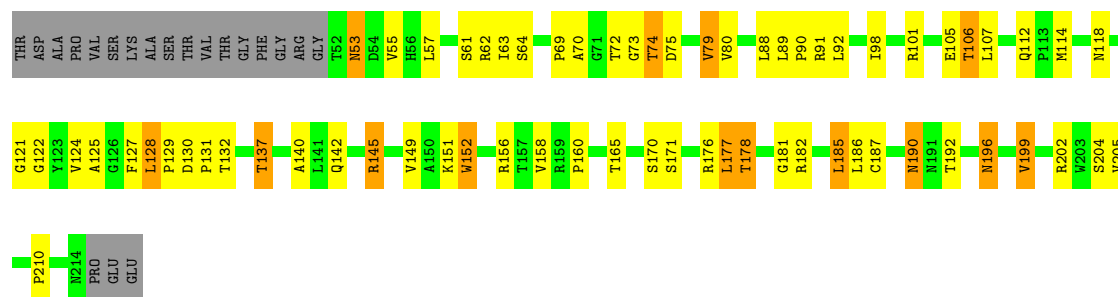
• Molecule 1: Coat protein

Chain O: 



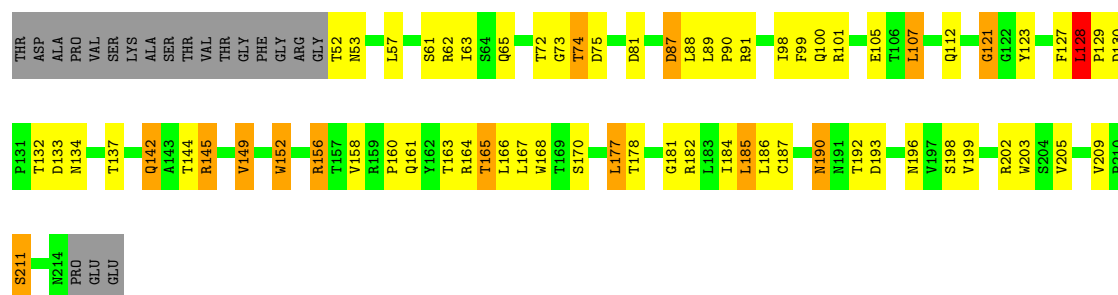
• Molecule 1: Coat protein

Chain P: 



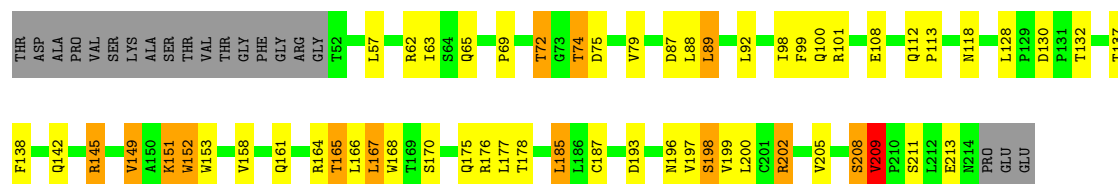
- Molecule 1: Coat protein

Chain Q: 51% 30% 8% 11%



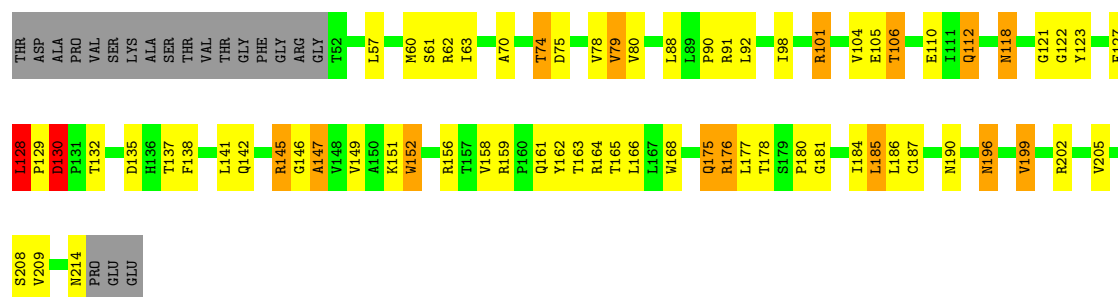
- Molecule 1: Coat protein

Chain R: 57% 24% 7% 11%



- Molecule 1: Coat protein

Chain S: 51% 30% 8% 11%

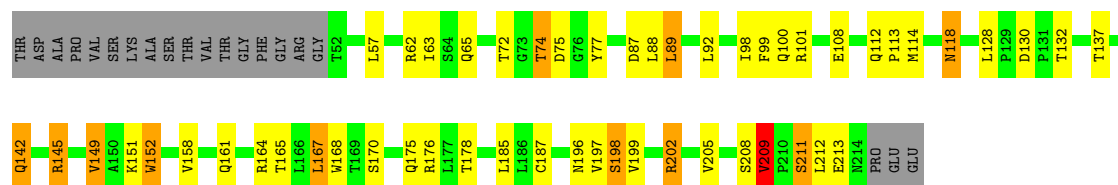


- Molecule 1: Coat protein

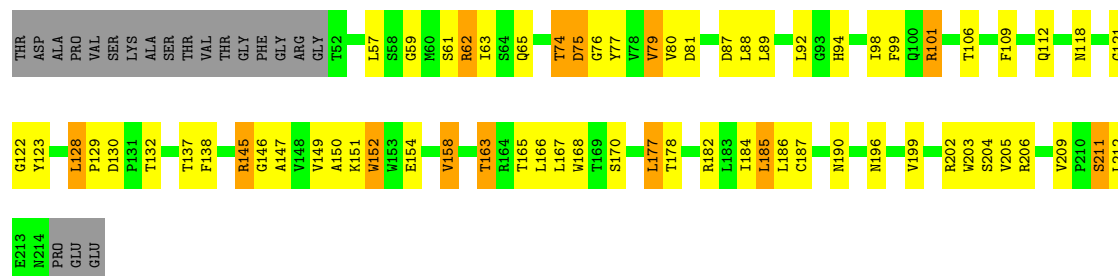
Chain T: 48% 32% 9% 11%



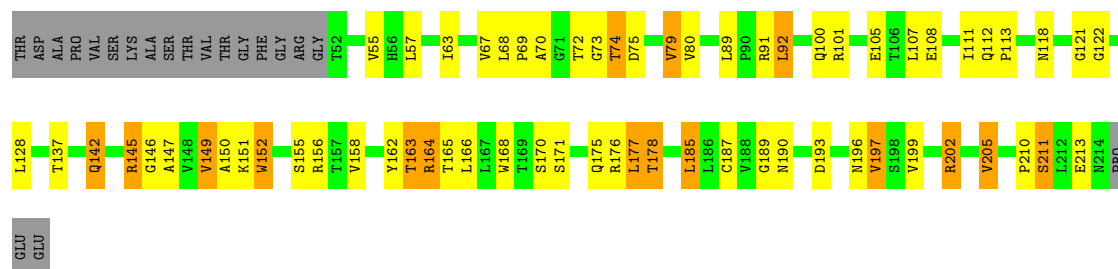
• Molecule 1: Coat protein



• Molecule 1: Coat protein

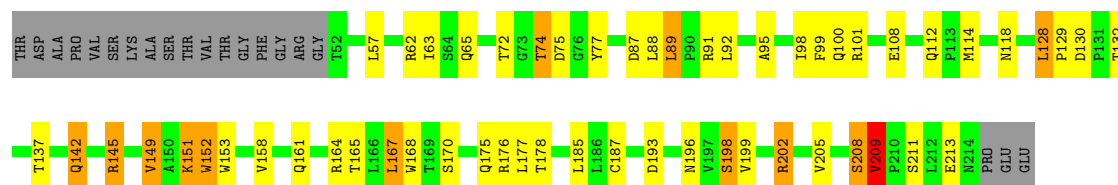


• Molecule 1: Coat protein



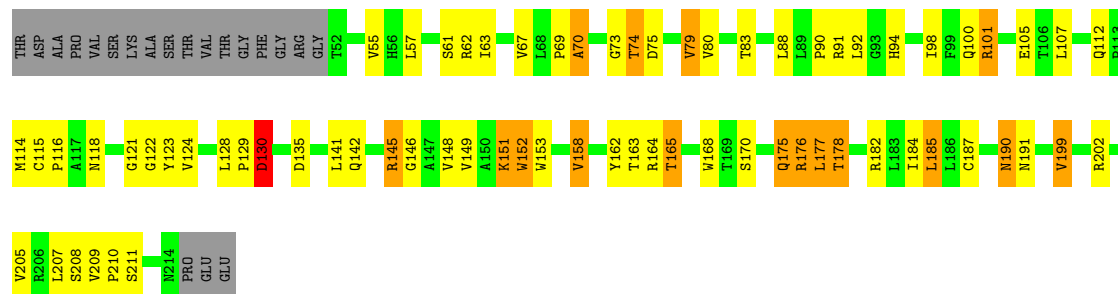
• Molecule 1: Coat protein





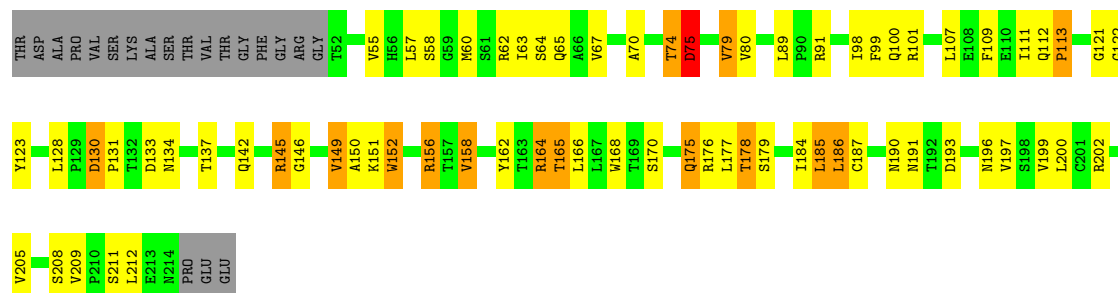
### • Molecule 1: Coat protein

Chain Y: 50% 30% 9% 11%



### • Molecule 1: Coat protein

Chain Z: 50% 30% 8% 11%



### • Molecule 1: Coat protein

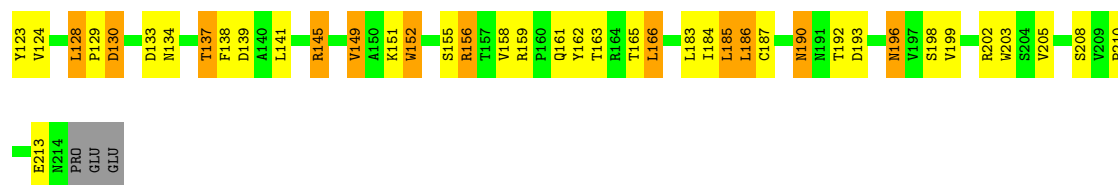
Chain 0: 59% 23% 7% 11%



### • Molecule 1: Coat protein

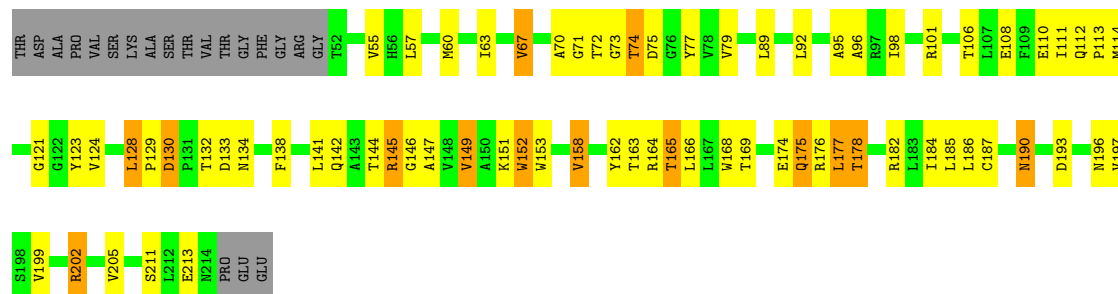
Chain 1: 51% 28% 9% 11%





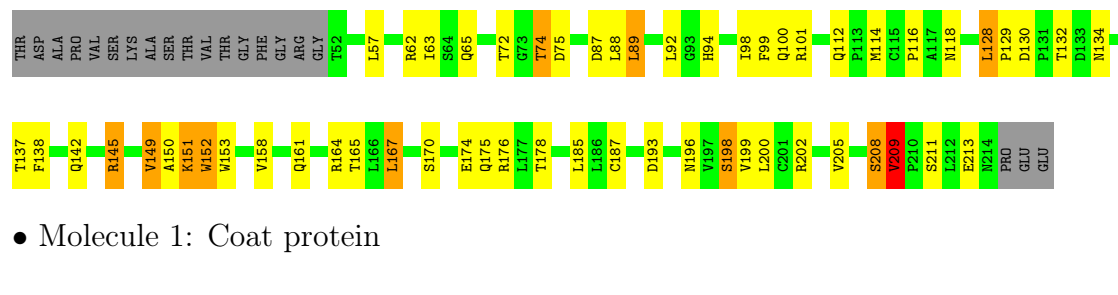
- Molecule 1: Coat protein

Chain 2: 49% 32% 8% 11%



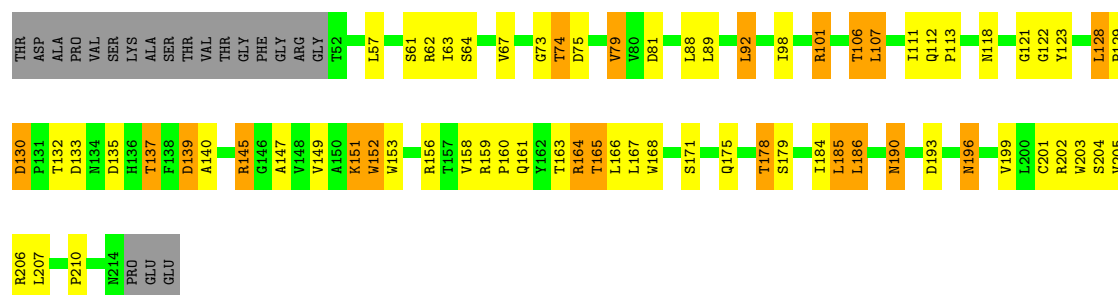
- Molecule 1: Coat protein

Chain 3: 58% 25% 5% 11%



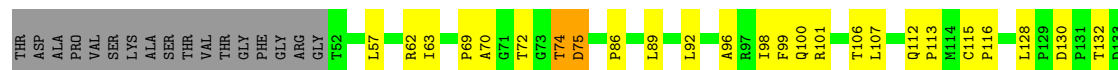
- Molecule 1: Coat protein

Chain 4: 51% 27% 11% 11%



- Molecule 1: Coat protein

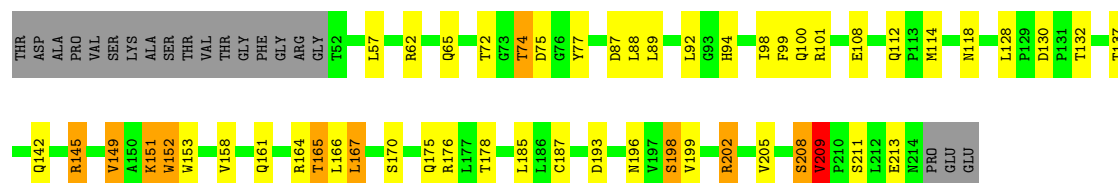
Chain 5: 55% 28% 6% 11%





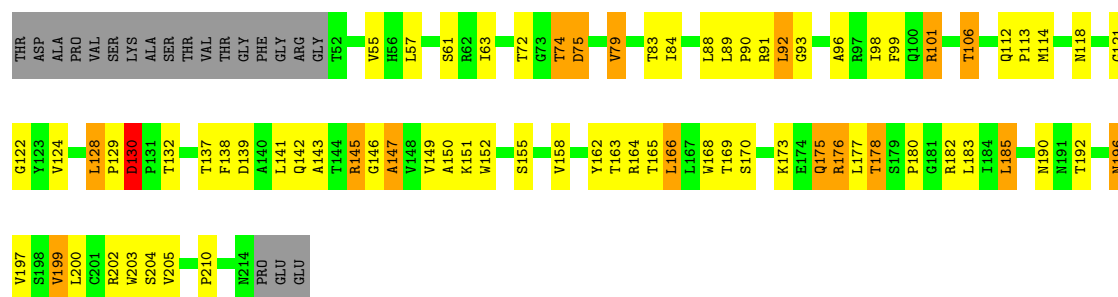
• Molecule 1: Coat protein

Chain 6: 61% 22% 5% • 11%



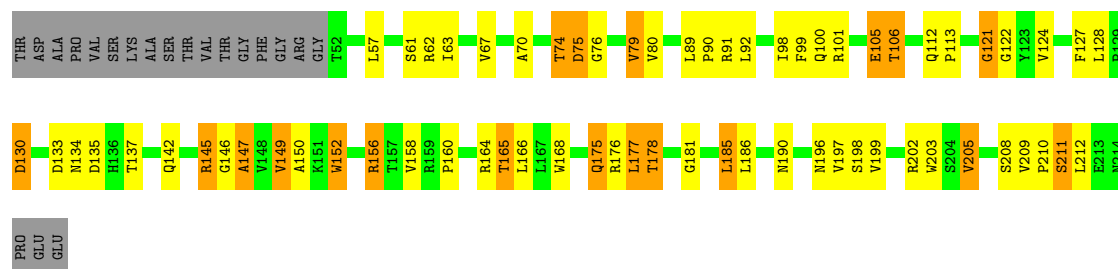
• Molecule 1: Coat protein

Chain 7: 48% 32% 9% • 11%



• Molecule 1: Coat protein

Chain 8: 52% 26% 10% 11%



• Molecule 1: Coat protein

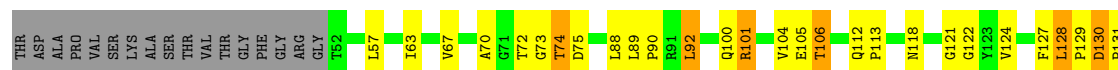
Chain 9: 56% 26% 7% • 11%





- Molecule 1: Coat protein

Chain a: 53% 26% 10% 11%



GLU

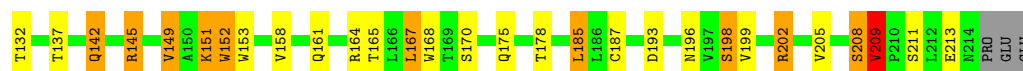
- Molecule 1: Coat protein

Chain b: 48% 33% 9% 11%



- Molecule 1: Coat protein

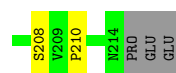
Chain c: 60% 21% 7% 11%



- Molecule 1: Coat protein

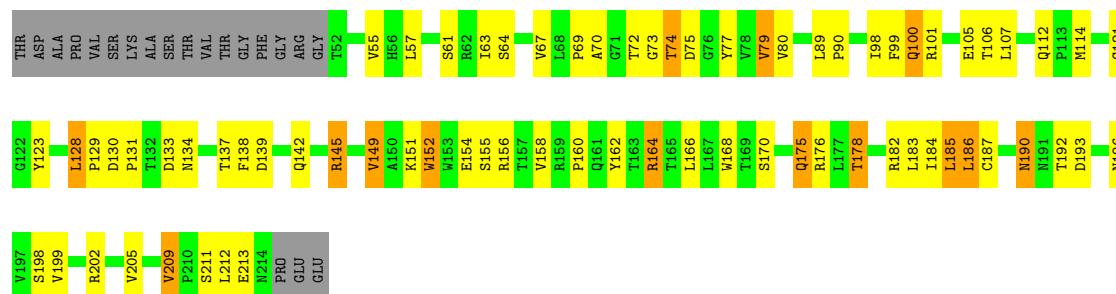
Chain d: 52% 30% 7% 11%





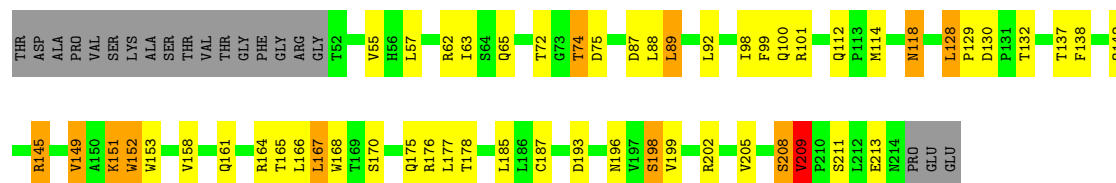
• Molecule 1: Coat protein

Chain e: 49% 32% 8% 11%



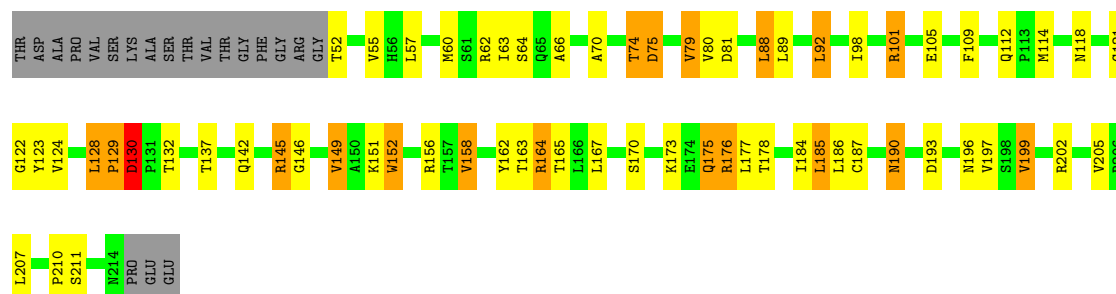
• Molecule 1: Coat protein

Chain f: 59% 23% 6% 11%



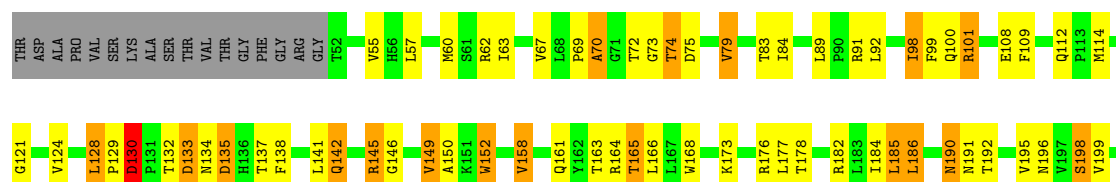
• Molecule 1: Coat protein

Chain g: 53% 26% 10% 11%



• Molecule 1: Coat protein

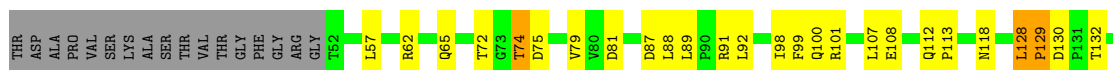
Chain h: 49% 28% 11% 11%





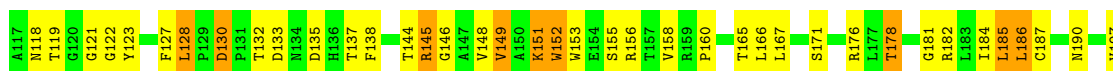
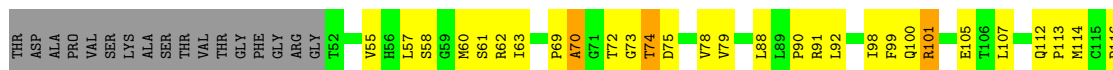
• Molecule 1: Coat protein

Chain i: 56% 26% 7% 11%



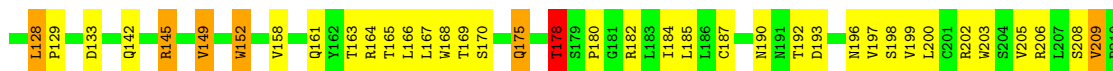
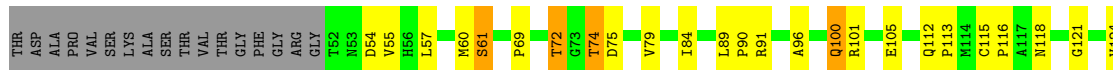
• Molecule 1: Coat protein

Chain j: 49% 32% 8% 11%



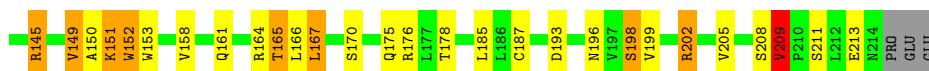
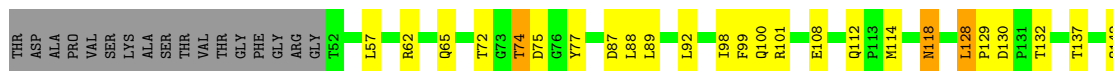
• Molecule 1: Coat protein

Chain k: 54% 30% 5% 11%



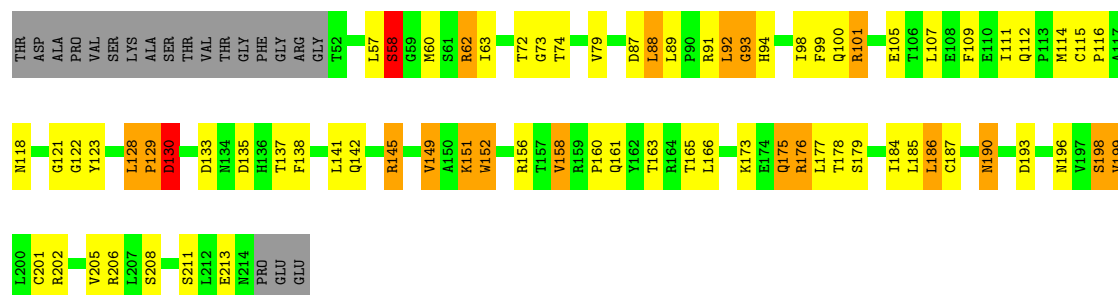
• Molecule 1: Coat protein

Chain l: 60% 22% 6% 11%



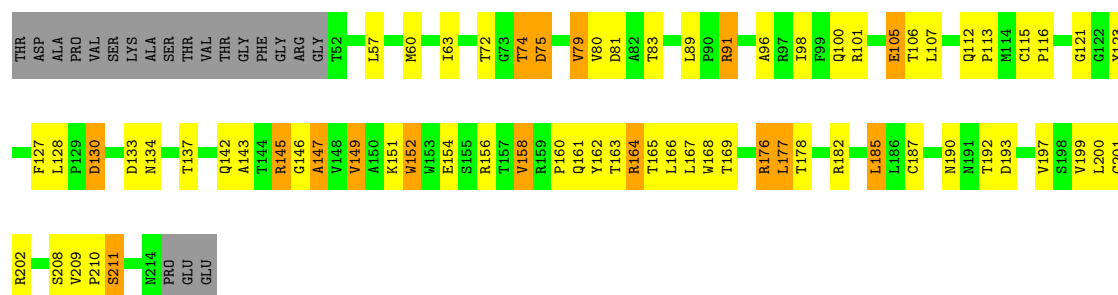
- Molecule 1: Coat protein

Chain m:  49% 30% 10% 11%



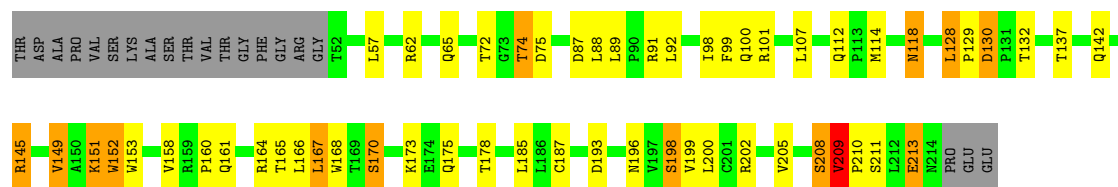
- Molecule 1: Coat protein

Chain n:  51% 30% 9% 11%



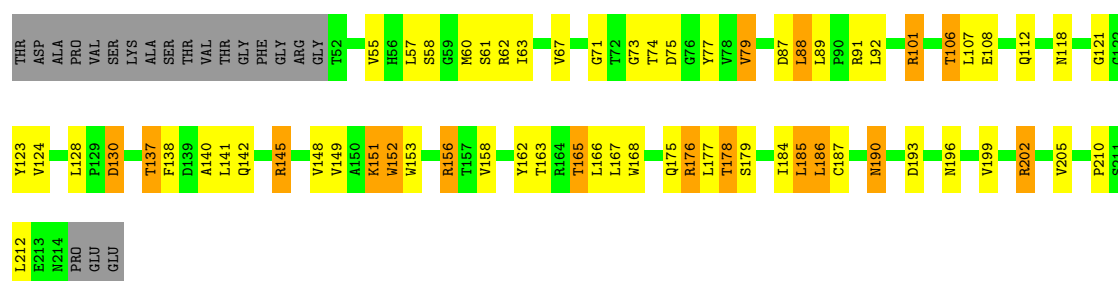
- Molecule 1: Coat protein

Chain o:  58% 23% 7% 11%



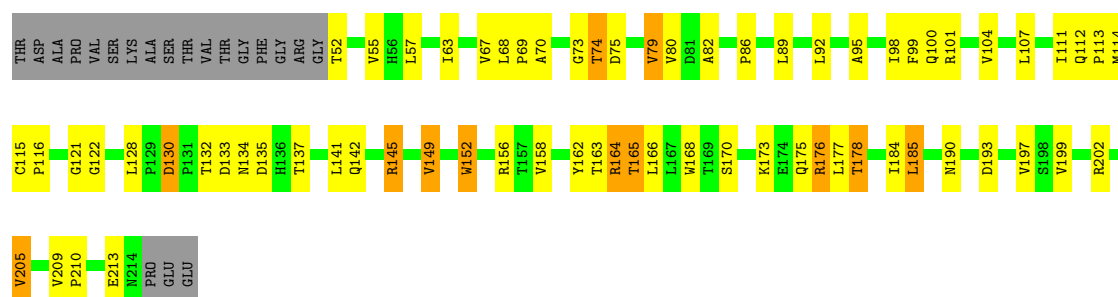
- Molecule 1: Coat protein

Chain p:  53% 27% 9% 11%



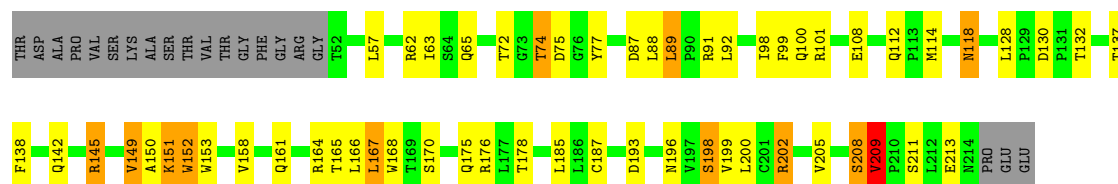
- Molecule 1: Coat protein

Chain q:  51% 31% 7% 11%



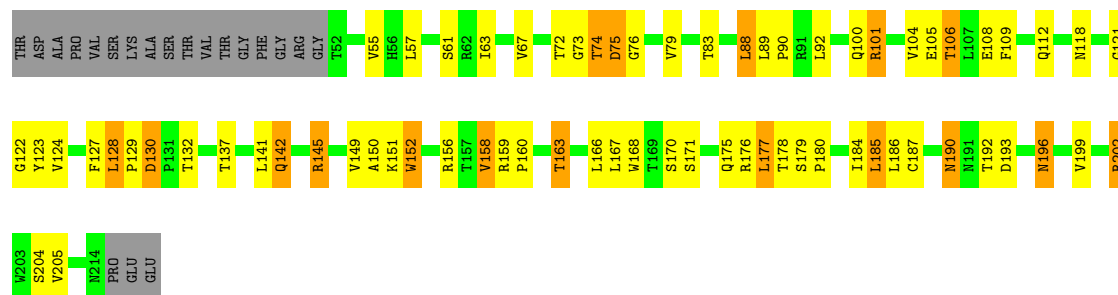
- Molecule 1: Coat protein

Chain r:  58% 25% 6% 11%



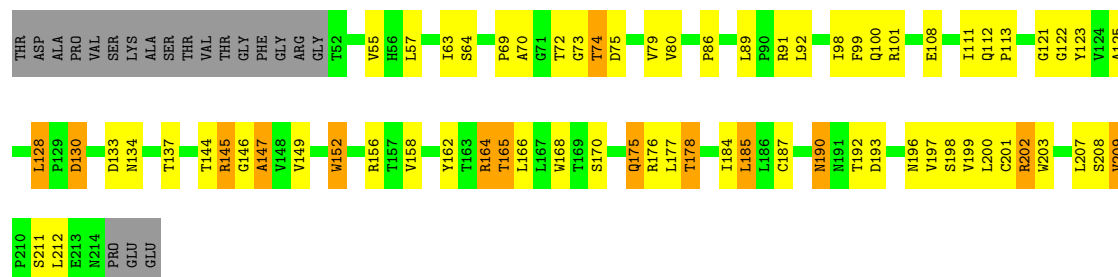
- Molecule 1: Coat protein

Chain s:  51% 29% 9% 11%



- Molecule 1: Coat protein

Chain t:  51% 31% 8% 11%



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|------|------|------|------|------|------|
| THR  | ASP  | ALA  | PRO  | VAL  | SER  | LYS  | ALA  | SER  | THR  | VAL  | THR  | GLY  | PHE  | GLY  | ARG  | GLY  | 752  | V55  | H56  | L57  | R62  | 163  | S64  | Q65  | T72  | G73  | T74  | D75  | G76  | G77  | G78  | V79  | D87  | L88  | L89  | L92  | G93  | H94  | 198 | F99 | Q100 | Q101 | E108 | Q112 | F113 | M114 | N118 | L128 | F129 |
| D130 | P131 | T132 | T137 | F138 | Q142 | R145 | V149 | A150 | M152 | W155 | V158 | Q161 | R164 | T165 | L166 | L167 | V168 | T169 | S170 | Q175 | R176 | L177 | T178 | L185 | L186 | C187 | N196 | V197 | S198 | V199 | R202 | V205 | S208 | Z209 | P210 | S211 | E213 | N214 | PRO | GLU | GLY  |      |      |      |      |      |      |      |      |

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 42                                                        | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 288.95Å 288.95Å 175.12Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 26.37 – 3.10<br>26.37 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.1 (26.37-3.10)<br>98.3 (26.37-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.25 (at 3.11Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0049                                             | Depositor        |
| R, $R_{free}$                                                           | 0.238 , 0.288<br>0.238 , 0.285                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 12823 reflections (4.92%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.018                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 22.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.448 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 75180                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 56.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

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   | 0     | 0.74         | 0/1281        | 0.95        | 0/1753        |
| 1   | 1     | 0.78         | 0/1281        | 1.00        | 3/1753 (0.2%) |
| 1   | 2     | 0.73         | 0/1281        | 0.99        | 0/1753        |
| 1   | 3     | 0.74         | 0/1281        | 0.94        | 0/1753        |
| 1   | 4     | 0.75         | 0/1281        | 1.03        | 2/1753 (0.1%) |
| 1   | 5     | 0.78         | 0/1281        | 0.99        | 0/1753        |
| 1   | 6     | 0.71         | 0/1281        | 0.95        | 0/1753        |
| 1   | 7     | 0.85         | 0/1281        | 1.04        | 1/1753 (0.1%) |
| 1   | 8     | 0.83         | 0/1281        | 1.10        | 2/1753 (0.1%) |
| 1   | 9     | 0.76         | 0/1281        | 0.97        | 0/1753        |
| 1   | A     | 0.77         | 0/1281        | 1.07        | 0/1753        |
| 1   | B     | 0.78         | 0/1281        | 1.00        | 1/1753 (0.1%) |
| 1   | C     | 0.72         | 0/1281        | 0.93        | 0/1753        |
| 1   | D     | 0.79         | 1/1281 (0.1%) | 1.03        | 1/1753 (0.1%) |
| 1   | E     | 0.78         | 0/1281        | 1.03        | 1/1753 (0.1%) |
| 1   | F     | 0.72         | 0/1281        | 0.95        | 0/1753        |
| 1   | G     | 0.85         | 1/1281 (0.1%) | 1.10        | 3/1753 (0.2%) |
| 1   | H     | 0.83         | 0/1281        | 1.08        | 3/1753 (0.2%) |
| 1   | I     | 0.77         | 0/1281        | 0.98        | 1/1753 (0.1%) |
| 1   | J     | 0.75         | 0/1281        | 1.02        | 0/1753        |
| 1   | K     | 0.75         | 0/1281        | 1.01        | 0/1753        |
| 1   | L     | 0.70         | 0/1281        | 0.93        | 0/1753        |
| 1   | M     | 0.83         | 0/1281        | 1.06        | 2/1753 (0.1%) |
| 1   | N     | 0.82         | 0/1281        | 1.14        | 8/1753 (0.5%) |
| 1   | O     | 0.75         | 0/1281        | 0.94        | 0/1753        |
| 1   | P     | 0.80         | 0/1281        | 1.03        | 1/1753 (0.1%) |
| 1   | Q     | 0.81         | 0/1281        | 1.01        | 2/1753 (0.1%) |
| 1   | R     | 0.72         | 0/1281        | 0.93        | 0/1753        |
| 1   | S     | 0.79         | 0/1281        | 1.03        | 5/1753 (0.3%) |
| 1   | T     | 0.82         | 1/1281 (0.1%) | 1.05        | 0/1753        |
| 1   | U     | 0.72         | 0/1281        | 0.95        | 0/1753        |
| 1   | V     | 0.80         | 0/1281        | 1.02        | 1/1753 (0.1%) |
| 1   | W     | 0.81         | 0/1281        | 1.02        | 3/1753 (0.2%) |
| 1   | X     | 0.73         | 0/1281        | 0.94        | 0/1753        |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | Y     | 0.82         | 1/1281 (0.1%)  | 1.04        | 2/1753 (0.1%)    |
| 1   | Z     | 0.75         | 0/1281         | 0.96        | 0/1753           |
| 1   | a     | 0.73         | 0/1281         | 0.97        | 3/1753 (0.2%)    |
| 1   | b     | 0.74         | 0/1281         | 0.97        | 2/1753 (0.1%)    |
| 1   | c     | 0.67         | 0/1281         | 0.92        | 0/1753           |
| 1   | d     | 0.83         | 0/1281         | 1.01        | 1/1753 (0.1%)    |
| 1   | e     | 0.78         | 0/1281         | 1.00        | 1/1753 (0.1%)    |
| 1   | f     | 0.67         | 0/1281         | 0.91        | 0/1753           |
| 1   | g     | 0.76         | 0/1281         | 1.01        | 4/1753 (0.2%)    |
| 1   | h     | 0.80         | 0/1281         | 1.06        | 5/1753 (0.3%)    |
| 1   | i     | 0.75         | 0/1281         | 0.97        | 1/1753 (0.1%)    |
| 1   | j     | 0.81         | 0/1281         | 1.06        | 3/1753 (0.2%)    |
| 1   | k     | 0.80         | 0/1281         | 1.04        | 5/1753 (0.3%)    |
| 1   | l     | 0.71         | 0/1281         | 0.95        | 0/1753           |
| 1   | m     | 0.85         | 1/1281 (0.1%)  | 1.10        | 7/1753 (0.4%)    |
| 1   | n     | 0.82         | 0/1281         | 1.07        | 2/1753 (0.1%)    |
| 1   | o     | 0.77         | 0/1281         | 0.96        | 0/1753           |
| 1   | p     | 0.80         | 0/1281         | 1.00        | 0/1753           |
| 1   | q     | 0.79         | 0/1281         | 1.03        | 1/1753 (0.1%)    |
| 1   | r     | 0.69         | 0/1281         | 0.94        | 2/1753 (0.1%)    |
| 1   | s     | 0.70         | 0/1281         | 0.97        | 1/1753 (0.1%)    |
| 1   | t     | 0.77         | 0/1281         | 1.00        | 3/1753 (0.2%)    |
| 1   | u     | 0.66         | 0/1281         | 0.92        | 0/1753           |
| 1   | v     | 0.77         | 0/1281         | 1.01        | 1/1753 (0.1%)    |
| 1   | w     | 0.77         | 0/1281         | 1.05        | 1/1753 (0.1%)    |
| 1   | x     | 0.73         | 0/1281         | 0.94        | 0/1753           |
| All | All   | 0.77         | 5/76860 (0.0%) | 1.00        | 85/105180 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 4     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | Y     | 0                   | 2                   |
| 1   | b     | 0                   | 1                   |
| 1   | m     | 0                   | 1                   |
| 1   | t     | 0                   | 1                   |
| 1   | w     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | T     | 130 | ASP  | CA-C  | -7.63 | 1.46        | 1.52     |
| 1   | G     | 130 | ASP  | CA-C  | -7.20 | 1.46        | 1.52     |
| 1   | Y     | 130 | ASP  | CA-C  | -5.86 | 1.47        | 1.52     |
| 1   | m     | 130 | ASP  | CA-C  | -5.51 | 1.46        | 1.52     |
| 1   | D     | 130 | ASP  | CA-C  | -5.24 | 1.48        | 1.52     |

All (85) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | N     | 159 | ARG  | CA-C-N  | -9.18 | 111.43      | 120.52   |
| 1   | N     | 159 | ARG  | C-N-CA  | -9.18 | 111.43      | 120.52   |
| 1   | n     | 208 | SER  | CA-C-N  | -8.29 | 115.64      | 122.85   |
| 1   | n     | 208 | SER  | C-N-CA  | -8.29 | 115.64      | 122.85   |
| 1   | h     | 130 | ASP  | CA-C-N  | -7.36 | 112.61      | 119.82   |
| 1   | h     | 130 | ASP  | C-N-CA  | -7.36 | 112.61      | 119.82   |
| 1   | a     | 163 | THR  | N-CA-C  | 7.19  | 119.98      | 111.71   |
| 1   | e     | 209 | VAL  | N-CA-C  | 7.04  | 115.75      | 107.73   |
| 1   | G     | 209 | VAL  | N-CA-C  | 7.03  | 115.11      | 108.15   |
| 1   | k     | 208 | SER  | CA-C-N  | -6.99 | 117.25      | 123.33   |
| 1   | k     | 208 | SER  | C-N-CA  | -6.99 | 117.25      | 123.33   |
| 1   | N     | 208 | SER  | CA-C-N  | -6.93 | 115.82      | 123.02   |
| 1   | N     | 208 | SER  | C-N-CA  | -6.93 | 115.82      | 123.02   |
| 1   | g     | 129 | PRO  | N-CA-C  | 6.66  | 121.61      | 114.68   |
| 1   | h     | 210 | PRO  | N-CA-C  | 6.65  | 121.65      | 111.34   |
| 1   | N     | 130 | ASP  | CA-C-N  | -6.61 | 113.34      | 119.82   |
| 1   | N     | 130 | ASP  | C-N-CA  | -6.61 | 113.34      | 119.82   |
| 1   | s     | 163 | THR  | N-CA-C  | 6.59  | 120.19      | 111.75   |
| 1   | h     | 191 | ASN  | N-CA-C  | 6.54  | 119.26      | 109.25   |
| 1   | m     | 130 | ASP  | N-CA-CB | 6.06  | 120.96      | 110.23   |
| 1   | G     | 130 | ASP  | CA-C-N  | -6.05 | 113.57      | 119.87   |
| 1   | G     | 130 | ASP  | C-N-CA  | -6.05 | 113.57      | 119.87   |
| 1   | g     | 130 | ASP  | N-CA-CB | 6.04  | 120.07      | 110.11   |
| 1   | k     | 209 | VAL  | N-CA-C  | 6.02  | 114.78      | 107.61   |
| 1   | Y     | 130 | ASP  | N-CA-CB | 5.89  | 121.62      | 110.42   |
| 1   | 4     | 128 | LEU  | CA-C-N  | 5.77  | 127.06      | 119.84   |
| 1   | 4     | 128 | LEU  | C-N-CA  | 5.77  | 127.06      | 119.84   |
| 1   | k     | 163 | THR  | N-CA-C  | 5.77  | 117.57      | 111.28   |
| 1   | a     | 130 | ASP  | CA-C-N  | -5.76 | 112.64      | 119.84   |
| 1   | a     | 130 | ASP  | C-N-CA  | -5.76 | 112.64      | 119.84   |
| 1   | j     | 176 | ARG  | N-CA-C  | -5.75 | 106.22      | 113.18   |
| 1   | P     | 70  | ALA  | N-CA-C  | 5.71  | 119.06      | 111.75   |
| 1   | W     | 155 | SER  | N-CA-C  | -5.68 | 103.03      | 110.53   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | Q     | 128 | LEU  | CA-C-N   | 5.64  | 126.38      | 120.12   |
| 1   | Q     | 128 | LEU  | C-N-CA   | 5.64  | 126.38      | 120.12   |
| 1   | H     | 197 | VAL  | N-CA-C   | 5.63  | 116.41      | 108.36   |
| 1   | 7     | 130 | ASP  | N-CA-CB  | 5.57  | 119.41      | 109.94   |
| 1   | b     | 128 | LEU  | CA-CB-CG | 5.57  | 135.78      | 116.30   |
| 1   | B     | 173 | LYS  | N-CA-C   | -5.55 | 105.14      | 111.14   |
| 1   | S     | 128 | LEU  | CA-C-N   | 5.55  | 126.78      | 119.84   |
| 1   | S     | 128 | LEU  | C-N-CA   | 5.55  | 126.78      | 119.84   |
| 1   | H     | 54  | ASP  | N-CA-C   | 5.54  | 118.26      | 110.23   |
| 1   | M     | 163 | THR  | N-CA-C   | 5.47  | 117.05      | 111.14   |
| 1   | d     | 98  | ILE  | N-CA-C   | -5.47 | 107.53      | 112.12   |
| 1   | g     | 132 | THR  | N-CA-C   | 5.46  | 116.92      | 110.97   |
| 1   | t     | 133 | ASP  | N-CA-C   | 5.46  | 117.61      | 109.25   |
| 1   | j     | 132 | THR  | N-CA-C   | 5.45  | 117.22      | 111.28   |
| 1   | j     | 171 | SER  | N-CA-C   | 5.44  | 117.59      | 109.59   |
| 1   | E     | 190 | ASN  | N-CA-C   | 5.41  | 118.22      | 108.48   |
| 1   | S     | 130 | ASP  | CA-C-N   | -5.40 | 113.09      | 119.84   |
| 1   | S     | 130 | ASP  | C-N-CA   | -5.40 | 113.09      | 119.84   |
| 1   | M     | 130 | ASP  | N-CA-C   | -5.38 | 100.79      | 109.40   |
| 1   | v     | 166 | LEU  | N-CA-C   | 5.34  | 117.42      | 108.23   |
| 1   | m     | 130 | ASP  | N-CA-C   | -5.32 | 100.89      | 109.40   |
| 1   | N     | 208 | SER  | N-CA-C   | 5.27  | 119.20      | 111.34   |
| 1   | V     | 163 | THR  | N-CA-C   | 5.24  | 117.39      | 111.11   |
| 1   | k     | 133 | ASP  | N-CA-C   | 5.21  | 117.74      | 109.24   |
| 1   | 8     | 130 | ASP  | CA-C-N   | -5.20 | 114.31      | 119.56   |
| 1   | 8     | 130 | ASP  | C-N-CA   | -5.20 | 114.31      | 119.56   |
| 1   | t     | 128 | LEU  | N-CA-CB  | 5.20  | 117.04      | 110.23   |
| 1   | S     | 209 | VAL  | N-CA-C   | 5.19  | 113.15      | 107.60   |
| 1   | I     | 129 | PRO  | N-CA-C   | 5.19  | 120.42      | 114.20   |
| 1   | m     | 190 | ASN  | N-CA-CB  | 5.18  | 119.07      | 110.63   |
| 1   | W     | 163 | THR  | N-CA-C   | 5.17  | 116.92      | 111.28   |
| 1   | h     | 84  | ILE  | CB-CA-C  | -5.17 | 105.65      | 111.23   |
| 1   | N     | 161 | GLN  | N-CA-C   | -5.15 | 101.77      | 109.95   |
| 1   | H     | 176 | ARG  | N-CA-C   | -5.13 | 106.97      | 113.18   |
| 1   | Y     | 130 | ASP  | CB-CA-C  | -5.13 | 100.95      | 109.15   |
| 1   | 1     | 68  | LEU  | CA-C-N   | -5.12 | 115.30      | 120.21   |
| 1   | 1     | 68  | LEU  | C-N-CA   | -5.12 | 115.30      | 120.21   |
| 1   | r     | 209 | VAL  | CA-C-N   | 5.11  | 125.11      | 119.89   |
| 1   | r     | 209 | VAL  | C-N-CA   | 5.11  | 125.11      | 119.89   |
| 1   | m     | 58  | SER  | N-CA-C   | 5.10  | 116.94      | 109.24   |
| 1   | b     | 128 | LEU  | N-CA-CB  | 5.10  | 116.91      | 110.23   |
| 1   | m     | 175 | GLN  | N-CA-C   | 5.09  | 118.81      | 112.59   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | l     | 133 | ASP  | N-CA-C   | 5.08  | 117.03      | 109.25   |
| 1   | t     | 128 | LEU  | CA-CB-CG | 5.08  | 134.06      | 116.30   |
| 1   | i     | 129 | PRO  | N-CA-C   | 5.07  | 120.29      | 114.20   |
| 1   | q     | 173 | LYS  | N-CA-C   | -5.05 | 105.23      | 111.40   |
| 1   | g     | 130 | ASP  | CB-CA-C  | -5.05 | 101.66      | 108.68   |
| 1   | D     | 133 | ASP  | N-CA-C   | 5.02  | 116.92      | 108.73   |
| 1   | m     | 208 | SER  | CA-C-N   | -5.01 | 117.13      | 122.85   |
| 1   | m     | 208 | SER  | C-N-CA   | -5.01 | 117.13      | 122.85   |
| 1   | W     | 171 | SER  | N-CA-C   | 5.01  | 117.56      | 110.10   |
| 1   | w     | 133 | ASP  | N-CA-C   | 5.01  | 117.77      | 109.46   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | 4     | 207 | LEU  | Peptide |
| 1   | E     | 207 | LEU  | Peptide |
| 1   | Y     | 129 | PRO  | Peptide |
| 1   | Y     | 207 | LEU  | Peptide |
| 1   | b     | 207 | LEU  | Peptide |
| 1   | m     | 129 | PRO  | Peptide |
| 1   | t     | 207 | LEU  | Peptide |
| 1   | w     | 207 | LEU  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 1253  | 0        | 1242     | 44      | 0            |
| 1   | 1     | 1253  | 0        | 1242     | 41      | 0            |
| 1   | 2     | 1253  | 0        | 1242     | 46      | 0            |
| 1   | 3     | 1253  | 0        | 1242     | 34      | 1            |
| 1   | 4     | 1253  | 0        | 1242     | 42      | 0            |
| 1   | 5     | 1253  | 0        | 1242     | 41      | 0            |
| 1   | 6     | 1253  | 0        | 1242     | 33      | 0            |
| 1   | 7     | 1253  | 0        | 1242     | 66      | 0            |
| 1   | 8     | 1253  | 0        | 1242     | 51      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 9     | 1253  | 0        | 1242     | 55      | 0            |
| 1   | A     | 1253  | 0        | 1242     | 39      | 0            |
| 1   | B     | 1253  | 0        | 1242     | 54      | 0            |
| 1   | C     | 1253  | 0        | 1242     | 29      | 0            |
| 1   | D     | 1253  | 0        | 1242     | 46      | 0            |
| 1   | E     | 1253  | 0        | 1242     | 59      | 0            |
| 1   | F     | 1253  | 0        | 1242     | 35      | 0            |
| 1   | G     | 1253  | 0        | 1242     | 56      | 0            |
| 1   | H     | 1253  | 0        | 1242     | 65      | 0            |
| 1   | I     | 1253  | 0        | 1242     | 59      | 0            |
| 1   | J     | 1253  | 0        | 1242     | 44      | 0            |
| 1   | K     | 1253  | 0        | 1242     | 50      | 0            |
| 1   | L     | 1253  | 0        | 1242     | 36      | 0            |
| 1   | M     | 1253  | 0        | 1242     | 61      | 0            |
| 1   | N     | 1253  | 0        | 1242     | 44      | 1            |
| 1   | O     | 1253  | 0        | 1242     | 40      | 0            |
| 1   | P     | 1253  | 0        | 1242     | 45      | 0            |
| 1   | Q     | 1253  | 0        | 1242     | 54      | 0            |
| 1   | R     | 1253  | 0        | 1242     | 32      | 0            |
| 1   | S     | 1253  | 0        | 1242     | 48      | 0            |
| 1   | T     | 1253  | 0        | 1242     | 51      | 0            |
| 1   | U     | 1253  | 0        | 1242     | 40      | 0            |
| 1   | V     | 1253  | 0        | 1242     | 45      | 0            |
| 1   | W     | 1253  | 0        | 1242     | 51      | 0            |
| 1   | X     | 1253  | 0        | 1242     | 38      | 0            |
| 1   | Y     | 1253  | 0        | 1242     | 61      | 0            |
| 1   | Z     | 1253  | 0        | 1242     | 57      | 0            |
| 1   | a     | 1253  | 0        | 1242     | 49      | 0            |
| 1   | b     | 1253  | 0        | 1242     | 51      | 0            |
| 1   | c     | 1253  | 0        | 1242     | 34      | 0            |
| 1   | d     | 1253  | 0        | 1242     | 39      | 0            |
| 1   | e     | 1253  | 0        | 1242     | 47      | 0            |
| 1   | f     | 1253  | 0        | 1242     | 35      | 0            |
| 1   | g     | 1253  | 0        | 1242     | 50      | 0            |
| 1   | h     | 1253  | 0        | 1242     | 62      | 0            |
| 1   | i     | 1253  | 0        | 1242     | 46      | 0            |
| 1   | j     | 1253  | 0        | 1242     | 52      | 0            |
| 1   | k     | 1253  | 0        | 1242     | 43      | 0            |
| 1   | l     | 1253  | 0        | 1242     | 31      | 0            |
| 1   | m     | 1253  | 0        | 1242     | 55      | 0            |
| 1   | n     | 1253  | 0        | 1242     | 49      | 0            |
| 1   | o     | 1253  | 0        | 1242     | 50      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | p     | 1253  | 0        | 1242     | 51      | 0            |
| 1   | q     | 1253  | 0        | 1242     | 53      | 0            |
| 1   | r     | 1253  | 0        | 1242     | 41      | 0            |
| 1   | s     | 1253  | 0        | 1242     | 45      | 0            |
| 1   | t     | 1253  | 0        | 1242     | 51      | 0            |
| 1   | u     | 1253  | 0        | 1242     | 37      | 0            |
| 1   | v     | 1253  | 0        | 1242     | 56      | 0            |
| 1   | w     | 1253  | 0        | 1242     | 50      | 0            |
| 1   | x     | 1253  | 0        | 1242     | 35      | 0            |
| All | All   | 75180 | 0        | 74520    | 2291    | 1            |

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 15.

All (2291) 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:N:101:ARG:HE  | 1:N:166:LEU:HD21 | 1.02                     | 1.07              |
| 1:n:101:ARG:HE  | 1:n:166:LEU:HD21 | 1.22                     | 1.05              |
| 1:T:101:ARG:HE  | 1:T:166:LEU:HD21 | 1.23                     | 1.03              |
| 1:Q:101:ARG:HE  | 1:Q:166:LEU:HD21 | 1.21                     | 1.02              |
| 1:H:91:ARG:O    | 1:M:98:ILE:HD11  | 1.61                     | 1.00              |
| 1:v:163:THR:HA  | 1:x:101:ARG:HH22 | 1.26                     | 1.00              |
| 1:Y:163:THR:HA  | 1:0:101:ARG:HH22 | 1.26                     | 0.99              |
| 1:1:152:TRP:HH2 | 1:1:187:CYS:HG   | 1.04                     | 0.98              |
| 1:m:163:THR:HA  | 1:o:101:ARG:HH22 | 1.29                     | 0.97              |
| 1:E:101:ARG:HE  | 1:E:166:LEU:HD21 | 1.30                     | 0.96              |
| 1:F:112:GLN:HG2 | 1:S:149:VAL:HG23 | 1.45                     | 0.96              |
| 1:I:112:GLN:HG2 | 1:Y:149:VAL:HG23 | 1.48                     | 0.94              |
| 1:H:121:GLY:HA3 | 1:H:152:TRP:HE3  | 1.33                     | 0.93              |
| 1:6:112:GLN:HG2 | 1:j:149:VAL:HG23 | 1.50                     | 0.92              |
| 1:p:152:TRP:HH2 | 1:p:187:CYS:HG   | 0.93                     | 0.91              |
| 1:H:101:ARG:HE  | 1:H:166:LEU:HD21 | 1.38                     | 0.89              |
| 1:N:101:ARG:NE  | 1:N:166:LEU:HD21 | 1.88                     | 0.89              |
| 1:D:168:TRP:HZ3 | 1:E:130:ASP:OD1  | 1.53                     | 0.89              |
| 1:T:101:ARG:NE  | 1:T:166:LEU:HD21 | 1.88                     | 0.89              |
| 1:i:112:GLN:HG2 | 1:p:149:VAL:HG23 | 1.55                     | 0.88              |
| 1:S:101:ARG:HE  | 1:S:166:LEU:HD21 | 1.38                     | 0.88              |
| 1:k:152:TRP:HH2 | 1:k:187:CYS:HG   | 0.94                     | 0.88              |
| 1:h:101:ARG:HE  | 1:h:166:LEU:HD21 | 1.38                     | 0.87              |
| 1:v:101:ARG:HE  | 1:v:166:LEU:HD21 | 1.40                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:73:GLY:O     | 1:w:190:ASN:HB3  | 1.74                     | 0.87              |
| 1:5:101:ARG:HE   | 1:5:166:LEU:HD21 | 1.40                     | 0.86              |
| 1:7:145:ARG:HE   | 1:7:145:ARG:N    | 1.74                     | 0.86              |
| 1:e:152:TRP:HH2  | 1:e:187:CYS:HG   | 1.24                     | 0.85              |
| 1:j:152:TRP:HH2  | 1:j:187:CYS:HG   | 1.23                     | 0.85              |
| 1:p:210:PRO:HG2  | 1:q:145:ARG:CD   | 2.07                     | 0.85              |
| 1:0:149:VAL:HG23 | 1:t:112:GLN:HG2  | 1.58                     | 0.85              |
| 1:D:101:ARG:HE   | 1:D:166:LEU:HD21 | 1.41                     | 0.84              |
| 1:Q:112:GLN:HG2  | 1:o:149:VAL:HG23 | 1.59                     | 0.84              |
| 1:P:210:PRO:HG2  | 1:Q:145:ARG:CD   | 2.08                     | 0.84              |
| 1:B:152:TRP:HH2  | 1:B:187:CYS:HG   | 1.25                     | 0.83              |
| 1:g:163:THR:HA   | 1:i:101:ARG:HH22 | 1.43                     | 0.83              |
| 1:H:120:GLY:N    | 1:H:192:THR:OG1  | 2.11                     | 0.83              |
| 1:P:121:GLY:HA3  | 1:P:152:TRP:HE3  | 1.43                     | 0.83              |
| 1:a:149:VAL:HG23 | 1:u:112:GLN:HG2  | 1.61                     | 0.82              |
| 1:j:152:TRP:HH2  | 1:j:187:CYS:SG   | 2.01                     | 0.82              |
| 1:O:94:HIS:HB2   | 1:X:98:ILE:HD11  | 1.60                     | 0.82              |
| 1:D:168:TRP:CZ3  | 1:E:130:ASP:OD1  | 2.33                     | 0.82              |
| 1:7:101:ARG:HE   | 1:7:166:LEU:HD21 | 1.44                     | 0.82              |
| 1:D:130:ASP:OD1  | 1:F:168:TRP:CH2  | 2.33                     | 0.81              |
| 1:W:121:GLY:HA3  | 1:W:152:TRP:HE3  | 1.44                     | 0.81              |
| 1:Z:101:ARG:HE   | 1:Z:166:LEU:HD21 | 1.44                     | 0.81              |
| 1:8:121:GLY:HA3  | 1:8:152:TRP:HE3  | 1.46                     | 0.81              |
| 1:1:152:TRP:HH2  | 1:1:187:CYS:SG   | 2.04                     | 0.81              |
| 1:I:149:VAL:HG23 | 1:M:112:GLN:HG2  | 1.62                     | 0.80              |
| 1:4:210:PRO:HG2  | 1:5:145:ARG:HD2  | 1.63                     | 0.80              |
| 1:S:163:THR:OG1  | 1:S:165:THR:HG22 | 1.82                     | 0.80              |
| 1:D:130:ASP:OD1  | 1:F:168:TRP:HH2  | 1.64                     | 0.80              |
| 1:7:145:ARG:HD3  | 1:9:210:PRO:HB2  | 1.64                     | 0.79              |
| 1:d:149:VAL:HG23 | 1:x:112:GLN:HG2  | 1.63                     | 0.79              |
| 1:w:152:TRP:HH2  | 1:w:187:CYS:HG   | 1.29                     | 0.79              |
| 1:t:73:GLY:O     | 1:t:190:ASN:HB3  | 1.82                     | 0.79              |
| 1:v:210:PRO:HG2  | 1:w:145:ARG:CD   | 2.13                     | 0.79              |
| 1:N:162:TYR:O    | 1:N:164:ARG:HG3  | 1.83                     | 0.79              |
| 1:Q:73:GLY:O     | 1:Q:190:ASN:HB3  | 1.82                     | 0.79              |
| 1:e:101:ARG:HE   | 1:e:166:LEU:HD21 | 1.46                     | 0.79              |
| 1:G:74:THR:O     | 1:G:75:ASP:C     | 2.24                     | 0.78              |
| 1:7:163:THR:HA   | 1:9:101:ARG:HH22 | 1.47                     | 0.78              |
| 1:A:91:ARG:O     | 1:E:98:ILE:HD11  | 1.81                     | 0.78              |
| 1:c:112:GLN:HG2  | 1:s:149:VAL:HG23 | 1.63                     | 0.78              |
| 1:p:121:GLY:HA3  | 1:p:152:TRP:HE3  | 1.49                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:4:101:ARG:HE   | 1:4:166:LEU:HD21 | 1.46                     | 0.78              |
| 1:2:73:GLY:O     | 1:2:190:ASN:HB3  | 1.84                     | 0.78              |
| 1:p:152:TRP:HH2  | 1:p:187:CYS:SG   | 2.04                     | 0.78              |
| 1:m:101:ARG:HE   | 1:m:166:LEU:HD21 | 1.48                     | 0.77              |
| 1:M:149:VAL:HG23 | 1:X:112:GLN:HG2  | 1.67                     | 0.77              |
| 1:7:118:ASN:HD21 | 1:o:118:ASN:HB2  | 1.49                     | 0.77              |
| 1:6:149:VAL:HG23 | 1:d:112:GLN:HG2  | 1.66                     | 0.77              |
| 1:E:152:TRP:HH2  | 1:E:187:CYS:HG   | 1.33                     | 0.76              |
| 1:E:101:ARG:NE   | 1:E:166:LEU:HD21 | 1.99                     | 0.76              |
| 1:O:112:GLN:HG2  | 1:V:149:VAL:HG23 | 1.68                     | 0.76              |
| 1:P:210:PRO:HG2  | 1:Q:145:ARG:HD2  | 1.65                     | 0.76              |
| 1:H:101:ARG:HE   | 1:H:166:LEU:CD2  | 1.98                     | 0.76              |
| 1:M:163:THR:HA   | 1:O:101:ARG:HH22 | 1.50                     | 0.76              |
| 1:K:101:ARG:HE   | 1:K:166:LEU:HD21 | 1.51                     | 0.76              |
| 1:R:149:VAL:HG23 | 1:n:112:GLN:HG2  | 1.68                     | 0.75              |
| 1:S:168:TRP:HZ3  | 1:T:130:ASP:OD1  | 1.69                     | 0.75              |
| 1:2:168:TRP:HB2  | 1:2:177:LEU:O    | 1.86                     | 0.75              |
| 1:W:112:GLN:HG2  | 1:x:149:VAL:HG23 | 1.69                     | 0.75              |
| 1:e:152:TRP:HH2  | 1:e:187:CYS:SG   | 2.09                     | 0.75              |
| 1:5:149:VAL:HG23 | 1:8:112:GLN:HG2  | 1.69                     | 0.75              |
| 1:B:152:TRP:HH2  | 1:B:187:CYS:SG   | 2.09                     | 0.74              |
| 1:b:112:GLN:HG2  | 1:h:149:VAL:CG2  | 2.17                     | 0.74              |
| 1:p:163:THR:HA   | 1:r:101:ARG:HH22 | 1.51                     | 0.74              |
| 1:T:98:ILE:HD11  | 1:k:91:ARG:O     | 1.88                     | 0.74              |
| 1:l:152:TRP:HH2  | 1:l:187:CYS:HG   | 1.34                     | 0.74              |
| 1:q:73:GLY:O     | 1:q:190:ASN:HB3  | 1.86                     | 0.74              |
| 1:C:112:GLN:HG2  | 1:P:149:VAL:HG23 | 1.69                     | 0.74              |
| 1:S:168:TRP:CZ3  | 1:T:130:ASP:OD1  | 2.39                     | 0.74              |
| 1:B:121:GLY:HA3  | 1:B:152:TRP:HE3  | 1.53                     | 0.73              |
| 1:S:163:THR:HA   | 1:U:101:ARG:HH22 | 1.53                     | 0.73              |
| 1:8:74:THR:O     | 1:8:75:ASP:C     | 2.31                     | 0.73              |
| 1:9:112:GLN:HG2  | 1:m:149:VAL:HG23 | 1.70                     | 0.73              |
| 1:G:149:VAL:HG23 | 1:0:112:GLN:HG2  | 1.70                     | 0.73              |
| 1:J:98:ILE:HG22  | 1:J:99:PHE:CD1   | 2.23                     | 0.73              |
| 1:7:145:ARG:CD   | 1:9:210:PRO:HB2  | 2.18                     | 0.73              |
| 1:s:121:GLY:HA3  | 1:s:152:TRP:HE3  | 1.53                     | 0.73              |
| 1:g:118:ASN:HD21 | 1:r:118:ASN:HB2  | 1.53                     | 0.73              |
| 1:g:149:VAL:HG23 | 1:r:112:GLN:HG2  | 1.71                     | 0.73              |
| 1:Y:112:GLN:HG2  | 1:w:149:VAL:HG23 | 1.71                     | 0.72              |
| 1:v:73:GLY:O     | 1:v:190:ASN:HB3  | 1.89                     | 0.72              |
| 1:h:100:GLN:HB2  | 1:h:209:VAL:HG22 | 1.72                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:7:74:THR:O     | 1:7:75:ASP:C     | 2.32                     | 0.72              |
| 1:Q:112:GLN:HG2  | 1:O:149:VAL:CG2  | 2.19                     | 0.72              |
| 1:m:176:ARG:HD2  | 1:O:168:TRP:CZ2  | 2.24                     | 0.72              |
| 1:S:130:ASP:OD1  | 1:U:100:GLN:CD   | 2.33                     | 0.72              |
| 1:h:73:GLY:O     | 1:h:190:ASN:HB3  | 1.89                     | 0.72              |
| 1:k:152:TRP:HH2  | 1:k:187:CYS:SG   | 2.09                     | 0.72              |
| 1:8:101:ARG:HE   | 1:8:166:LEU:HD21 | 1.55                     | 0.72              |
| 1:T:74:THR:O     | 1:T:75:ASP:C     | 2.33                     | 0.72              |
| 1:3:149:VAL:HG23 | 1:q:112:GLN:HG2  | 1.71                     | 0.72              |
| 1:g:175:GLN:HA   | 1:g:178:THR:HG22 | 1.72                     | 0.72              |
| 1:l:152:TRP:HH2  | 1:l:187:CYS:SG   | 2.12                     | 0.72              |
| 1:C:114:MET:SD   | 1:P:122:GLY:HA3  | 2.30                     | 0.72              |
| 1:Y:152:TRP:HH2  | 1:Y:187:CYS:HG   | 1.35                     | 0.71              |
| 1:H:98:ILE:HD11  | 1:M:91:ARG:O     | 1.90                     | 0.71              |
| 1:j:210:PRO:HG2  | 1:k:145:ARG:CD   | 2.21                     | 0.71              |
| 1:q:121:GLY:HA3  | 1:q:152:TRP:HE3  | 1.56                     | 0.71              |
| 1:H:121:GLY:HA3  | 1:H:152:TRP:CE3  | 2.20                     | 0.71              |
| 1:j:63:ILE:HB    | 1:j:199:VAL:HG22 | 1.72                     | 0.71              |
| 1:n:152:TRP:HH2  | 1:n:187:CYS:HG   | 1.39                     | 0.71              |
| 1:E:100:GLN:HB2  | 1:E:209:VAL:HG22 | 1.73                     | 0.71              |
| 1:E:149:VAL:CG2  | 1:N:112:GLN:HG2  | 2.21                     | 0.71              |
| 1:P:112:GLN:HG2  | 1:q:149:VAL:HG23 | 1.71                     | 0.71              |
| 1:2:101:ARG:HE   | 1:2:166:LEU:HD21 | 1.55                     | 0.71              |
| 1:w:121:GLY:HA3  | 1:w:152:TRP:HE3  | 1.53                     | 0.71              |
| 1:Q:168:TRP:HB2  | 1:Q:177:LEU:O    | 1.90                     | 0.70              |
| 1:b:55:VAL:HG13  | 1:g:55:VAL:HG13  | 1.73                     | 0.70              |
| 1:c:149:VAL:HG23 | 1:g:112:GLN:HG2  | 1.73                     | 0.70              |
| 1:m:145:ARG:HE   | 1:m:145:ARG:N    | 1.88                     | 0.70              |
| 1:H:100:GLN:HB2  | 1:H:209:VAL:HG22 | 1.72                     | 0.70              |
| 1:n:130:ASP:OD2  | 1:n:176:ARG:NH2  | 2.23                     | 0.70              |
| 1:J:149:VAL:HG23 | 1:3:112:GLN:HG2  | 1.71                     | 0.70              |
| 1:H:175:GLN:HA   | 1:H:178:THR:HG23 | 1.72                     | 0.70              |
| 1:K:145:ARG:N    | 1:K:145:ARG:HE   | 1.89                     | 0.70              |
| 1:l:145:ARG:HE   | 1:l:145:ARG:N    | 1.90                     | 0.70              |
| 1:D:163:THR:HA   | 1:F:101:ARG:HH22 | 1.56                     | 0.70              |
| 1:T:55:VAL:HG13  | 1:k:55:VAL:HG13  | 1.72                     | 0.70              |
| 1:n:101:ARG:NE   | 1:n:166:LEU:HD21 | 2.03                     | 0.70              |
| 1:8:133:ASP:OD2  | 1:8:135:ASP:HB2  | 1.92                     | 0.70              |
| 1:E:152:TRP:HH2  | 1:E:187:CYS:SG   | 2.15                     | 0.69              |
| 1:d:130:ASP:HB2  | 1:d:132:THR:OG1  | 1.91                     | 0.69              |
| 1:D:145:ARG:HE   | 1:D:145:ARG:N    | 1.90                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:101:ARG:HE   | 1:w:166:LEU:HD21 | 1.57                     | 0.69              |
| 1:4:130:ASP:HB2  | 1:4:132:THR:OG1  | 1.92                     | 0.69              |
| 1:L:98:ILE:HD11  | 1:3:94:HIS:HB2   | 1.74                     | 0.69              |
| 1:N:175:GLN:HA   | 1:N:178:THR:HG23 | 1.74                     | 0.69              |
| 1:f:112:GLN:HG2  | 1:v:149:VAL:HG23 | 1.74                     | 0.69              |
| 1:G:176:ARG:HD2  | 1:I:168:TRP:CZ2  | 2.28                     | 0.69              |
| 1:Z:112:GLN:HG2  | 1:u:149:VAL:HG23 | 1.75                     | 0.69              |
| 1:a:141:LEU:HD21 | 1:a:184:ILE:HB   | 1.75                     | 0.69              |
| 1:o:145:ARG:HE   | 1:o:145:ARG:N    | 1.91                     | 0.68              |
| 1:H:106:THR:OG1  | 1:H:204:SER:HB3  | 1.93                     | 0.68              |
| 1:W:63:ILE:HD11  | 1:W:89:LEU:CD2   | 2.24                     | 0.68              |
| 1:Q:145:ARG:HE   | 1:Q:145:ARG:N    | 1.92                     | 0.68              |
| 1:7:168:TRP:HZ3  | 1:8:130:ASP:OD1  | 1.76                     | 0.68              |
| 1:w:152:TRP:HH2  | 1:w:187:CYS:SG   | 2.16                     | 0.68              |
| 1:M:63:ILE:HB    | 1:M:199:VAL:HG22 | 1.74                     | 0.68              |
| 1:G:112:GLN:HG2  | 1:L:149:VAL:HG23 | 1.75                     | 0.68              |
| 1:P:121:GLY:HA3  | 1:P:152:TRP:CE3  | 2.29                     | 0.68              |
| 1:3:145:ARG:HE   | 1:3:145:ARG:N    | 1.92                     | 0.68              |
| 1:4:163:THR:HA   | 1:6:101:ARG:HH22 | 1.59                     | 0.68              |
| 1:L:112:GLN:HG2  | 1:1:149:VAL:HG23 | 1.76                     | 0.68              |
| 1:R:152:TRP:HH2  | 1:R:187:CYS:SG   | 2.17                     | 0.68              |
| 1:D:118:ASN:HD21 | 1:U:118:ASN:HB2  | 1.59                     | 0.67              |
| 1:K:74:THR:O     | 1:K:75:ASP:C     | 2.38                     | 0.67              |
| 1:Y:118:ASN:HB2  | 1:w:118:ASN:HD21 | 1.59                     | 0.67              |
| 1:Z:101:ARG:HE   | 1:Z:166:LEU:CD2  | 2.07                     | 0.67              |
| 1:d:98:ILE:HG22  | 1:d:99:PHE:CD1   | 2.29                     | 0.67              |
| 1:I:145:ARG:HE   | 1:I:145:ARG:N    | 1.91                     | 0.67              |
| 1:6:145:ARG:HE   | 1:6:145:ARG:N    | 1.93                     | 0.67              |
| 1:9:114:MET:SD   | 1:m:122:GLY:HA3  | 2.35                     | 0.67              |
| 1:c:145:ARG:HE   | 1:c:145:ARG:N    | 1.92                     | 0.67              |
| 1:x:145:ARG:HE   | 1:x:145:ARG:N    | 1.92                     | 0.67              |
| 1:Z:175:GLN:HA   | 1:Z:178:THR:HG23 | 1.75                     | 0.67              |
| 1:n:121:GLY:HA3  | 1:n:152:TRP:HE3  | 1.60                     | 0.67              |
| 1:G:145:ARG:HE   | 1:G:145:ARG:N    | 1.92                     | 0.67              |
| 1:h:62:ARG:HD2   | 1:h:198:SER:HB3  | 1.76                     | 0.67              |
| 1:A:60:MET:O     | 1:F:142:GLN:NE2  | 2.28                     | 0.67              |
| 1:W:101:ARG:HE   | 1:W:166:LEU:HD21 | 1.60                     | 0.67              |
| 1:4:149:VAL:HG23 | 1:l:112:GLN:HG2  | 1.76                     | 0.67              |
| 1:a:130:ASP:HB3  | 1:a:132:THR:OG1  | 1.95                     | 0.67              |
| 1:C:145:ARG:HE   | 1:C:145:ARG:N    | 1.92                     | 0.67              |
| 1:b:100:GLN:OE1  | 1:c:130:ASP:OD1  | 2.13                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:118:ASN:HB2  | 1:s:118:ASN:HD21 | 1.59                     | 0.67              |
| 1:C:149:VAL:HG23 | 1:J:112:GLN:HG2  | 1.76                     | 0.66              |
| 1:T:112:GLN:HG2  | 1:l:149:VAL:HG23 | 1.77                     | 0.66              |
| 1:4:112:GLN:HG2  | 1:9:149:VAL:HG23 | 1.76                     | 0.66              |
| 1:a:121:GLY:HA3  | 1:a:152:TRP:HE3  | 1.59                     | 0.66              |
| 1:n:74:THR:O     | 1:n:75:ASP:C     | 2.37                     | 0.66              |
| 1:r:145:ARG:HE   | 1:r:145:ARG:N    | 1.93                     | 0.66              |
| 1:t:100:GLN:HB2  | 1:t:209:VAL:HG22 | 1.78                     | 0.66              |
| 1:B:91:ARG:O     | 1:J:98:ILE:HD11  | 1.96                     | 0.66              |
| 1:X:145:ARG:HE   | 1:X:145:ARG:N    | 1.93                     | 0.66              |
| 1:p:168:TRP:HZ3  | 1:q:130:ASP:OD1  | 1.77                     | 0.66              |
| 1:a:112:GLN:HG2  | 1:f:149:VAL:HG23 | 1.76                     | 0.66              |
| 1:g:176:ARG:HD2  | 1:i:168:TRP:CZ2  | 2.30                     | 0.66              |
| 1:L:145:ARG:HE   | 1:L:145:ARG:N    | 1.94                     | 0.66              |
| 1:9:145:ARG:HE   | 1:9:145:ARG:N    | 1.93                     | 0.66              |
| 1:K:121:GLY:HA3  | 1:K:152:TRP:HE3  | 1.61                     | 0.66              |
| 1:P:152:TRP:HH2  | 1:P:187:CYS:HG   | 1.44                     | 0.66              |
| 1:N:100:GLN:HB2  | 1:N:209:VAL:HG22 | 1.77                     | 0.66              |
| 1:T:149:VAL:HG23 | 1:m:112:GLN:HG2  | 1.76                     | 0.66              |
| 1:7:145:ARG:N    | 1:7:145:ARG:NE   | 2.42                     | 0.66              |
| 1:u:145:ARG:HE   | 1:u:145:ARG:N    | 1.94                     | 0.66              |
| 1:s:176:ARG:O    | 1:s:177:LEU:HD13 | 1.96                     | 0.66              |
| 1:F:145:ARG:HE   | 1:F:145:ARG:N    | 1.94                     | 0.65              |
| 1:t:121:GLY:HA3  | 1:t:152:TRP:HE3  | 1.61                     | 0.65              |
| 1:0:145:ARG:N    | 1:0:145:ARG:HE   | 1.94                     | 0.65              |
| 1:Z:74:THR:O     | 1:Z:75:ASP:C     | 2.40                     | 0.65              |
| 1:Z:149:VAL:HG23 | 1:v:112:GLN:HG2  | 1.77                     | 0.65              |
| 1:b:152:TRP:HH2  | 1:b:187:CYS:HG   | 1.44                     | 0.65              |
| 1:P:152:TRP:HH2  | 1:P:187:CYS:SG   | 2.19                     | 0.65              |
| 1:7:91:ARG:O     | 1:h:98:ILE:HD11  | 1.96                     | 0.65              |
| 1:b:101:ARG:HE   | 1:b:166:LEU:HD21 | 1.61                     | 0.65              |
| 1:E:74:THR:O     | 1:E:75:ASP:C     | 2.40                     | 0.65              |
| 1:t:101:ARG:HE   | 1:t:166:LEU:HD21 | 1.62                     | 0.65              |
| 1:H:101:ARG:NE   | 1:H:166:LEU:HD21 | 2.10                     | 0.65              |
| 1:Y:112:GLN:HG2  | 1:w:149:VAL:CG2  | 2.27                     | 0.65              |
| 1:6:112:GLN:HG2  | 1:j:149:VAL:CG2  | 2.26                     | 0.65              |
| 1:w:121:GLY:CA   | 1:w:152:TRP:HE3  | 2.10                     | 0.65              |
| 1:8:149:VAL:HG23 | 1:h:112:GLN:HG2  | 1.76                     | 0.65              |
| 1:O:145:ARG:HE   | 1:O:145:ARG:N    | 1.94                     | 0.65              |
| 1:1:196:ASN:HD22 | 1:1:196:ASN:C    | 2.05                     | 0.64              |
| 1:1:210:PRO:HG2  | 1:2:145:ARG:CD   | 2.26                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:118:ASN:HD21 | 1:j:118:ASN:HB2  | 1.62                     | 0.64              |
| 1:d:74:THR:HG23  | 1:d:190:ASN:OD1  | 1.97                     | 0.64              |
| 1:B:61:SER:OG    | 1:B:90:PRO:HD2   | 1.98                     | 0.64              |
| 1:P:106:THR:HG23 | 1:P:204:SER:HB3  | 1.79                     | 0.64              |
| 1:R:145:ARG:HE   | 1:R:145:ARG:N    | 1.96                     | 0.64              |
| 1:f:145:ARG:HE   | 1:f:145:ARG:N    | 1.95                     | 0.64              |
| 1:t:98:ILE:HG22  | 1:t:99:PHE:CD1   | 2.32                     | 0.64              |
| 1:I:91:ARG:NE    | 1:0:98:ILE:HG23  | 2.13                     | 0.64              |
| 1:b:121:GLY:HA3  | 1:b:152:TRP:HE3  | 1.62                     | 0.64              |
| 1:T:101:ARG:HE   | 1:T:166:LEU:CD2  | 2.05                     | 0.64              |
| 1:a:101:ARG:HE   | 1:a:166:LEU:HD21 | 1.61                     | 0.64              |
| 1:Q:152:TRP:HH2  | 1:Q:187:CYS:HG   | 1.44                     | 0.64              |
| 1:V:146:GLY:HA3  | 1:V:158:VAL:HG23 | 1.80                     | 0.64              |
| 1:l:190:ASN:N    | 1:l:190:ASN:OD1  | 2.29                     | 0.64              |
| 1:m:145:ARG:N    | 1:m:145:ARG:NE   | 2.46                     | 0.64              |
| 1:G:121:GLY:HA3  | 1:G:152:TRP:HE3  | 1.62                     | 0.64              |
| 1:g:122:GLY:HA3  | 1:r:114:MET:SD   | 2.37                     | 0.64              |
| 1:M:122:GLY:HA3  | 1:X:114:MET:SD   | 2.38                     | 0.64              |
| 1:a:167:LEU:HD23 | 1:a:179:SER:N    | 2.12                     | 0.64              |
| 1:W:142:GLN:HE22 | 1:j:60:MET:HG2   | 1.61                     | 0.64              |
| 1:S:145:ARG:N    | 1:S:145:ARG:HE   | 1.96                     | 0.64              |
| 1:0:152:TRP:HH2  | 1:0:187:CYS:HG   | 1.46                     | 0.63              |
| 1:g:74:THR:O     | 1:g:75:ASP:C     | 2.41                     | 0.63              |
| 1:A:210:PRO:HG2  | 1:B:145:ARG:CD   | 2.27                     | 0.63              |
| 1:b:100:GLN:HB2  | 1:b:209:VAL:HG22 | 1.79                     | 0.63              |
| 1:t:74:THR:O     | 1:t:75:ASP:C     | 2.40                     | 0.63              |
| 1:D:122:GLY:HA3  | 1:U:114:MET:SD   | 2.38                     | 0.63              |
| 1:Y:210:PRO:HG2  | 1:Z:145:ARG:HD2  | 1.81                     | 0.63              |
| 1:j:210:PRO:HG2  | 1:k:145:ARG:HD2  | 1.79                     | 0.63              |
| 1:n:145:ARG:N    | 1:n:145:ARG:HE   | 1.96                     | 0.63              |
| 1:A:69:PRO:HD2   | 1:A:72:THR:OG1   | 1.99                     | 0.63              |
| 1:7:55:VAL:HG13  | 1:h:55:VAL:HG13  | 1.79                     | 0.63              |
| 1:a:104:VAL:HG21 | 1:a:180:PRO:HG3  | 1.79                     | 0.63              |
| 1:a:122:GLY:HA3  | 1:u:114:MET:SD   | 2.39                     | 0.63              |
| 1:m:130:ASP:OD1  | 1:o:100:GLN:NE2  | 2.31                     | 0.63              |
| 1:o:62:ARG:HD2   | 1:o:198:SER:HB3  | 1.80                     | 0.63              |
| 1:L:114:MET:SD   | 1:l:122:GLY:HA3  | 2.37                     | 0.63              |
| 1:U:142:GLN:NE2  | 1:k:60:MET:O     | 2.31                     | 0.63              |
| 1:0:149:VAL:CG2  | 1:t:112:GLN:HG2  | 2.27                     | 0.63              |
| 1:2:149:VAL:HG23 | 1:s:112:GLN:HG2  | 1.79                     | 0.63              |
| 1:5:74:THR:O     | 1:5:75:ASP:C     | 2.42                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:122:GLY:HA3  | 1:x:114:MET:SD   | 2.38                     | 0.63              |
| 1:S:121:GLY:HA3  | 1:S:152:TRP:HE3  | 1.63                     | 0.63              |
| 1:p:58:SER:O     | 1:p:91:ARG:NH1   | 2.32                     | 0.63              |
| 1:l:98:ILE:HG23  | 1:O:91:ARG:NE    | 2.14                     | 0.63              |
| 1:O:94:HIS:CB    | 1:X:98:ILE:HD11  | 2.29                     | 0.63              |
| 1:W:92:LEU:HD11  | 1:W:205:VAL:HG11 | 1.81                     | 0.63              |
| 1:Y:175:GLN:HA   | 1:Y:178:THR:HG22 | 1.81                     | 0.63              |
| 1:Z:121:GLY:HA3  | 1:Z:152:TRP:HE3  | 1.64                     | 0.63              |
| 1:M:98:ILE:HG22  | 1:M:99:PHE:CD1   | 2.33                     | 0.63              |
| 1:U:145:ARG:HE   | 1:U:145:ARG:N    | 1.97                     | 0.63              |
| 1:q:79:VAL:CG2   | 1:q:185:LEU:HD13 | 2.29                     | 0.63              |
| 1:Y:210:PRO:HG2  | 1:Z:145:ARG:CD   | 2.28                     | 0.62              |
| 1:i:145:ARG:HE   | 1:i:145:ARG:N    | 1.95                     | 0.62              |
| 1:t:69:PRO:HD2   | 1:t:72:THR:OG1   | 1.99                     | 0.62              |
| 1:R:152:TRP:HH2  | 1:R:187:CYS:HG   | 1.44                     | 0.62              |
| 1:A:149:VAL:HG23 | 1:R:112:GLN:HG2  | 1.81                     | 0.62              |
| 1:M:130:ASP:OD1  | 1:M:130:ASP:N    | 2.31                     | 0.62              |
| 1:Z:146:GLY:HA3  | 1:Z:158:VAL:HG23 | 1.81                     | 0.62              |
| 1:Z:152:TRP:HH2  | 1:Z:187:CYS:HG   | 1.47                     | 0.62              |
| 1:Y:152:TRP:HH2  | 1:Y:187:CYS:SG   | 2.22                     | 0.62              |
| 1:1:55:VAL:HG13  | 1:s:55:VAL:HG13  | 1.82                     | 0.62              |
| 1:7:112:GLN:HG2  | 1:i:149:VAL:HG23 | 1.81                     | 0.62              |
| 1:X:149:VAL:HG23 | 1:w:112:GLN:HG2  | 1.81                     | 0.62              |
| 1:h:101:ARG:NE   | 1:h:166:LEU:HD21 | 2.14                     | 0.62              |
| 1:n:100:GLN:HG2  | 1:n:211:SER:CB   | 2.29                     | 0.62              |
| 1:H:91:ARG:NH1   | 1:M:98:ILE:HG23  | 2.15                     | 0.62              |
| 1:Y:91:ARG:O     | 1:v:98:ILE:HD11  | 2.00                     | 0.62              |
| 1:4:122:GLY:HA3  | 1:l:114:MET:SD   | 2.39                     | 0.62              |
| 1:5:152:TRP:HH2  | 1:5:187:CYS:HG   | 1.47                     | 0.62              |
| 1:a:127:PHE:HB3  | 1:a:160:PRO:HB3  | 1.82                     | 0.62              |
| 1:b:113:PRO:HA   | 1:b:197:VAL:HA   | 1.80                     | 0.62              |
| 1:N:145:ARG:HE   | 1:N:145:ARG:N    | 1.98                     | 0.62              |
| 1:V:98:ILE:HG22  | 1:V:99:PHE:CD1   | 2.34                     | 0.62              |
| 1:V:211:SER:OG   | 1:V:212:LEU:N    | 2.30                     | 0.62              |
| 1:V:163:THR:HA   | 1:X:101:ARG:HH22 | 1.64                     | 0.62              |
| 1:c:62:ARG:HD2   | 1:c:198:SER:HB3  | 1.82                     | 0.62              |
| 1:d:130:ASP:N    | 1:d:130:ASP:OD1  | 2.31                     | 0.62              |
| 1:n:162:TYR:O    | 1:n:164:ARG:HG3  | 2.00                     | 0.62              |
| 1:s:127:PHE:HB3  | 1:s:160:PRO:HB3  | 1.82                     | 0.62              |
| 1:P:63:ILE:HD11  | 1:P:89:LEU:HD21  | 1.82                     | 0.62              |
| 1:q:73:GLY:O     | 1:q:190:ASN:CB   | 2.46                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:168:TRP:CH2  | 1:b:176:ARG:HD2  | 2.35                     | 0.61              |
| 1:b:74:THR:O     | 1:b:75:ASP:C     | 2.43                     | 0.61              |
| 1:w:100:GLN:HB2  | 1:w:209:VAL:HG23 | 1.80                     | 0.61              |
| 1:s:121:GLY:HA3  | 1:s:152:TRP:CE3  | 2.35                     | 0.61              |
| 1:v:152:TRP:HH2  | 1:v:187:CYS:HG   | 1.48                     | 0.61              |
| 1:8:149:VAL:CG2  | 1:h:112:GLN:HG2  | 2.29                     | 0.61              |
| 1:b:149:VAL:CG2  | 1:e:112:GLN:HG2  | 2.30                     | 0.61              |
| 1:S:112:GLN:HG2  | 1:n:149:VAL:HG23 | 1.82                     | 0.61              |
| 1:4:210:PRO:HG2  | 1:5:145:ARG:CD   | 2.30                     | 0.61              |
| 1:B:121:GLY:HA3  | 1:B:152:TRP:CE3  | 2.35                     | 0.61              |
| 1:a:145:ARG:HE   | 1:a:145:ARG:N    | 1.98                     | 0.61              |
| 1:h:108:GLU:HB2  | 1:h:202:ARG:HG2  | 1.81                     | 0.61              |
| 1:D:112:GLN:HG2  | 1:O:149:VAL:HG23 | 1.83                     | 0.61              |
| 1:V:63:ILE:HD11  | 1:V:89:LEU:HD21  | 1.81                     | 0.61              |
| 1:Y:98:ILE:HD11  | 1:v:91:ARG:O     | 2.00                     | 0.61              |
| 1:Z:109:PHE:HB2  | 1:Z:158:VAL:HG13 | 1.83                     | 0.61              |
| 1:4:145:ARG:HE   | 1:4:145:ARG:N    | 1.98                     | 0.61              |
| 1:G:63:ILE:HD11  | 1:G:89:LEU:HD21  | 1.82                     | 0.61              |
| 1:M:101:ARG:HE   | 1:M:166:LEU:HD21 | 1.66                     | 0.61              |
| 1:W:63:ILE:HD11  | 1:W:89:LEU:HD21  | 1.82                     | 0.61              |
| 1:W:121:GLY:HA3  | 1:W:152:TRP:CE3  | 2.32                     | 0.61              |
| 1:1:98:ILE:HG22  | 1:1:99:PHE:CD1   | 2.34                     | 0.61              |
| 1:T:79:VAL:HG23  | 1:T:80:VAL:HG23  | 1.82                     | 0.61              |
| 1:U:149:VAL:HG23 | 1:k:112:GLN:HG2  | 1.82                     | 0.61              |
| 1:h:163:THR:OG1  | 1:h:165:THR:HG22 | 2.00                     | 0.61              |
| 1:C:152:TRP:HH2  | 1:C:187:CYS:SG   | 2.24                     | 0.61              |
| 1:I:91:ARG:O     | 1:0:98:ILE:HD11  | 2.01                     | 0.61              |
| 1:h:98:ILE:HG22  | 1:h:99:PHE:CD1   | 2.36                     | 0.61              |
| 1:G:79:VAL:HG23  | 1:G:80:VAL:HG23  | 1.83                     | 0.61              |
| 1:V:112:GLN:HG2  | 1:k:149:VAL:HG23 | 1.82                     | 0.61              |
| 1:N:101:ARG:HE   | 1:N:166:LEU:CD2  | 1.95                     | 0.60              |
| 1:Y:175:GLN:HA   | 1:Y:178:THR:CG2  | 2.29                     | 0.60              |
| 1:m:184:ILE:HG22 | 1:m:186:LEU:HD13 | 1.83                     | 0.60              |
| 1:N:100:GLN:HB2  | 1:N:209:VAL:CG2  | 2.31                     | 0.60              |
| 1:3:152:TRP:HH2  | 1:3:187:CYS:HG   | 1.49                     | 0.60              |
| 1:v:168:TRP:HZ3  | 1:w:130:ASP:OD1  | 1.83                     | 0.60              |
| 1:Y:55:VAL:HG13  | 1:v:55:VAL:HG13  | 1.82                     | 0.60              |
| 1:Z:168:TRP:HZ3  | 1:0:130:ASP:OD1  | 1.83                     | 0.60              |
| 1:7:101:ARG:NE   | 1:7:166:LEU:HD21 | 2.14                     | 0.60              |
| 1:H:196:ASN:C    | 1:H:196:ASN:HD22 | 2.08                     | 0.60              |
| 1:8:101:ARG:NE   | 1:8:166:LEU:HD21 | 2.16                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:210:PRO:HG2  | 1:e:145:ARG:CD   | 2.31                     | 0.60              |
| 1:5:101:ARG:HE   | 1:5:166:LEU:CD2  | 2.13                     | 0.60              |
| 1:q:101:ARG:HE   | 1:q:166:LEU:HD21 | 1.67                     | 0.60              |
| 1:M:69:PRO:HD2   | 1:M:72:THR:OG1   | 2.01                     | 0.60              |
| 1:S:91:ARG:O     | 1:m:98:ILE:HD11  | 2.00                     | 0.60              |
| 1:G:163:THR:HA   | 1:I:101:ARG:HH22 | 1.67                     | 0.60              |
| 1:2:182:ARG:HG3  | 1:2:184:ILE:HD11 | 1.84                     | 0.60              |
| 1:E:98:ILE:HG22  | 1:E:99:PHE:CD1   | 2.37                     | 0.60              |
| 1:Q:61:SER:OG    | 1:Q:90:PRO:HD2   | 2.00                     | 0.60              |
| 1:2:73:GLY:O     | 1:2:190:ASN:CB   | 2.49                     | 0.60              |
| 1:9:62:ARG:HD2   | 1:9:198:SER:HB3  | 1.84                     | 0.60              |
| 1:d:149:VAL:CG2  | 1:x:112:GLN:HG2  | 2.32                     | 0.60              |
| 1:N:63:ILE:HD11  | 1:N:89:LEU:HD21  | 1.82                     | 0.60              |
| 1:1:130:ASP:N    | 1:1:130:ASP:OD1  | 2.35                     | 0.60              |
| 1:d:152:TRP:HH2  | 1:d:187:CYS:SG   | 2.25                     | 0.60              |
| 1:O:152:TRP:HH2  | 1:O:187:CYS:SG   | 2.25                     | 0.59              |
| 1:Y:145:ARG:HE   | 1:Y:145:ARG:N    | 2.00                     | 0.59              |
| 1:x:62:ARG:HD2   | 1:x:198:SER:HB3  | 1.84                     | 0.59              |
| 1:B:145:ARG:HE   | 1:B:145:ARG:N    | 2.00                     | 0.59              |
| 1:1:210:PRO:HG2  | 1:2:145:ARG:HD2  | 1.84                     | 0.59              |
| 1:8:168:TRP:HZ3  | 1:9:130:ASP:OD1  | 1.84                     | 0.59              |
| 1:p:63:ILE:HD11  | 1:p:89:LEU:HD21  | 1.84                     | 0.59              |
| 1:p:73:GLY:O     | 1:p:190:ASN:HB3  | 2.00                     | 0.59              |
| 1:u:62:ARG:HD2   | 1:u:198:SER:HB3  | 1.83                     | 0.59              |
| 1:2:112:GLN:HG2  | 1:r:149:VAL:HG23 | 1.82                     | 0.59              |
| 1:6:62:ARG:HD2   | 1:6:198:SER:HB3  | 1.84                     | 0.59              |
| 1:h:146:GLY:HA3  | 1:h:158:VAL:HG23 | 1.85                     | 0.59              |
| 1:G:121:GLY:CA   | 1:G:152:TRP:HE3  | 2.15                     | 0.59              |
| 1:W:121:GLY:CA   | 1:W:152:TRP:HE3  | 2.15                     | 0.59              |
| 1:4:163:THR:OG1  | 1:4:165:THR:HG22 | 2.03                     | 0.59              |
| 1:b:74:THR:O     | 1:b:76:GLY:N     | 2.35                     | 0.59              |
| 1:l:145:ARG:N    | 1:l:145:ARG:NE   | 2.51                     | 0.59              |
| 1:N:166:LEU:HD23 | 1:N:166:LEU:O    | 2.03                     | 0.59              |
| 1:P:73:GLY:O     | 1:P:190:ASN:HB3  | 2.03                     | 0.59              |
| 1:7:89:LEU:HD13  | 1:7:203:TRP:CD1  | 2.38                     | 0.59              |
| 1:H:202:ARG:HG3  | 1:H:202:ARG:O    | 2.03                     | 0.59              |
| 1:M:149:VAL:CG2  | 1:X:112:GLN:HG2  | 2.33                     | 0.59              |
| 1:9:152:TRP:HH2  | 1:9:187:CYS:HG   | 1.51                     | 0.59              |
| 1:i:62:ARG:HD2   | 1:i:198:SER:HB3  | 1.85                     | 0.59              |
| 1:A:121:GLY:HA3  | 1:A:152:TRP:HE3  | 1.67                     | 0.59              |
| 1:6:152:TRP:HH2  | 1:6:187:CYS:HG   | 1.50                     | 0.59              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:h:74:THR:O    | 1:h:75:ASP:C     | 2.45                     | 0.59              |
| 1:t:101:ARG:HB2 | 1:t:208:SER:HB2  | 1.85                     | 0.59              |
| 1:B:132:THR:OG1 | 1:B:176:ARG:NH2  | 2.35                     | 0.59              |
| 1:G:176:ARG:CZ  | 1:I:168:TRP:CE3  | 2.86                     | 0.59              |
| 1:M:74:THR:O    | 1:M:75:ASP:C     | 2.46                     | 0.59              |
| 1:O:62:ARG:HD2  | 1:O:198:SER:HB3  | 1.84                     | 0.59              |
| 1:P:130:ASP:HB3 | 1:P:132:THR:OG1  | 2.03                     | 0.58              |
| 1:n:145:ARG:N   | 1:n:145:ARG:NE   | 2.50                     | 0.58              |
| 1:A:112:GLN:HG2 | 1:F:149:VAL:HG23 | 1.85                     | 0.58              |
| 1:H:79:VAL:HG23 | 1:H:80:VAL:HG23  | 1.84                     | 0.58              |
| 1:Z:121:GLY:HA3 | 1:Z:152:TRP:CE3  | 2.38                     | 0.58              |
| 1:x:74:THR:O    | 1:x:75:ASP:C     | 2.47                     | 0.58              |
| 1:D:176:ARG:NH1 | 1:F:168:TRP:CE3  | 2.71                     | 0.58              |
| 1:F:62:ARG:HD2  | 1:F:198:SER:HB3  | 1.85                     | 0.58              |
| 1:R:62:ARG:HD2  | 1:R:198:SER:HB3  | 1.85                     | 0.58              |
| 1:Y:94:HIS:HB2  | 1:v:98:ILE:HD11  | 1.85                     | 0.58              |
| 1:3:152:TRP:HH2 | 1:3:187:CYS:SG   | 2.25                     | 0.58              |
| 1:4:74:THR:O    | 1:4:75:ASP:C     | 2.47                     | 0.58              |
| 1:5:98:ILE:HG22 | 1:5:99:PHE:CD1   | 2.38                     | 0.58              |
| 1:d:130:ASP:O   | 1:d:132:THR:N    | 2.35                     | 0.58              |
| 1:d:152:TRP:HH2 | 1:d:187:CYS:HG   | 1.50                     | 0.58              |
| 1:7:121:GLY:O   | 1:o:114:MET:HB3  | 2.03                     | 0.58              |
| 1:r:152:TRP:HH2 | 1:r:187:CYS:HG   | 1.51                     | 0.58              |
| 1:m:63:ILE:HD11 | 1:m:89:LEU:HD21  | 1.85                     | 0.58              |
| 1:v:106:THR:HA  | 1:v:162:TYR:OH   | 2.04                     | 0.58              |
| 1:Q:87:ASP:OD1  | 1:Q:87:ASP:N     | 2.34                     | 0.58              |
| 1:2:152:TRP:HH2 | 1:2:187:CYS:SG   | 2.26                     | 0.58              |
| 1:5:168:TRP:CZ3 | 1:6:176:ARG:NH2  | 2.71                     | 0.58              |
| 1:6:114:MET:SD  | 1:j:122:GLY:HA3  | 2.44                     | 0.58              |
| 1:n:100:GLN:HB2 | 1:n:209:VAL:HG23 | 1.84                     | 0.58              |
| 1:J:74:THR:O    | 1:J:75:ASP:C     | 2.47                     | 0.58              |
| 1:S:175:GLN:HA  | 1:S:178:THR:HG22 | 1.86                     | 0.58              |
| 1:7:63:ILE:HD11 | 1:7:89:LEU:CD2   | 2.34                     | 0.58              |
| 1:g:176:ARG:NH2 | 1:i:168:TRP:CZ3  | 2.71                     | 0.58              |
| 1:q:130:ASP:OD2 | 1:q:176:ARG:NH2  | 2.36                     | 0.58              |
| 1:M:81:ASP:C    | 1:M:81:ASP:OD1   | 2.47                     | 0.58              |
| 1:C:130:ASP:HB3 | 1:C:132:THR:OG1  | 2.04                     | 0.58              |
| 1:4:73:GLY:O    | 1:4:190:ASN:HB3  | 2.04                     | 0.58              |
| 1:G:145:ARG:N   | 1:G:145:ARG:NE   | 2.51                     | 0.58              |
| 1:T:98:ILE:HG22 | 1:T:99:PHE:CD1   | 2.39                     | 0.58              |
| 1:U:62:ARG:HD2  | 1:U:198:SER:HB3  | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:152:TRP:HH2  | 1:X:187:CYS:HG   | 1.51                     | 0.58              |
| 1:O:62:ARG:HD2   | 1:O:198:SER:HB3  | 1.85                     | 0.58              |
| 1:s:192:THR:O    | 1:s:192:THR:HG22 | 2.03                     | 0.58              |
| 1:P:55:VAL:HG13  | 1:p:55:VAL:HG13  | 1.86                     | 0.57              |
| 1:t:63:ILE:HD11  | 1:t:89:LEU:CD2   | 2.34                     | 0.57              |
| 1:W:111:ILE:HG22 | 1:W:113:PRO:HD3  | 1.87                     | 0.57              |
| 1:o:152:TRP:HH2  | 1:o:187:CYS:HG   | 1.51                     | 0.57              |
| 1:L:62:ARG:HD2   | 1:L:198:SER:HB3  | 1.86                     | 0.57              |
| 1:5:62:ARG:HD2   | 1:5:198:SER:HB3  | 1.84                     | 0.57              |
| 1:q:92:LEU:HD11  | 1:q:205:VAL:HG11 | 1.85                     | 0.57              |
| 1:w:124:VAL:HG13 | 1:w:186:LEU:HB2  | 1.85                     | 0.57              |
| 1:8:100:GLN:OE1  | 1:9:130:ASP:OD1  | 2.22                     | 0.57              |
| 1:x:152:TRP:HH2  | 1:x:187:CYS:HG   | 1.50                     | 0.57              |
| 1:Z:122:GLY:HA3  | 1:v:114:MET:SD   | 2.44                     | 0.57              |
| 1:e:130:ASP:HB2  | 1:e:133:ASP:HB2  | 1.86                     | 0.57              |
| 1:s:167:LEU:HD23 | 1:s:179:SER:N    | 2.19                     | 0.57              |
| 1:A:63:ILE:HB    | 1:A:199:VAL:HG22 | 1.85                     | 0.57              |
| 1:T:106:THR:HA   | 1:T:162:TYR:OH   | 2.04                     | 0.57              |
| 1:e:73:GLY:O     | 1:e:190:ASN:HB3  | 2.03                     | 0.57              |
| 1:f:62:ARG:HD2   | 1:f:198:SER:HB3  | 1.86                     | 0.57              |
| 1:H:210:PRO:HG2  | 1:I:145:ARG:HD2  | 1.86                     | 0.57              |
| 1:I:145:ARG:N    | 1:I:145:ARG:NE   | 2.52                     | 0.57              |
| 1:K:100:GLN:HB2  | 1:K:209:VAL:HG23 | 1.86                     | 0.57              |
| 1:P:91:ARG:NH2   | 1:p:210:PRO:HB3  | 2.19                     | 0.57              |
| 1:D:210:PRO:HG2  | 1:E:145:ARG:HD2  | 1.86                     | 0.57              |
| 1:Y:79:VAL:HG23  | 1:Y:80:VAL:HG23  | 1.85                     | 0.57              |
| 1:Z:91:ARG:O     | 1:t:98:ILE:HD11  | 2.04                     | 0.57              |
| 1:Z:184:ILE:HG22 | 1:Z:186:LEU:HD13 | 1.85                     | 0.57              |
| 1:3:62:ARG:HD2   | 1:3:198:SER:HB3  | 1.85                     | 0.57              |
| 1:g:145:ARG:HE   | 1:g:145:ARG:N    | 2.03                     | 0.57              |
| 1:m:152:TRP:HH2  | 1:m:187:CYS:SG   | 2.28                     | 0.57              |
| 1:n:79:VAL:HG23  | 1:n:80:VAL:HG23  | 1.87                     | 0.57              |
| 1:s:83:THR:O     | 1:s:88:LEU:HD12  | 2.05                     | 0.57              |
| 1:A:152:TRP:HH2  | 1:A:187:CYS:SG   | 2.28                     | 0.57              |
| 1:j:113:PRO:HA   | 1:j:197:VAL:HA   | 1.86                     | 0.57              |
| 1:N:145:ARG:N    | 1:N:145:ARG:NE   | 2.53                     | 0.57              |
| 1:c:152:TRP:HH2  | 1:c:187:CYS:SG   | 2.27                     | 0.57              |
| 1:h:83:THR:HA    | 1:h:182:ARG:HB3  | 1.86                     | 0.57              |
| 1:s:175:GLN:HA   | 1:s:178:THR:HG22 | 1.87                     | 0.57              |
| 1:C:145:ARG:N    | 1:C:145:ARG:NE   | 2.53                     | 0.56              |
| 1:I:62:ARG:NH1   | 1:I:65:GLN:NE2   | 2.53                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:152:TRP:HH2  | 1:L:187:CYS:HG   | 1.53                     | 0.56              |
| 1:g:145:ARG:N    | 1:g:145:ARG:NE   | 2.53                     | 0.56              |
| 1:H:168:TRP:HZ3  | 1:I:130:ASP:CG   | 2.12                     | 0.56              |
| 1:O:62:ARG:NH1   | 1:O:65:GLN:NE2   | 2.53                     | 0.56              |
| 1:2:145:ARG:HE   | 1:2:145:ARG:N    | 2.02                     | 0.56              |
| 1:9:74:THR:O     | 1:9:75:ASP:C     | 2.49                     | 0.56              |
| 1:s:141:LEU:HD21 | 1:s:184:ILE:HB   | 1.86                     | 0.56              |
| 1:x:145:ARG:N    | 1:x:145:ARG:NE   | 2.53                     | 0.56              |
| 1:I:62:ARG:HD2   | 1:I:198:SER:HB3  | 1.86                     | 0.56              |
| 1:3:130:ASP:HB3  | 1:3:132:THR:OG1  | 2.05                     | 0.56              |
| 1:5:98:ILE:HD11  | 1:d:91:ARG:O     | 2.05                     | 0.56              |
| 1:b:111:ILE:HG21 | 1:b:123:TYR:CE2  | 2.41                     | 0.56              |
| 1:c:152:TRP:HH2  | 1:c:187:CYS:HG   | 1.53                     | 0.56              |
| 1:h:89:LEU:HD13  | 1:h:203:TRP:CD1  | 2.41                     | 0.56              |
| 1:p:210:PRO:HG2  | 1:q:145:ARG:HD3  | 1.85                     | 0.56              |
| 1:r:145:ARG:N    | 1:r:145:ARG:NE   | 2.54                     | 0.56              |
| 1:s:163:THR:HA   | 1:u:101:ARG:HH22 | 1.69                     | 0.56              |
| 1:M:146:GLY:HA3  | 1:M:158:VAL:HG23 | 1.88                     | 0.56              |
| 1:P:125:ALA:HB2  | 1:P:185:LEU:HD23 | 1.88                     | 0.56              |
| 1:3:145:ARG:N    | 1:3:145:ARG:NE   | 2.53                     | 0.56              |
| 1:7:149:VAL:HG23 | 1:o:112:GLN:HG2  | 1.86                     | 0.56              |
| 1:b:149:VAL:HG22 | 1:e:112:GLN:HG2  | 1.87                     | 0.56              |
| 1:e:121:GLY:HA3  | 1:e:152:TRP:HB2  | 1.86                     | 0.56              |
| 1:h:121:GLY:CA   | 1:h:152:TRP:HE3  | 2.17                     | 0.56              |
| 1:l:62:ARG:NH1   | 1:l:65:GLN:NE2   | 2.53                     | 0.56              |
| 1:r:152:TRP:HH2  | 1:r:187:CYS:SG   | 2.29                     | 0.56              |
| 1:A:125:ALA:HB2  | 1:A:185:LEU:HD23 | 1.87                     | 0.56              |
| 1:H:145:ARG:HE   | 1:H:145:ARG:N    | 2.04                     | 0.56              |
| 1:Q:121:GLY:HA3  | 1:Q:152:TRP:HE3  | 1.70                     | 0.56              |
| 1:X:145:ARG:N    | 1:X:145:ARG:NE   | 2.54                     | 0.56              |
| 1:r:62:ARG:HD2   | 1:r:198:SER:HB3  | 1.86                     | 0.56              |
| 1:t:100:GLN:OE1  | 1:u:130:ASP:OD1  | 2.23                     | 0.56              |
| 1:t:175:GLN:HA   | 1:t:178:THR:HG22 | 1.88                     | 0.56              |
| 1:B:145:ARG:N    | 1:B:145:ARG:NE   | 2.53                     | 0.56              |
| 1:T:152:TRP:HH2  | 1:T:187:CYS:SG   | 2.29                     | 0.56              |
| 1:2:130:ASP:OD2  | 1:2:132:THR:OG1  | 2.23                     | 0.56              |
| 1:c:145:ARG:N    | 1:c:145:ARG:NE   | 2.53                     | 0.56              |
| 1:h:69:PRO:O     | 1:h:70:ALA:C     | 2.48                     | 0.56              |
| 1:o:145:ARG:N    | 1:o:145:ARG:NE   | 2.53                     | 0.56              |
| 1:K:145:ARG:N    | 1:K:145:ARG:NE   | 2.54                     | 0.56              |
| 1:T:112:GLN:HG2  | 1:l:149:VAL:CG2  | 2.35                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:121:GLY:HA3  | 1:a:152:TRP:CE3  | 2.40                     | 0.56              |
| 1:g:81:ASP:C     | 1:g:81:ASP:OD1   | 2.49                     | 0.56              |
| 1:p:101:ARG:HE   | 1:p:166:LEU:HD21 | 1.69                     | 0.56              |
| 1:v:210:PRO:HG2  | 1:w:145:ARG:NE   | 2.21                     | 0.56              |
| 1:E:69:PRO:HD2   | 1:E:72:THR:OG1   | 2.05                     | 0.56              |
| 1:E:149:VAL:HG23 | 1:N:112:GLN:HG2  | 1.87                     | 0.56              |
| 1:E:166:LEU:O    | 1:E:166:LEU:HD23 | 2.06                     | 0.56              |
| 1:1:145:ARG:HE   | 1:1:145:ARG:N    | 2.04                     | 0.56              |
| 1:6:94:HIS:HB2   | 1:l:98:ILE:HD11  | 1.87                     | 0.56              |
| 1:6:145:ARG:N    | 1:6:145:ARG:NE   | 2.53                     | 0.56              |
| 1:q:145:ARG:HE   | 1:q:145:ARG:N    | 2.04                     | 0.56              |
| 1:F:112:GLN:HG2  | 1:S:149:VAL:CG2  | 2.27                     | 0.56              |
| 1:e:168:TRP:CZ3  | 1:f:176:ARG:NH2  | 2.74                     | 0.56              |
| 1:F:145:ARG:N    | 1:F:145:ARG:NE   | 2.54                     | 0.56              |
| 1:K:168:TRP:CZ3  | 1:L:176:ARG:NH2  | 2.74                     | 0.56              |
| 1:1:163:THR:HA   | 1:3:101:ARG:HH22 | 1.71                     | 0.56              |
| 1:7:122:GLY:HA3  | 1:o:114:MET:SD   | 2.46                     | 0.56              |
| 1:8:175:GLN:HA   | 1:8:178:THR:HG23 | 1.87                     | 0.56              |
| 1:t:86:PRO:HA    | 1:t:92:LEU:HD23  | 1.87                     | 0.56              |
| 1:E:106:THR:HA   | 1:E:162:TYR:OH   | 2.06                     | 0.55              |
| 1:Q:152:TRP:HH2  | 1:Q:187:CYS:SG   | 2.29                     | 0.55              |
| 1:X:74:THR:O     | 1:X:75:ASP:C     | 2.49                     | 0.55              |
| 1:0:152:TRP:HH2  | 1:0:187:CYS:SG   | 2.28                     | 0.55              |
| 1:e:168:TRP:CH2  | 1:f:176:ARG:HD2  | 2.40                     | 0.55              |
| 1:h:145:ARG:N    | 1:h:145:ARG:NE   | 2.54                     | 0.55              |
| 1:o:130:ASP:HB3  | 1:o:132:THR:OG1  | 2.05                     | 0.55              |
| 1:v:146:GLY:HA3  | 1:v:158:VAL:HG23 | 1.88                     | 0.55              |
| 1:B:108:GLU:OE1  | 1:B:202:ARG:NH1  | 2.39                     | 0.55              |
| 1:B:109:PHE:HB2  | 1:B:158:VAL:HG13 | 1.88                     | 0.55              |
| 1:X:152:TRP:HH2  | 1:X:187:CYS:SG   | 2.28                     | 0.55              |
| 1:2:152:TRP:HH2  | 1:2:187:CYS:HG   | 1.52                     | 0.55              |
| 1:m:58:SER:O     | 1:m:91:ARG:NH1   | 2.39                     | 0.55              |
| 1:J:98:ILE:HG22  | 1:J:99:PHE:CE1   | 2.41                     | 0.55              |
| 1:K:111:ILE:HG22 | 1:K:113:PRO:HD3  | 1.89                     | 0.55              |
| 1:T:152:TRP:HH2  | 1:T:187:CYS:HG   | 1.55                     | 0.55              |
| 1:d:130:ASP:C    | 1:d:132:THR:N    | 2.63                     | 0.55              |
| 1:B:149:VAL:CG2  | 1:E:112:GLN:HG2  | 2.37                     | 0.55              |
| 1:I:175:GLN:HA   | 1:I:178:THR:HG22 | 1.88                     | 0.55              |
| 1:P:63:ILE:HD11  | 1:P:89:LEU:CD2   | 2.37                     | 0.55              |
| 1:Q:145:ARG:N    | 1:Q:145:ARG:NE   | 2.54                     | 0.55              |
| 1:V:74:THR:O     | 1:V:75:ASP:C     | 2.49                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:Z:130:ASP:OD1 | 1:Z:176:ARG:NH2  | 2.39                     | 0.55              |
| 1:a:176:ARG:O   | 1:a:177:LEU:HD13 | 2.06                     | 0.55              |
| 1:g:79:VAL:HG23 | 1:g:80:VAL:HG23  | 1.88                     | 0.55              |
| 1:m:166:LEU:O   | 1:m:166:LEU:HD23 | 2.06                     | 0.55              |
| 1:u:175:GLN:HA  | 1:u:178:THR:HG22 | 1.89                     | 0.55              |
| 1:H:190:ASN:OD1 | 1:H:190:ASN:N    | 2.39                     | 0.55              |
| 1:Q:63:ILE:HD11 | 1:Q:89:LEU:HD21  | 1.88                     | 0.55              |
| 1:U:152:TRP:HH2 | 1:U:187:CYS:SG   | 2.29                     | 0.55              |
| 1:7:192:THR:O   | 1:7:192:THR:HG22 | 2.06                     | 0.55              |
| 1:n:79:VAL:CG2  | 1:n:185:LEU:HD13 | 2.36                     | 0.55              |
| 1:B:79:VAL:CG2  | 1:B:185:LEU:HD13 | 2.35                     | 0.55              |
| 1:D:101:ARG:NE  | 1:D:166:LEU:HD21 | 2.17                     | 0.55              |
| 1:G:55:VAL:HG13 | 1:K:55:VAL:HG13  | 1.89                     | 0.55              |
| 1:7:210:PRO:HG2 | 1:8:145:ARG:CD   | 2.37                     | 0.55              |
| 1:j:74:THR:O    | 1:j:75:ASP:C     | 2.50                     | 0.55              |
| 1:n:146:GLY:HA3 | 1:n:158:VAL:HG23 | 1.87                     | 0.55              |
| 1:o:152:TRP:HH2 | 1:o:187:CYS:SG   | 2.29                     | 0.55              |
| 1:t:168:TRP:CZ3 | 1:u:176:ARG:NH2  | 2.75                     | 0.55              |
| 1:w:106:THR:OG1 | 1:w:204:SER:HB3  | 2.07                     | 0.55              |
| 1:G:130:ASP:CG  | 1:I:168:TRP:CH2  | 2.84                     | 0.55              |
| 1:P:176:ARG:O   | 1:P:177:LEU:HD13 | 2.07                     | 0.55              |
| 1:Y:130:ASP:CG  | 1:O:168:TRP:CH2  | 2.85                     | 0.55              |
| 1:h:67:VAL:HG13 | 1:h:67:VAL:O     | 2.06                     | 0.55              |
| 1:J:125:ALA:HB2 | 1:J:185:LEU:HD23 | 1.89                     | 0.55              |
| 1:O:145:ARG:N   | 1:O:145:ARG:NE   | 2.54                     | 0.55              |
| 1:k:100:GLN:HB2 | 1:k:209:VAL:HG23 | 1.89                     | 0.55              |
| 1:m:176:ARG:CZ  | 1:o:168:TRP:CE3  | 2.90                     | 0.55              |
| 1:p:210:PRO:HG2 | 1:q:145:ARG:HD2  | 1.89                     | 0.55              |
| 1:s:196:ASN:C   | 1:s:196:ASN:HD22 | 2.14                     | 0.55              |
| 1:u:145:ARG:N   | 1:u:145:ARG:NE   | 2.54                     | 0.55              |
| 1:H:69:PRO:O    | 1:H:70:ALA:C     | 2.50                     | 0.55              |
| 1:N:79:VAL:HG23 | 1:N:80:VAL:HG23  | 1.88                     | 0.55              |
| 1:Z:149:VAL:O   | 1:Z:156:ARG:NH2  | 2.40                     | 0.55              |
| 1:i:130:ASP:HB3 | 1:i:132:THR:OG1  | 2.07                     | 0.55              |
| 1:l:62:ARG:HD2  | 1:l:198:SER:HB3  | 1.87                     | 0.55              |
| 1:O:145:ARG:N   | 1:O:145:ARG:NE   | 2.54                     | 0.54              |
| 1:2:149:VAL:CG2 | 1:s:112:GLN:HG2  | 2.37                     | 0.54              |
| 1:4:98:ILE:HG23 | 1:8:91:ARG:HD2   | 1.89                     | 0.54              |
| 1:9:175:GLN:HA  | 1:9:178:THR:HG22 | 1.89                     | 0.54              |
| 1:a:112:GLN:HG2 | 1:f:149:VAL:CG2  | 2.37                     | 0.54              |
| 1:b:86:PRO:HA   | 1:b:92:LEU:HD23  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:175:GLN:HA   | 1:c:178:THR:HG22 | 1.89                     | 0.54              |
| 1:g:190:ASN:N    | 1:g:190:ASN:OD1  | 2.39                     | 0.54              |
| 1:n:166:LEU:O    | 1:n:166:LEU:HD23 | 2.06                     | 0.54              |
| 1:s:100:GLN:OE1  | 1:t:130:ASP:OD1  | 2.24                     | 0.54              |
| 1:N:63:ILE:HD11  | 1:N:89:LEU:CD2   | 2.37                     | 0.54              |
| 1:7:145:ARG:NE   | 1:7:145:ARG:H    | 2.06                     | 0.54              |
| 1:a:89:LEU:O     | 1:a:90:PRO:C     | 2.50                     | 0.54              |
| 1:x:175:GLN:HA   | 1:x:178:THR:HG22 | 1.88                     | 0.54              |
| 1:H:100:GLN:HB2  | 1:H:209:VAL:CG2  | 2.36                     | 0.54              |
| 1:J:62:ARG:NH1   | 1:J:65:GLN:HE21  | 2.06                     | 0.54              |
| 1:L:62:ARG:NH1   | 1:L:65:GLN:NE2   | 2.56                     | 0.54              |
| 1:W:122:GLY:HA3  | 1:j:114:MET:SD   | 2.47                     | 0.54              |
| 1:Z:152:TRP:HH2  | 1:Z:187:CYS:SG   | 2.30                     | 0.54              |
| 1:5:152:TRP:HH2  | 1:5:187:CYS:SG   | 2.29                     | 0.54              |
| 1:7:145:ARG:HD3  | 1:9:210:PRO:CB   | 2.36                     | 0.54              |
| 1:9:145:ARG:N    | 1:9:145:ARG:NE   | 2.55                     | 0.54              |
| 1:f:118:ASN:HB2  | 1:v:118:ASN:HD21 | 1.71                     | 0.54              |
| 1:A:55:VAL:HG13  | 1:E:55:VAL:HG13  | 1.89                     | 0.54              |
| 1:C:62:ARG:HD2   | 1:C:198:SER:HB3  | 1.88                     | 0.54              |
| 1:K:73:GLY:O     | 1:K:190:ASN:HB3  | 2.07                     | 0.54              |
| 1:4:133:ASP:OD2  | 1:4:135:ASP:HB2  | 2.06                     | 0.54              |
| 1:6:62:ARG:NH1   | 1:6:65:GLN:NE2   | 2.54                     | 0.54              |
| 1:b:163:THR:OG1  | 1:b:165:THR:HG22 | 2.08                     | 0.54              |
| 1:E:100:GLN:OE1  | 1:F:130:ASP:OD1  | 2.24                     | 0.54              |
| 1:K:121:GLY:HA3  | 1:K:152:TRP:CE3  | 2.42                     | 0.54              |
| 1:0:130:ASP:HB3  | 1:0:132:THR:OG1  | 2.08                     | 0.54              |
| 1:7:145:ARG:HE   | 1:7:145:ARG:H    | 1.52                     | 0.54              |
| 1:b:122:GLY:HA3  | 1:e:114:MET:SD   | 2.47                     | 0.54              |
| 1:k:113:PRO:HA   | 1:k:197:VAL:HA   | 1.90                     | 0.54              |
| 1:E:146:GLY:HA3  | 1:E:158:VAL:HG23 | 1.90                     | 0.54              |
| 1:Y:74:THR:O     | 1:Y:75:ASP:C     | 2.51                     | 0.54              |
| 1:4:111:ILE:HG22 | 1:4:113:PRO:HD3  | 1.88                     | 0.54              |
| 1:c:130:ASP:HB3  | 1:c:132:THR:OG1  | 2.07                     | 0.54              |
| 1:l:100:GLN:HB3  | 1:l:209:VAL:CG2  | 2.37                     | 0.54              |
| 1:F:175:GLN:HA   | 1:F:178:THR:HG22 | 1.89                     | 0.54              |
| 1:W:168:TRP:CZ3  | 1:X:176:ARG:NH2  | 2.76                     | 0.54              |
| 1:Y:163:THR:OG1  | 1:Y:165:THR:HG22 | 2.06                     | 0.54              |
| 1:b:175:GLN:HA   | 1:b:178:THR:CG2  | 2.38                     | 0.54              |
| 1:d:130:ASP:C    | 1:d:132:THR:H    | 2.16                     | 0.54              |
| 1:p:121:GLY:CA   | 1:p:152:TRP:HE3  | 2.20                     | 0.54              |
| 1:u:152:TRP:HH2  | 1:u:187:CYS:HG   | 1.55                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:108:GLU:OE1  | 1:w:202:ARG:NH1  | 2.41                     | 0.54              |
| 1:E:175:GLN:HA   | 1:E:178:THR:HG23 | 1.87                     | 0.54              |
| 1:J:210:PRO:HG2  | 1:K:145:ARG:CD   | 2.37                     | 0.54              |
| 1:W:149:VAL:CG2  | 1:j:112:GLN:HG2  | 2.37                     | 0.54              |
| 1:4:79:VAL:CG2   | 1:4:185:LEU:HD13 | 2.38                     | 0.54              |
| 1:9:112:GLN:HG2  | 1:m:149:VAL:CG2  | 2.37                     | 0.54              |
| 1:e:151:LYS:NZ   | 1:e:154:GLU:OE1  | 2.40                     | 0.54              |
| 1:i:145:ARG:N    | 1:i:145:ARG:NE   | 2.56                     | 0.54              |
| 1:L:145:ARG:N    | 1:L:145:ARG:NE   | 2.54                     | 0.54              |
| 1:0:74:THR:O     | 1:0:75:ASP:C     | 2.50                     | 0.54              |
| 1:7:63:ILE:HD11  | 1:7:89:LEU:HD23  | 1.90                     | 0.54              |
| 1:g:124:VAL:HG13 | 1:g:186:LEU:HB2  | 1.90                     | 0.54              |
| 1:g:176:ARG:CZ   | 1:i:168:TRP:CE3  | 2.91                     | 0.54              |
| 1:h:133:ASP:OD2  | 1:h:135:ASP:HB2  | 2.08                     | 0.54              |
| 1:k:121:GLY:HA3  | 1:k:152:TRP:HE3  | 1.73                     | 0.54              |
| 1:J:152:TRP:HH2  | 1:J:187:CYS:HG   | 1.55                     | 0.54              |
| 1:T:166:LEU:HD23 | 1:T:166:LEU:O    | 2.08                     | 0.54              |
| 1:Y:91:ARG:NH2   | 1:v:210:PRO:HB3  | 2.23                     | 0.54              |
| 1:e:130:ASP:CB   | 1:e:133:ASP:HB2  | 2.38                     | 0.54              |
| 1:p:184:ILE:HG22 | 1:p:186:LEU:HD13 | 1.90                     | 0.54              |
| 1:R:100:GLN:HB3  | 1:R:209:VAL:CG2  | 2.39                     | 0.53              |
| 1:R:145:ARG:N    | 1:R:145:ARG:NE   | 2.56                     | 0.53              |
| 1:S:130:ASP:CG   | 1:U:168:TRP:HH2  | 2.16                     | 0.53              |
| 1:V:145:ARG:HE   | 1:V:145:ARG:N    | 2.06                     | 0.53              |
| 1:5:63:ILE:HD11  | 1:5:89:LEU:HD21  | 1.91                     | 0.53              |
| 1:5:100:GLN:HB2  | 1:5:209:VAL:HG22 | 1.90                     | 0.53              |
| 1:6:130:ASP:HB3  | 1:6:132:THR:OG1  | 2.08                     | 0.53              |
| 1:f:145:ARG:N    | 1:f:145:ARG:NE   | 2.56                     | 0.53              |
| 1:l:130:ASP:HB3  | 1:l:132:THR:OG1  | 2.07                     | 0.53              |
| 1:s:104:VAL:HG21 | 1:s:180:PRO:HG3  | 1.89                     | 0.53              |
| 1:s:124:VAL:HG13 | 1:s:186:LEU:HB2  | 1.89                     | 0.53              |
| 1:E:79:VAL:HG23  | 1:E:80:VAL:HG23  | 1.91                     | 0.53              |
| 1:4:63:ILE:HD11  | 1:4:201:CYS:HB3  | 1.90                     | 0.53              |
| 1:m:145:ARG:CD   | 1:o:210:PRO:HB2  | 2.38                     | 0.53              |
| 1:u:62:ARG:NH1   | 1:u:65:GLN:NE2   | 2.56                     | 0.53              |
| 1:D:121:GLY:HA3  | 1:D:152:TRP:CE3  | 2.44                     | 0.53              |
| 1:H:96:ALA:HB1   | 1:H:169:THR:HB   | 1.91                     | 0.53              |
| 1:O:74:THR:O     | 1:O:75:ASP:C     | 2.51                     | 0.53              |
| 1:Q:62:ARG:NH1   | 1:Q:65:GLN:HE21  | 2.06                     | 0.53              |
| 1:R:130:ASP:HB3  | 1:R:132:THR:OG1  | 2.08                     | 0.53              |
| 1:T:73:GLY:O     | 1:T:190:ASN:HB3  | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:162:TYR:O    | 1:Z:164:ARG:HG3  | 2.09                     | 0.53              |
| 1:e:162:TYR:O    | 1:e:164:ARG:HG3  | 2.09                     | 0.53              |
| 1:j:69:PRO:O     | 1:j:70:ALA:C     | 2.51                     | 0.53              |
| 1:k:145:ARG:HE   | 1:k:145:ARG:N    | 2.06                     | 0.53              |
| 1:t:101:ARG:HB2  | 1:t:208:SER:CB   | 2.39                     | 0.53              |
| 1:B:149:VAL:HG23 | 1:E:112:GLN:HG2  | 1.89                     | 0.53              |
| 1:C:100:GLN:HB3  | 1:C:209:VAL:CG2  | 2.38                     | 0.53              |
| 1:D:149:VAL:HG23 | 1:U:112:GLN:HG2  | 1.89                     | 0.53              |
| 1:L:175:GLN:HA   | 1:L:178:THR:HG22 | 1.90                     | 0.53              |
| 1:M:69:PRO:HG2   | 1:M:72:THR:HG21  | 1.90                     | 0.53              |
| 1:Q:74:THR:O     | 1:Q:75:ASP:C     | 2.52                     | 0.53              |
| 1:T:100:GLN:HB2  | 1:T:209:VAL:HG22 | 1.90                     | 0.53              |
| 1:Y:98:ILE:HG23  | 1:v:91:ARG:NH2   | 2.23                     | 0.53              |
| 1:2:175:GLN:HA   | 1:2:178:THR:HG22 | 1.90                     | 0.53              |
| 1:9:114:MET:SD   | 1:m:122:GLY:CA   | 2.96                     | 0.53              |
| 1:b:112:GLN:HG2  | 1:h:149:VAL:HG23 | 1.88                     | 0.53              |
| 1:b:120:GLY:N    | 1:b:192:THR:OG1  | 2.41                     | 0.53              |
| 1:j:135:ASP:OD1  | 1:j:137:THR:HG22 | 2.08                     | 0.53              |
| 1:O:152:TRP:HH2  | 1:O:187:CYS:HG   | 1.56                     | 0.53              |
| 1:S:121:GLY:CA   | 1:S:152:TRP:HE3  | 2.22                     | 0.53              |
| 1:X:62:ARG:HD2   | 1:X:198:SER:HB3  | 1.90                     | 0.53              |
| 1:f:175:GLN:HA   | 1:f:178:THR:HG22 | 1.90                     | 0.53              |
| 1:n:166:LEU:HD23 | 1:n:166:LEU:C    | 2.34                     | 0.53              |
| 1:q:121:GLY:HA3  | 1:q:152:TRP:CE3  | 2.41                     | 0.53              |
| 1:D:121:GLY:HA3  | 1:D:152:TRP:HE3  | 1.73                     | 0.53              |
| 1:L:130:ASP:HB3  | 1:L:132:THR:OG1  | 2.09                     | 0.53              |
| 1:P:114:MET:SD   | 1:q:122:GLY:HA3  | 2.49                     | 0.53              |
| 1:S:130:ASP:CG   | 1:U:168:TRP:CH2  | 2.86                     | 0.53              |
| 1:Y:145:ARG:N    | 1:Y:145:ARG:NE   | 2.55                     | 0.53              |
| 1:h:163:THR:OG1  | 1:h:165:THR:CG2  | 2.57                     | 0.53              |
| 1:v:109:PHE:HB2  | 1:v:158:VAL:HG13 | 1.89                     | 0.53              |
| 1:A:175:GLN:HB2  | 1:A:178:THR:CG2  | 2.39                     | 0.53              |
| 1:N:162:TYR:O    | 1:N:164:ARG:CG   | 2.56                     | 0.53              |
| 1:3:62:ARG:NH1   | 1:3:65:GLN:NE2   | 2.56                     | 0.53              |
| 1:7:124:VAL:HG23 | 1:7:149:VAL:HG12 | 1.90                     | 0.53              |
| 1:a:145:ARG:N    | 1:a:145:ARG:NE   | 2.57                     | 0.53              |
| 1:g:121:GLY:HA3  | 1:g:152:TRP:HE3  | 1.74                     | 0.53              |
| 1:k:89:LEU:HD13  | 1:k:203:TRP:CD1  | 2.44                     | 0.53              |
| 1:r:62:ARG:NH1   | 1:r:65:GLN:NE2   | 2.57                     | 0.53              |
| 1:W:100:GLN:OE1  | 1:X:130:ASP:OD1  | 2.26                     | 0.53              |
| 1:2:130:ASP:HB3  | 1:2:133:ASP:H    | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:r:100:GLN:HB3  | 1:r:209:VAL:CG2  | 2.39                     | 0.53              |
| 1:B:96:ALA:HB1   | 1:B:169:THR:HB   | 1.91                     | 0.53              |
| 1:Y:141:LEU:HD21 | 1:Y:184:ILE:HB   | 1.90                     | 0.53              |
| 1:6:100:GLN:HB3  | 1:6:209:VAL:CG2  | 2.39                     | 0.53              |
| 1:a:100:GLN:OE1  | 1:b:130:ASP:OD1  | 2.26                     | 0.53              |
| 1:h:63:ILE:HD11  | 1:h:89:LEU:CD2   | 2.39                     | 0.53              |
| 1:i:175:GLN:HA   | 1:i:178:THR:HG22 | 1.90                     | 0.53              |
| 1:w:145:ARG:HE   | 1:w:145:ARG:N    | 2.06                     | 0.53              |
| 1:I:122:GLY:HA3  | 1:M:114:MET:SD   | 2.48                     | 0.53              |
| 1:R:74:THR:O     | 1:R:75:ASP:C     | 2.52                     | 0.53              |
| 1:T:121:GLY:HA3  | 1:T:152:TRP:HE3  | 1.74                     | 0.53              |
| 1:9:91:ARG:NE    | 1:o:98:ILE:HG23  | 2.24                     | 0.53              |
| 1:r:175:GLN:HA   | 1:r:178:THR:HG22 | 1.90                     | 0.53              |
| 1:I:98:ILE:HD11  | 1:0:91:ARG:O     | 2.10                     | 0.52              |
| 1:R:62:ARG:NH1   | 1:R:65:GLN:NE2   | 2.57                     | 0.52              |
| 1:R:175:GLN:HA   | 1:R:178:THR:HG22 | 1.91                     | 0.52              |
| 1:U:130:ASP:HB3  | 1:U:132:THR:OG1  | 2.09                     | 0.52              |
| 1:U:145:ARG:N    | 1:U:145:ARG:NE   | 2.57                     | 0.52              |
| 1:X:130:ASP:HB3  | 1:X:132:THR:OG1  | 2.08                     | 0.52              |
| 1:2:145:ARG:N    | 1:2:145:ARG:NE   | 2.57                     | 0.52              |
| 1:4:145:ARG:N    | 1:4:145:ARG:NE   | 2.56                     | 0.52              |
| 1:7:130:ASP:OD1  | 1:9:100:GLN:NE2  | 2.42                     | 0.52              |
| 1:e:211:SER:OG   | 1:e:212:LEU:N    | 2.42                     | 0.52              |
| 1:u:152:TRP:HH2  | 1:u:187:CYS:SG   | 2.31                     | 0.52              |
| 1:B:67:VAL:HG13  | 1:B:67:VAL:O     | 2.09                     | 0.52              |
| 1:B:100:GLN:HB2  | 1:B:209:VAL:O    | 2.10                     | 0.52              |
| 1:C:175:GLN:HA   | 1:C:178:THR:HG22 | 1.92                     | 0.52              |
| 1:N:107:LEU:HD22 | 1:N:109:PHE:CZ   | 2.44                     | 0.52              |
| 1:V:98:ILE:HD11  | 1:j:91:ARG:O     | 2.09                     | 0.52              |
| 1:X:100:GLN:HB3  | 1:X:209:VAL:CG2  | 2.39                     | 0.52              |
| 1:Z:145:ARG:N    | 1:Z:145:ARG:NE   | 2.56                     | 0.52              |
| 1:f:101:ARG:HG2  | 1:f:167:LEU:O    | 2.10                     | 0.52              |
| 1:g:121:GLY:HA3  | 1:g:152:TRP:CE3  | 2.44                     | 0.52              |
| 1:w:100:GLN:HB2  | 1:w:209:VAL:CG2  | 2.39                     | 0.52              |
| 1:x:100:GLN:HB3  | 1:x:209:VAL:CG2  | 2.40                     | 0.52              |
| 1:H:109:PHE:HB2  | 1:H:158:VAL:HG13 | 1.91                     | 0.52              |
| 1:a:168:TRP:CZ3  | 1:b:176:ARG:HD2  | 2.45                     | 0.52              |
| 1:e:168:TRP:CZ3  | 1:f:176:ARG:CZ   | 2.93                     | 0.52              |
| 1:h:63:ILE:HD11  | 1:h:89:LEU:HD21  | 1.92                     | 0.52              |
| 1:i:62:ARG:NH1   | 1:i:65:GLN:NE2   | 2.57                     | 0.52              |
| 1:S:106:THR:HA   | 1:S:162:TYR:OH   | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:123:TYR:HB2  | 1:T:185:LEU:HD21 | 1.92                     | 0.52              |
| 1:U:62:ARG:NH1   | 1:U:65:GLN:NE2   | 2.56                     | 0.52              |
| 1:1:74:THR:O     | 1:1:75:ASP:C     | 2.52                     | 0.52              |
| 1:c:114:MET:SD   | 1:s:122:GLY:HA3  | 2.49                     | 0.52              |
| 1:q:111:ILE:HG22 | 1:q:113:PRO:HD3  | 1.91                     | 0.52              |
| 1:A:210:PRO:HB3  | 1:E:91:ARG:NH1   | 2.24                     | 0.52              |
| 1:I:74:THR:O     | 1:I:75:ASP:C     | 2.52                     | 0.52              |
| 1:V:152:TRP:HH2  | 1:V:187:CYS:SG   | 2.32                     | 0.52              |
| 1:k:61:SER:HB3   | 1:k:90:PRO:HD2   | 1.90                     | 0.52              |
| 1:o:62:ARG:NH1   | 1:o:65:GLN:NE2   | 2.58                     | 0.52              |
| 1:T:74:THR:O     | 1:T:76:GLY:N     | 2.43                     | 0.52              |
| 1:U:74:THR:O     | 1:U:75:ASP:C     | 2.52                     | 0.52              |
| 1:X:62:ARG:NH1   | 1:X:65:GLN:NE2   | 2.58                     | 0.52              |
| 1:4:63:ILE:HD11  | 1:4:89:LEU:HD21  | 1.91                     | 0.52              |
| 1:o:100:GLN:HB3  | 1:o:209:VAL:CG2  | 2.40                     | 0.52              |
| 1:G:98:ILE:HG23  | 1:K:91:ARG:NH1   | 2.24                     | 0.52              |
| 1:G:145:ARG:CD   | 1:I:210:PRO:HB2  | 2.39                     | 0.52              |
| 1:K:168:TRP:CE3  | 1:L:176:ARG:CZ   | 2.93                     | 0.52              |
| 1:0:100:GLN:HB3  | 1:0:209:VAL:CG2  | 2.40                     | 0.52              |
| 1:3:175:GLN:HA   | 1:3:178:THR:HG22 | 1.91                     | 0.52              |
| 1:f:130:ASP:HB3  | 1:f:132:THR:OG1  | 2.10                     | 0.52              |
| 1:h:210:PRO:HG2  | 1:i:145:ARG:HD2  | 1.92                     | 0.52              |
| 1:q:175:GLN:HA   | 1:q:178:THR:CG2  | 2.40                     | 0.52              |
| 1:v:130:ASP:OD1  | 1:x:100:GLN:CD   | 2.53                     | 0.52              |
| 1:H:98:ILE:HG22  | 1:H:99:PHE:CD1   | 2.44                     | 0.52              |
| 1:J:168:TRP:N    | 1:J:177:LEU:O    | 2.42                     | 0.52              |
| 1:L:74:THR:O     | 1:L:75:ASP:C     | 2.51                     | 0.52              |
| 1:L:100:GLN:HB3  | 1:L:209:VAL:CG2  | 2.39                     | 0.52              |
| 1:U:175:GLN:HA   | 1:U:178:THR:HG22 | 1.91                     | 0.52              |
| 1:W:145:ARG:HE   | 1:W:145:ARG:N    | 2.07                     | 0.52              |
| 1:Y:123:TYR:HB2  | 1:Y:185:LEU:CD2  | 2.40                     | 0.52              |
| 1:Y:210:PRO:HB3  | 1:v:91:ARG:NH2   | 2.25                     | 0.52              |
| 1:8:89:LEU:HD13  | 1:8:203:TRP:CD1  | 2.44                     | 0.52              |
| 1:b:63:ILE:HD11  | 1:b:89:LEU:HD21  | 1.91                     | 0.52              |
| 1:e:98:ILE:HG22  | 1:e:99:PHE:CD1   | 2.45                     | 0.52              |
| 1:f:114:MET:SD   | 1:v:122:GLY:HA2  | 2.50                     | 0.52              |
| 1:p:108:GLU:OE1  | 1:p:202:ARG:NH1  | 2.42                     | 0.52              |
| 1:U:209:VAL:HG23 | 1:U:209:VAL:O    | 2.09                     | 0.52              |
| 1:V:62:ARG:CZ    | 1:V:65:GLN:HE21  | 2.23                     | 0.52              |
| 1:X:175:GLN:HA   | 1:X:178:THR:HG22 | 1.92                     | 0.52              |
| 1:c:98:ILE:HD11  | 1:u:94:HIS:HB2   | 1.91                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:c:100:GLN:HB3 | 1:c:209:VAL:CG2  | 2.39                     | 0.52              |
| 1:d:127:PHE:HB3 | 1:d:160:PRO:HB3  | 1.92                     | 0.52              |
| 1:i:100:GLN:HB3 | 1:i:209:VAL:CG2  | 2.39                     | 0.52              |
| 1:q:74:THR:O    | 1:q:75:ASP:C     | 2.53                     | 0.52              |
| 1:F:74:THR:O    | 1:F:75:ASP:C     | 2.53                     | 0.52              |
| 1:I:114:MET:SD  | 1:Y:122:GLY:HA3  | 2.50                     | 0.52              |
| 1:N:69:PRO:HD2  | 1:N:72:THR:HG21  | 1.90                     | 0.52              |
| 1:O:100:GLN:HB3 | 1:O:209:VAL:CG2  | 2.39                     | 0.52              |
| 1:T:114:MET:HE2 | 1:l:150:ALA:C    | 2.34                     | 0.52              |
| 1:3:100:GLN:HB3 | 1:3:209:VAL:CG2  | 2.39                     | 0.52              |
| 1:7:143:ALA:CB  | 1:9:212:LEU:HB2  | 2.40                     | 0.52              |
| 1:h:79:VAL:CG2  | 1:h:185:LEU:HD13 | 2.39                     | 0.52              |
| 1:h:210:PRO:HG2 | 1:i:145:ARG:CD   | 2.40                     | 0.52              |
| 1:q:100:GLN:HB2 | 1:q:209:VAL:CG2  | 2.39                     | 0.52              |
| 1:9:152:TRP:HH2 | 1:9:187:CYS:SG   | 2.33                     | 0.51              |
| 1:g:109:PHE:HB2 | 1:g:158:VAL:HG13 | 1.93                     | 0.51              |
| 1:o:74:THR:O    | 1:o:75:ASP:C     | 2.53                     | 0.51              |
| 1:v:145:ARG:HE  | 1:v:145:ARG:N    | 2.08                     | 0.51              |
| 1:L:152:TRP:HH2 | 1:L:187:CYS:SG   | 2.32                     | 0.51              |
| 1:P:79:VAL:HG23 | 1:P:80:VAL:HG23  | 1.93                     | 0.51              |
| 1:S:98:ILE:HD11 | 1:m:91:ARG:O     | 2.10                     | 0.51              |
| 1:U:100:GLN:HB3 | 1:U:209:VAL:CG2  | 2.40                     | 0.51              |
| 1:5:145:ARG:N   | 1:5:145:ARG:NE   | 2.58                     | 0.51              |
| 1:e:145:ARG:HE  | 1:e:145:ARG:N    | 2.08                     | 0.51              |
| 1:g:146:GLY:HA3 | 1:g:158:VAL:HG23 | 1.90                     | 0.51              |
| 1:t:123:TYR:HB2 | 1:t:185:LEU:CD2  | 2.40                     | 0.51              |
| 1:u:130:ASP:HB3 | 1:u:132:THR:OG1  | 2.08                     | 0.51              |
| 1:w:79:VAL:CG2  | 1:w:185:LEU:HD13 | 2.40                     | 0.51              |
| 1:H:61:SER:HB3  | 1:H:90:PRO:HD2   | 1.92                     | 0.51              |
| 1:M:106:THR:HA  | 1:M:162:TYR:OH   | 2.09                     | 0.51              |
| 1:5:168:TRP:CZ3 | 1:6:176:ARG:CZ   | 2.93                     | 0.51              |
| 1:9:91:ARG:O    | 1:o:98:ILE:HD11  | 2.11                     | 0.51              |
| 1:h:168:TRP:HZ3 | 1:i:130:ASP:CG   | 2.18                     | 0.51              |
| 1:n:63:ILE:HD11 | 1:n:89:LEU:CD2   | 2.40                     | 0.51              |
| 1:q:121:GLY:CA  | 1:q:152:TRP:HE3  | 2.22                     | 0.51              |
| 1:r:74:THR:O    | 1:r:75:ASP:C     | 2.53                     | 0.51              |
| 1:s:101:ARG:HE  | 1:s:166:LEU:HD21 | 1.75                     | 0.51              |
| 1:t:121:GLY:HA3 | 1:t:152:TRP:CE3  | 2.43                     | 0.51              |
| 1:u:100:GLN:HB3 | 1:u:209:VAL:CG2  | 2.41                     | 0.51              |
| 1:v:108:GLU:OE1 | 1:v:202:ARG:NH1  | 2.42                     | 0.51              |
| 1:x:152:TRP:HH2 | 1:x:187:CYS:SG   | 2.33                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:124:VAL:HB   | 1:A:149:VAL:HG12 | 1.92                     | 0.51              |
| 1:F:62:ARG:NH1   | 1:F:65:GLN:NE2   | 2.58                     | 0.51              |
| 1:W:100:GLN:HG2  | 1:W:211:SER:CB   | 2.41                     | 0.51              |
| 1:3:74:THR:O     | 1:3:75:ASP:C     | 2.53                     | 0.51              |
| 1:8:79:VAL:HG23  | 1:8:80:VAL:HG23  | 1.92                     | 0.51              |
| 1:t:146:GLY:O    | 1:t:147:ALA:O    | 2.28                     | 0.51              |
| 1:E:121:GLY:HA3  | 1:E:152:TRP:HB2  | 1.91                     | 0.51              |
| 1:K:63:ILE:HD11  | 1:K:89:LEU:HD21  | 1.93                     | 0.51              |
| 1:K:100:GLN:HB2  | 1:K:209:VAL:CG2  | 2.41                     | 0.51              |
| 1:Y:100:GLN:HG2  | 1:Y:211:SER:HB3  | 1.92                     | 0.51              |
| 1:g:101:ARG:HG2  | 1:g:167:LEU:O    | 2.11                     | 0.51              |
| 1:Q:127:PHE:CZ   | 1:Q:181:GLY:HA3  | 2.46                     | 0.51              |
| 1:a:63:ILE:HD11  | 1:a:89:LEU:HD21  | 1.93                     | 0.51              |
| 1:f:74:THR:O     | 1:f:75:ASP:C     | 2.53                     | 0.51              |
| 1:g:152:TRP:HH2  | 1:g:187:CYS:SG   | 2.33                     | 0.51              |
| 1:l:175:GLN:HA   | 1:l:178:THR:HG22 | 1.92                     | 0.51              |
| 1:s:79:VAL:CG2   | 1:s:185:LEU:HD13 | 2.40                     | 0.51              |
| 1:C:62:ARG:NH1   | 1:C:65:GLN:NE2   | 2.58                     | 0.51              |
| 1:H:101:ARG:NH1  | 1:H:168:TRP:CZ2  | 2.79                     | 0.51              |
| 1:H:130:ASP:OD2  | 1:H:176:ARG:NH2  | 2.44                     | 0.51              |
| 1:J:145:ARG:N    | 1:J:145:ARG:NE   | 2.59                     | 0.51              |
| 1:M:60:MET:HE1   | 1:M:110:GLU:OE1  | 2.10                     | 0.51              |
| 1:T:101:ARG:HB2  | 1:T:208:SER:HB2  | 1.92                     | 0.51              |
| 1:V:77:TYR:C     | 1:V:77:TYR:CD1   | 2.89                     | 0.51              |
| 1:2:111:ILE:HG21 | 1:2:123:TYR:CE2  | 2.46                     | 0.51              |
| 1:5:146:GLY:HA3  | 1:5:158:VAL:HG23 | 1.92                     | 0.51              |
| 1:6:175:GLN:HA   | 1:6:178:THR:HG22 | 1.91                     | 0.51              |
| 1:8:63:ILE:HD11  | 1:8:89:LEU:HD21  | 1.93                     | 0.51              |
| 1:f:100:GLN:HB3  | 1:f:209:VAL:CG2  | 2.41                     | 0.51              |
| 1:h:100:GLN:N    | 1:h:209:VAL:O    | 2.40                     | 0.51              |
| 1:D:91:ARG:O     | 1:N:98:ILE:HD11  | 2.11                     | 0.51              |
| 1:F:100:GLN:HB3  | 1:F:209:VAL:CG2  | 2.40                     | 0.51              |
| 1:F:130:ASP:HB3  | 1:F:132:THR:OG1  | 2.11                     | 0.51              |
| 1:G:118:ASN:HD21 | 1:O:118:ASN:HB2  | 1.75                     | 0.51              |
| 1:J:130:ASP:C    | 1:J:132:THR:H    | 2.19                     | 0.51              |
| 1:Q:98:ILE:HD11  | 1:n:91:ARG:O     | 2.10                     | 0.51              |
| 1:W:122:GLY:CA   | 1:j:114:MET:SD   | 2.99                     | 0.51              |
| 1:9:100:GLN:HB3  | 1:9:209:VAL:CG2  | 2.41                     | 0.51              |
| 1:d:210:PRO:HG2  | 1:e:145:ARG:HD2  | 1.93                     | 0.51              |
| 1:f:62:ARG:NH1   | 1:f:65:GLN:NE2   | 2.59                     | 0.51              |
| 1:w:100:GLN:OE1  | 1:x:130:ASP:OD1  | 2.28                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:74:THR:O     | 1:C:75:ASP:C     | 2.52                     | 0.51              |
| 1:E:78:VAL:HG22  | 1:E:186:LEU:HD11 | 1.92                     | 0.51              |
| 1:E:130:ASP:OD2  | 1:E:176:ARG:NH2  | 2.43                     | 0.51              |
| 1:G:167:LEU:N    | 1:G:167:LEU:HD12 | 2.26                     | 0.51              |
| 1:I:98:ILE:HG23  | 1:O:91:ARG:HE    | 1.76                     | 0.51              |
| 1:S:176:ARG:HD2  | 1:U:168:TRP:CZ2  | 2.45                     | 0.51              |
| 1:4:106:THR:HG23 | 1:4:204:SER:HB3  | 1.93                     | 0.51              |
| 1:4:167:LEU:HD23 | 1:4:179:SER:N    | 2.26                     | 0.51              |
| 1:r:130:ASP:HB3  | 1:r:132:THR:OG1  | 2.10                     | 0.51              |
| 1:s:130:ASP:OD1  | 1:u:100:GLN:CD   | 2.54                     | 0.51              |
| 1:D:131:PRO:HB2  | 1:D:175:GLN:NE2  | 2.25                     | 0.51              |
| 1:Q:100:GLN:HB2  | 1:Q:209:VAL:HG22 | 1.92                     | 0.51              |
| 1:e:131:PRO:HA   | 1:e:182:ARG:HD2  | 1.93                     | 0.51              |
| 1:J:210:PRO:HG2  | 1:K:145:ARG:NE   | 2.26                     | 0.50              |
| 1:K:62:ARG:HD2   | 1:K:198:SER:HB3  | 1.93                     | 0.50              |
| 1:2:146:GLY:HA3  | 1:2:158:VAL:HG23 | 1.93                     | 0.50              |
| 1:9:130:ASP:HB3  | 1:9:132:THR:OG1  | 2.12                     | 0.50              |
| 1:c:62:ARG:NH1   | 1:c:65:GLN:NE2   | 2.58                     | 0.50              |
| 1:c:101:ARG:HG2  | 1:c:167:LEU:O    | 2.11                     | 0.50              |
| 1:D:142:GLN:HA   | 1:D:147:ALA:HB1  | 1.93                     | 0.50              |
| 1:J:122:GLY:HA3  | 1:3:114:MET:SD   | 2.51                     | 0.50              |
| 1:S:145:ARG:N    | 1:S:145:ARG:NE   | 2.59                     | 0.50              |
| 1:k:96:ALA:HB1   | 1:k:169:THR:HB   | 1.93                     | 0.50              |
| 1:E:61:SER:HB3   | 1:E:90:PRO:HD2   | 1.94                     | 0.50              |
| 1:G:101:ARG:HE   | 1:G:166:LEU:HD21 | 1.76                     | 0.50              |
| 1:L:101:ARG:HG2  | 1:L:167:LEU:O    | 2.11                     | 0.50              |
| 1:L:114:MET:SD   | 1:1:122:GLY:CA   | 2.98                     | 0.50              |
| 1:M:176:ARG:HD2  | 1:O:168:TRP:CZ2  | 2.45                     | 0.50              |
| 1:O:130:ASP:HB3  | 1:O:132:THR:OG1  | 2.12                     | 0.50              |
| 1:9:98:ILE:HG23  | 1:o:91:ARG:NE    | 2.25                     | 0.50              |
| 1:a:124:VAL:O    | 1:a:185:LEU:HD23 | 2.11                     | 0.50              |
| 1:b:69:PRO:HD2   | 1:b:72:THR:OG1   | 2.11                     | 0.50              |
| 1:d:106:THR:HG23 | 1:d:204:SER:HB3  | 1.92                     | 0.50              |
| 1:m:101:ARG:NE   | 1:m:166:LEU:HD21 | 2.22                     | 0.50              |
| 1:n:81:ASP:CG    | 1:n:81:ASP:O     | 2.54                     | 0.50              |
| 1:p:130:ASP:OD1  | 1:r:100:GLN:CD   | 2.54                     | 0.50              |
| 1:v:152:TRP:HH2  | 1:v:187:CYS:SG   | 2.35                     | 0.50              |
| 1:D:113:PRO:HA   | 1:D:197:VAL:HA   | 1.93                     | 0.50              |
| 1:I:130:ASP:HB3  | 1:I:132:THR:OG1  | 2.10                     | 0.50              |
| 1:O:62:ARG:NH1   | 1:O:65:GLN:NE2   | 2.59                     | 0.50              |
| 1:1:184:ILE:HG22 | 1:1:186:LEU:HD13 | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:5:145:ARG:N    | 1:5:145:ARG:HE   | 2.08                     | 0.50              |
| 1:7:122:GLY:HA2  | 1:7:150:ALA:O    | 2.12                     | 0.50              |
| 1:7:183:LEU:C    | 1:7:183:LEU:HD13 | 2.37                     | 0.50              |
| 1:g:79:VAL:CG2   | 1:g:185:LEU:HD13 | 2.42                     | 0.50              |
| 1:n:63:ILE:HD11  | 1:n:89:LEU:HD21  | 1.93                     | 0.50              |
| 1:q:100:GLN:HB2  | 1:q:209:VAL:HG22 | 1.93                     | 0.50              |
| 1:q:145:ARG:N    | 1:q:145:ARG:NE   | 2.58                     | 0.50              |
| 1:u:74:THR:O     | 1:u:75:ASP:C     | 2.54                     | 0.50              |
| 1:B:114:MET:SD   | 1:K:122:GLY:HA3  | 2.52                     | 0.50              |
| 1:B:124:VAL:HG11 | 1:B:138:PHE:CD2  | 2.46                     | 0.50              |
| 1:D:183:LEU:C    | 1:D:183:LEU:HD13 | 2.36                     | 0.50              |
| 1:H:74:THR:O     | 1:H:75:ASP:C     | 2.54                     | 0.50              |
| 1:N:152:TRP:HH2  | 1:N:187:CYS:HG   | 1.59                     | 0.50              |
| 1:O:175:GLN:HA   | 1:O:178:THR:HG22 | 1.93                     | 0.50              |
| 1:6:101:ARG:HG2  | 1:6:167:LEU:O    | 2.11                     | 0.50              |
| 1:a:130:ASP:OD1  | 1:c:168:TRP:HH2  | 1.94                     | 0.50              |
| 1:j:151:LYS:HD2  | 1:j:153:TRP:CZ2  | 2.47                     | 0.50              |
| 1:o:175:GLN:HA   | 1:o:178:THR:HG22 | 1.91                     | 0.50              |
| 1:N:168:TRP:HZ3  | 1:O:130:ASP:OD1  | 1.95                     | 0.50              |
| 1:S:78:VAL:HG22  | 1:S:186:LEU:HD11 | 1.94                     | 0.50              |
| 1:a:118:ASN:HD21 | 1:u:118:ASN:HB2  | 1.77                     | 0.50              |
| 1:g:66:ALA:HB3   | 1:g:197:VAL:CG1  | 2.42                     | 0.50              |
| 1:p:137:THR:HG23 | 1:p:140:ALA:HB3  | 1.92                     | 0.50              |
| 1:D:145:ARG:N    | 1:D:145:ARG:NE   | 2.60                     | 0.50              |
| 1:G:130:ASP:CG   | 1:I:168:TRP:HH2  | 2.18                     | 0.50              |
| 1:I:100:GLN:HB3  | 1:I:209:VAL:CG2  | 2.42                     | 0.50              |
| 1:9:62:ARG:NH1   | 1:9:65:GLN:NE2   | 2.60                     | 0.50              |
| 1:b:121:GLY:HA3  | 1:b:152:TRP:CE3  | 2.44                     | 0.50              |
| 1:d:122:GLY:CA   | 1:x:114:MET:SD   | 2.99                     | 0.50              |
| 1:j:116:PRO:O    | 1:j:119:THR:OG1  | 2.20                     | 0.50              |
| 1:v:124:VAL:HG13 | 1:v:186:LEU:HB2  | 1.92                     | 0.50              |
| 1:D:124:VAL:HG23 | 1:D:149:VAL:HG12 | 1.93                     | 0.50              |
| 1:E:100:GLN:CB   | 1:E:209:VAL:HG22 | 2.42                     | 0.50              |
| 1:E:145:ARG:N    | 1:E:145:ARG:NE   | 2.59                     | 0.50              |
| 1:O:175:GLN:HA   | 1:O:178:THR:HG22 | 1.92                     | 0.50              |
| 1:Q:101:ARG:NE   | 1:Q:166:LEU:HD21 | 2.06                     | 0.50              |
| 1:T:61:SER:CB    | 1:T:90:PRO:HD2   | 2.41                     | 0.50              |
| 1:V:121:GLY:CA   | 1:V:152:TRP:HE3  | 2.24                     | 0.50              |
| 1:Y:123:TYR:HB2  | 1:Y:185:LEU:HD21 | 1.94                     | 0.50              |
| 1:Z:113:PRO:HG2  | 1:Z:152:TRP:O    | 2.12                     | 0.50              |
| 1:4:89:LEU:HD13  | 1:4:203:TRP:CD1  | 2.47                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:78:VAL:HA    | 1:j:186:LEU:HD12 | 1.93                     | 0.50              |
| 1:n:146:GLY:O    | 1:n:147:ALA:C    | 2.54                     | 0.50              |
| 1:x:62:ARG:NH1   | 1:x:65:GLN:NE2   | 2.60                     | 0.50              |
| 1:E:83:THR:HA    | 1:E:182:ARG:HB3  | 1.93                     | 0.50              |
| 1:G:60:MET:O     | 1:L:142:GLN:NE2  | 2.45                     | 0.50              |
| 1:V:121:GLY:HA2  | 1:V:152:TRP:HE3  | 1.77                     | 0.50              |
| 1:V:152:TRP:HH2  | 1:V:187:CYS:HG   | 1.60                     | 0.50              |
| 1:W:118:ASN:ND2  | 1:j:118:ASN:HB2  | 2.27                     | 0.50              |
| 1:h:145:ARG:N    | 1:h:145:ARG:HE   | 2.10                     | 0.50              |
| 1:E:133:ASP:OD2  | 1:E:135:ASP:HB2  | 2.12                     | 0.49              |
| 1:M:130:ASP:OD1  | 1:O:100:GLN:NE2  | 2.45                     | 0.49              |
| 1:6:152:TRP:HH2  | 1:6:187:CYS:SG   | 2.33                     | 0.49              |
| 1:8:211:SER:OG   | 1:8:212:LEU:N    | 2.45                     | 0.49              |
| 1:w:141:LEU:HD21 | 1:w:184:ILE:HB   | 1.94                     | 0.49              |
| 1:A:163:THR:HA   | 1:C:101:ARG:HH22 | 1.78                     | 0.49              |
| 1:D:176:ARG:CZ   | 1:F:168:TRP:CE3  | 2.95                     | 0.49              |
| 1:8:121:GLY:HA3  | 1:8:152:TRP:CE3  | 2.36                     | 0.49              |
| 1:p:145:ARG:HE   | 1:p:145:ARG:N    | 2.09                     | 0.49              |
| 1:K:123:TYR:OH   | 1:K:156:ARG:HB2  | 2.12                     | 0.49              |
| 1:Z:113:PRO:HA   | 1:Z:197:VAL:HA   | 1.95                     | 0.49              |
| 1:5:100:GLN:HB2  | 1:5:209:VAL:CG2  | 2.42                     | 0.49              |
| 1:8:62:ARG:HD2   | 1:8:198:SER:HB3  | 1.94                     | 0.49              |
| 1:a:163:THR:HA   | 1:c:101:ARG:HH22 | 1.77                     | 0.49              |
| 1:d:168:TRP:N    | 1:d:177:LEU:O    | 2.45                     | 0.49              |
| 1:p:121:GLY:HA3  | 1:p:152:TRP:CE3  | 2.39                     | 0.49              |
| 1:E:63:ILE:HD12  | 1:E:88:LEU:HD13  | 1.94                     | 0.49              |
| 1:G:176:ARG:NH2  | 1:I:168:TRP:CZ3  | 2.81                     | 0.49              |
| 1:H:91:ARG:NH1   | 1:M:98:ILE:O     | 2.43                     | 0.49              |
| 1:V:94:HIS:HB2   | 1:j:98:ILE:HD11  | 1.95                     | 0.49              |
| 1:Y:176:ARG:HD2  | 1:O:168:TRP:CZ2  | 2.48                     | 0.49              |
| 1:4:139:ASP:OD1  | 1:4:139:ASP:N    | 2.46                     | 0.49              |
| 1:6:74:THR:O     | 1:6:75:ASP:C     | 2.53                     | 0.49              |
| 1:7:138:PHE:CD1  | 1:7:138:PHE:C    | 2.90                     | 0.49              |
| 1:j:73:GLY:O     | 1:j:190:ASN:HB3  | 2.11                     | 0.49              |
| 1:n:152:TRP:HH2  | 1:n:187:CYS:SG   | 2.34                     | 0.49              |
| 1:s:63:ILE:HD11  | 1:s:89:LEU:HD21  | 1.94                     | 0.49              |
| 1:B:115:CYS:HB2  | 1:B:116:PRO:HD2  | 1.94                     | 0.49              |
| 1:B:130:ASP:HB3  | 1:B:133:ASP:H    | 1.77                     | 0.49              |
| 1:H:210:PRO:CG   | 1:I:145:ARG:HD2  | 2.41                     | 0.49              |
| 1:N:130:ASP:OD2  | 1:N:176:ARG:NH2  | 2.45                     | 0.49              |
| 1:V:79:VAL:CG2   | 1:V:185:LEU:HD13 | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:111:ILE:HG21 | 1:Z:123:TYR:CE2  | 2.47                     | 0.49              |
| 1:2:60:MET:SD    | 1:2:202:ARG:HB2  | 2.53                     | 0.49              |
| 1:3:149:VAL:CG2  | 1:q:112:GLN:HG2  | 2.41                     | 0.49              |
| 1:8:100:GLN:HB2  | 1:8:209:VAL:HG23 | 1.94                     | 0.49              |
| 1:a:89:LEU:O     | 1:a:92:LEU:N     | 2.45                     | 0.49              |
| 1:s:123:TYR:CZ   | 1:s:150:ALA:HB3  | 2.47                     | 0.49              |
| 1:D:144:THR:HB   | 1:D:145:ARG:HH21 | 1.78                     | 0.49              |
| 1:M:143:ALA:HB1  | 1:X:91:ARG:HD2   | 1.95                     | 0.49              |
| 1:P:53:ASN:OD1   | 1:P:53:ASN:N     | 2.45                     | 0.49              |
| 1:R:101:ARG:HG2  | 1:R:167:LEU:O    | 2.13                     | 0.49              |
| 1:S:61:SER:HB3   | 1:S:90:PRO:HD2   | 1.95                     | 0.49              |
| 1:Y:210:PRO:HG2  | 1:Z:145:ARG:NE   | 2.28                     | 0.49              |
| 1:1:98:ILE:HG22  | 1:1:99:PHE:CE1   | 2.46                     | 0.49              |
| 1:2:168:TRP:CZ3  | 1:3:176:ARG:NH2  | 2.80                     | 0.49              |
| 1:7:63:ILE:HB    | 1:7:199:VAL:CG2  | 2.43                     | 0.49              |
| 1:7:149:VAL:HG22 | 1:o:200:LEU:HD11 | 1.94                     | 0.49              |
| 1:b:123:TYR:HB2  | 1:b:185:LEU:CD2  | 2.43                     | 0.49              |
| 1:b:125:ALA:O    | 1:b:147:ALA:HA   | 2.12                     | 0.49              |
| 1:c:74:THR:O     | 1:c:75:ASP:C     | 2.56                     | 0.49              |
| 1:h:101:ARG:HB2  | 1:h:208:SER:HB2  | 1.94                     | 0.49              |
| 1:w:141:LEU:HD22 | 1:w:186:LEU:HD22 | 1.94                     | 0.49              |
| 1:D:74:THR:O     | 1:D:75:ASP:C     | 2.55                     | 0.49              |
| 1:K:176:ARG:O    | 1:K:177:LEU:HD13 | 2.13                     | 0.49              |
| 1:K:211:SER:OG   | 1:K:212:LEU:N    | 2.45                     | 0.49              |
| 1:Q:130:ASP:OD2  | 1:Q:132:THR:OG1  | 2.31                     | 0.49              |
| 1:N:98:ILE:HG22  | 1:N:99:PHE:CD1   | 2.47                     | 0.49              |
| 1:Q:123:TYR:OH   | 1:Q:156:ARG:HB2  | 2.12                     | 0.49              |
| 1:b:112:GLN:HG2  | 1:h:149:VAL:HG22 | 1.94                     | 0.49              |
| 1:e:63:ILE:HD11  | 1:e:89:LEU:HD21  | 1.95                     | 0.49              |
| 1:n:113:PRO:HA   | 1:n:197:VAL:HA   | 1.93                     | 0.49              |
| 1:p:152:TRP:CH2  | 1:p:187:CYS:SG   | 2.90                     | 0.49              |
| 1:x:130:ASP:HB3  | 1:x:132:THR:OG1  | 2.12                     | 0.49              |
| 1:H:112:GLN:HG2  | 1:N:149:VAL:CG2  | 2.43                     | 0.49              |
| 1:H:210:PRO:HG2  | 1:I:145:ARG:CD   | 2.41                     | 0.49              |
| 1:I:114:MET:SD   | 1:Y:122:GLY:CA   | 3.01                     | 0.49              |
| 1:J:123:TYR:HA   | 1:J:186:LEU:O    | 2.13                     | 0.49              |
| 1:X:209:VAL:HG23 | 1:X:209:VAL:O    | 2.13                     | 0.49              |
| 1:9:98:ILE:HD11  | 1:o:91:ARG:O     | 2.13                     | 0.49              |
| 1:r:101:ARG:HG2  | 1:r:167:LEU:O    | 2.12                     | 0.49              |
| 1:s:61:SER:HB3   | 1:s:90:PRO:HD2   | 1.95                     | 0.49              |
| 1:s:79:VAL:CG1   | 1:s:187:CYS:SG   | 3.01                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:178:THR:O    | 1:A:178:THR:OG1  | 2.27                     | 0.49              |
| 1:F:114:MET:SD   | 1:S:122:GLY:HA3  | 2.53                     | 0.49              |
| 1:O:118:ASN:HB2  | 1:V:118:ASN:HD21 | 1.78                     | 0.49              |
| 1:P:192:THR:O    | 1:P:192:THR:HG22 | 2.13                     | 0.49              |
| 1:X:101:ARG:HG2  | 1:X:167:LEU:O    | 2.13                     | 0.49              |
| 1:a:175:GLN:HA   | 1:a:178:THR:HG22 | 1.94                     | 0.49              |
| 1:j:145:ARG:NE   | 1:j:145:ARG:N    | 2.60                     | 0.49              |
| 1:n:163:THR:OG1  | 1:n:165:THR:HG22 | 2.13                     | 0.49              |
| 1:u:209:VAL:HG23 | 1:u:209:VAL:O    | 2.12                     | 0.49              |
| 1:H:81:ASP:OD1   | 1:H:81:ASP:C     | 2.56                     | 0.48              |
| 1:H:210:PRO:HD2  | 1:I:145:ARG:HD2  | 1.94                     | 0.48              |
| 1:J:152:TRP:HH2  | 1:J:187:CYS:SG   | 2.36                     | 0.48              |
| 1:T:175:GLN:HA   | 1:T:178:THR:HG23 | 1.94                     | 0.48              |
| 1:T:210:PRO:HD2  | 1:U:145:ARG:HD2  | 1.94                     | 0.48              |
| 1:2:92:LEU:HD12  | 1:2:95:ALA:HB3   | 1.94                     | 0.48              |
| 1:2:163:THR:OG1  | 1:2:165:THR:HG22 | 2.13                     | 0.48              |
| 1:8:210:PRO:HG2  | 1:9:145:ARG:HD2  | 1.95                     | 0.48              |
| 1:i:152:TRP:HH2  | 1:i:187:CYS:SG   | 2.36                     | 0.48              |
| 1:q:141:LEU:HD21 | 1:q:184:ILE:HB   | 1.93                     | 0.48              |
| 1:s:145:ARG:HE   | 1:s:145:ARG:N    | 2.11                     | 0.48              |
| 1:v:145:ARG:N    | 1:v:145:ARG:NE   | 2.61                     | 0.48              |
| 1:B:98:ILE:HG22  | 1:B:99:PHE:CD1   | 2.48                     | 0.48              |
| 1:G:142:GLN:NE2  | 1:0:60:MET:O     | 2.45                     | 0.48              |
| 1:I:91:ARG:CZ    | 1:0:98:ILE:HG23  | 2.43                     | 0.48              |
| 1:J:100:GLN:HG2  | 1:J:211:SER:OG   | 2.14                     | 0.48              |
| 1:K:146:GLY:O    | 1:K:147:ALA:C    | 2.56                     | 0.48              |
| 1:T:171:SER:O    | 1:U:176:ARG:NH1  | 2.45                     | 0.48              |
| 1:W:63:ILE:HD11  | 1:W:89:LEU:HD23  | 1.93                     | 0.48              |
| 1:1:123:TYR:OH   | 1:1:156:ARG:HB2  | 2.13                     | 0.48              |
| 1:5:149:VAL:CG2  | 1:8:112:GLN:HG2  | 2.42                     | 0.48              |
| 1:7:196:ASN:C    | 1:7:196:ASN:HD22 | 2.20                     | 0.48              |
| 1:8:150:ALA:HB2  | 1:8:156:ARG:HE   | 1.78                     | 0.48              |
| 1:8:150:ALA:O    | 1:h:114:MET:HE2  | 2.13                     | 0.48              |
| 1:g:210:PRO:HG2  | 1:h:145:ARG:HD2  | 1.95                     | 0.48              |
| 1:n:100:GLN:HB2  | 1:n:209:VAL:CG2  | 2.43                     | 0.48              |
| 1:B:74:THR:O     | 1:B:75:ASP:C     | 2.56                     | 0.48              |
| 1:F:152:TRP:HH2  | 1:F:187:CYS:HG   | 1.61                     | 0.48              |
| 1:M:134:ASN:O    | 1:M:136:HIS:CG   | 2.67                     | 0.48              |
| 1:Q:62:ARG:NH1   | 1:Q:65:GLN:NE2   | 2.61                     | 0.48              |
| 1:Q:112:GLN:CG   | 1:o:149:VAL:HG23 | 2.37                     | 0.48              |
| 1:S:63:ILE:HB    | 1:S:199:VAL:HG22 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:122:GLY:HA3  | 1:m:114:MET:SD   | 2.52                     | 0.48              |
| 1:W:149:VAL:HG23 | 1:j:112:GLN:HG2  | 1.94                     | 0.48              |
| 1:e:106:THR:HA   | 1:e:162:TYR:OH   | 2.13                     | 0.48              |
| 1:A:74:THR:O     | 1:A:75:ASP:C     | 2.56                     | 0.48              |
| 1:M:122:GLY:CA   | 1:X:114:MET:SD   | 3.01                     | 0.48              |
| 1:W:145:ARG:N    | 1:W:145:ARG:NE   | 2.62                     | 0.48              |
| 1:2:113:PRO:HA   | 1:2:197:VAL:HA   | 1.95                     | 0.48              |
| 1:5:106:THR:OG1  | 1:5:204:SER:HB3  | 2.13                     | 0.48              |
| 1:6:114:MET:HB3  | 1:j:121:GLY:O    | 2.12                     | 0.48              |
| 1:7:83:THR:HA    | 1:7:182:ARG:HB3  | 1.95                     | 0.48              |
| 1:8:113:PRO:HA   | 1:8:197:VAL:HA   | 1.95                     | 0.48              |
| 1:e:168:TRP:CE3  | 1:f:176:ARG:CZ   | 2.97                     | 0.48              |
| 1:j:178:THR:O    | 1:j:178:THR:OG1  | 2.31                     | 0.48              |
| 1:m:98:ILE:HG22  | 1:m:99:PHE:CD1   | 2.48                     | 0.48              |
| 1:s:67:VAL:HG13  | 1:s:67:VAL:O     | 2.13                     | 0.48              |
| 1:v:163:THR:HA   | 1:x:101:ARG:NH2  | 2.11                     | 0.48              |
| 1:v:176:ARG:NH1  | 1:x:168:TRP:CE3  | 2.82                     | 0.48              |
| 1:B:112:GLN:HG2  | 1:K:149:VAL:CG2  | 2.43                     | 0.48              |
| 1:C:101:ARG:HG2  | 1:C:167:LEU:O    | 2.13                     | 0.48              |
| 1:M:121:GLY:HA3  | 1:M:152:TRP:HB2  | 1.96                     | 0.48              |
| 1:O:101:ARG:HG2  | 1:O:167:LEU:O    | 2.12                     | 0.48              |
| 1:8:166:LEU:HD23 | 1:8:166:LEU:C    | 2.39                     | 0.48              |
| 1:i:113:PRO:O    | 1:p:151:LYS:HE3  | 2.14                     | 0.48              |
| 1:w:121:GLY:HA3  | 1:w:152:TRP:CE3  | 2.43                     | 0.48              |
| 1:A:176:ARG:O    | 1:A:177:LEU:HD13 | 2.13                     | 0.48              |
| 1:D:104:VAL:HG11 | 1:D:107:LEU:HG   | 1.94                     | 0.48              |
| 1:O:94:HIS:HB2   | 1:X:98:ILE:CD1   | 2.38                     | 0.48              |
| 1:T:63:ILE:HD11  | 1:T:89:LEU:HD23  | 1.95                     | 0.48              |
| 1:T:123:TYR:HB2  | 1:T:185:LEU:CD2  | 2.43                     | 0.48              |
| 1:Y:100:GLN:HB2  | 1:Y:209:VAL:HB   | 1.95                     | 0.48              |
| 1:1:114:MET:SD   | 1:t:122:GLY:HA3  | 2.53                     | 0.48              |
| 1:q:98:ILE:HG22  | 1:q:99:PHE:CD1   | 2.49                     | 0.48              |
| 1:A:145:ARG:HE   | 1:A:145:ARG:N    | 2.11                     | 0.48              |
| 1:G:166:LEU:C    | 1:G:167:LEU:HD12 | 2.39                     | 0.48              |
| 1:H:121:GLY:CA   | 1:H:152:TRP:HE3  | 2.17                     | 0.48              |
| 1:J:167:LEU:HD23 | 1:J:179:SER:N    | 2.29                     | 0.48              |
| 1:K:67:VAL:O     | 1:K:69:PRO:HD3   | 2.13                     | 0.48              |
| 1:S:91:ARG:HD2   | 1:n:143:ALA:HB1  | 1.94                     | 0.48              |
| 1:V:145:ARG:N    | 1:V:145:ARG:NE   | 2.61                     | 0.48              |
| 1:W:108:GLU:OE1  | 1:W:202:ARG:NH1  | 2.46                     | 0.48              |
| 1:Z:212:LEU:HG   | 1:Z:212:LEU:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:55:VAL:HG13  | 1:q:55:VAL:HG13  | 1.94                     | 0.48              |
| 1:5:106:THR:HA   | 1:5:162:TYR:OH   | 2.13                     | 0.48              |
| 1:e:183:LEU:C    | 1:e:184:ILE:HD13 | 2.37                     | 0.48              |
| 1:h:101:ARG:HB2  | 1:h:208:SER:CB   | 2.43                     | 0.48              |
| 1:p:167:LEU:C    | 1:p:168:TRP:CD1  | 2.92                     | 0.48              |
| 1:q:63:ILE:HD11  | 1:q:89:LEU:HD21  | 1.95                     | 0.48              |
| 1:A:112:GLN:OE1  | 1:A:155:SER:OG   | 2.31                     | 0.48              |
| 1:H:113:PRO:HA   | 1:H:197:VAL:HA   | 1.96                     | 0.48              |
| 1:P:114:MET:HB3  | 1:q:121:GLY:O    | 2.13                     | 0.48              |
| 1:0:101:ARG:HG2  | 1:0:167:LEU:O    | 2.14                     | 0.48              |
| 1:7:98:ILE:HG23  | 1:h:91:ARG:NH1   | 2.29                     | 0.48              |
| 1:e:182:ARG:HG3  | 1:e:184:ILE:HD11 | 1.94                     | 0.48              |
| 1:h:165:THR:HG23 | 1:h:166:LEU:N    | 2.29                     | 0.48              |
| 1:l:209:VAL:HG23 | 1:l:209:VAL:O    | 2.13                     | 0.48              |
| 1:t:165:THR:HG23 | 1:t:166:LEU:N    | 2.29                     | 0.48              |
| 1:u:101:ARG:HG2  | 1:u:167:LEU:O    | 2.14                     | 0.48              |
| 1:v:163:THR:OG1  | 1:v:165:THR:HG22 | 2.12                     | 0.48              |
| 1:F:118:ASN:HB2  | 1:S:118:ASN:HD21 | 1.79                     | 0.48              |
| 1:G:127:PHE:HB3  | 1:G:160:PRO:HB3  | 1.95                     | 0.48              |
| 1:G:162:TYR:O    | 1:G:164:ARG:HG3  | 2.14                     | 0.48              |
| 1:M:176:ARG:CZ   | 1:O:168:TRP:CE3  | 2.97                     | 0.48              |
| 1:V:122:GLY:HA2  | 1:V:150:ALA:O    | 2.13                     | 0.48              |
| 1:5:130:ASP:C    | 1:5:132:THR:H    | 2.21                     | 0.48              |
| 1:j:61:SER:HB3   | 1:j:90:PRO:HD2   | 1.96                     | 0.48              |
| 1:L:209:VAL:HG23 | 1:L:209:VAL:O    | 2.13                     | 0.48              |
| 1:W:113:PRO:HA   | 1:W:197:VAL:HA   | 1.95                     | 0.48              |
| 1:2:141:LEU:O    | 1:2:144:THR:OG1  | 2.23                     | 0.48              |
| 1:2:175:GLN:HA   | 1:2:178:THR:CG2  | 2.43                     | 0.48              |
| 1:8:100:GLN:HB2  | 1:8:209:VAL:CG2  | 2.44                     | 0.48              |
| 1:a:146:GLY:HA3  | 1:a:158:VAL:HG23 | 1.96                     | 0.48              |
| 1:q:101:ARG:NH1  | 1:q:168:TRP:CZ2  | 2.82                     | 0.48              |
| 1:B:55:VAL:HG13  | 1:J:55:VAL:HG13  | 1.96                     | 0.47              |
| 1:G:113:PRO:HA   | 1:G:197:VAL:HA   | 1.95                     | 0.47              |
| 1:M:184:ILE:HG22 | 1:M:186:LEU:HD13 | 1.96                     | 0.47              |
| 1:1:101:ARG:HE   | 1:1:166:LEU:HD21 | 1.79                     | 0.47              |
| 1:9:98:ILE:HG22  | 1:9:99:PHE:CD1   | 2.48                     | 0.47              |
| 1:i:101:ARG:HG2  | 1:i:167:LEU:O    | 2.14                     | 0.47              |
| 1:n:106:THR:HA   | 1:n:162:TYR:OH   | 2.13                     | 0.47              |
| 1:n:121:GLY:HA3  | 1:n:152:TRP:CE3  | 2.43                     | 0.47              |
| 1:D:214:ASN:HD21 | 1:E:137:THR:HG21 | 1.80                     | 0.47              |
| 1:H:106:THR:OG1  | 1:H:204:SER:CB   | 2.62                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:210:PRO:HG2  | 1:Q:145:ARG:HD3  | 1.93                     | 0.47              |
| 1:Y:61:SER:HB3   | 1:Y:90:PRO:HD2   | 1.96                     | 0.47              |
| 1:1:115:CYS:HB2  | 1:1:116:PRO:HD2  | 1.96                     | 0.47              |
| 1:k:168:TRP:CZ3  | 1:l:176:ARG:NH2  | 2.82                     | 0.47              |
| 1:p:176:ARG:HD2  | 1:r:168:TRP:CZ2  | 2.50                     | 0.47              |
| 1:t:146:GLY:O    | 1:t:147:ALA:C    | 2.57                     | 0.47              |
| 1:A:149:VAL:CG2  | 1:R:200:LEU:HD11 | 2.44                     | 0.47              |
| 1:H:146:GLY:O    | 1:H:147:ALA:C    | 2.57                     | 0.47              |
| 1:J:130:ASP:C    | 1:J:132:THR:N    | 2.72                     | 0.47              |
| 1:K:113:PRO:HA   | 1:K:197:VAL:HA   | 1.96                     | 0.47              |
| 1:V:80:VAL:HB    | 1:V:185:LEU:HB2  | 1.97                     | 0.47              |
| 1:2:114:MET:HE2  | 1:r:150:ALA:C    | 2.40                     | 0.47              |
| 1:e:168:TRP:CZ2  | 1:f:176:ARG:HD2  | 2.49                     | 0.47              |
| 1:j:98:ILE:HG22  | 1:j:99:PHE:CD1   | 2.49                     | 0.47              |
| 1:l:101:ARG:HG2  | 1:l:167:LEU:O    | 2.14                     | 0.47              |
| 1:q:175:GLN:HA   | 1:q:178:THR:HG23 | 1.95                     | 0.47              |
| 1:G:176:ARG:CZ   | 1:I:168:TRP:CZ3  | 2.98                     | 0.47              |
| 1:H:145:ARG:N    | 1:H:145:ARG:NE   | 2.62                     | 0.47              |
| 1:I:149:VAL:HG22 | 1:M:200:LEU:HD11 | 1.97                     | 0.47              |
| 1:J:79:VAL:CG2   | 1:J:185:LEU:HD13 | 2.44                     | 0.47              |
| 1:J:145:ARG:N    | 1:J:145:ARG:HE   | 2.13                     | 0.47              |
| 1:L:98:ILE:HD11  | 1:3:94:HIS:CB    | 2.44                     | 0.47              |
| 1:V:109:PHE:HB2  | 1:V:158:VAL:HG13 | 1.96                     | 0.47              |
| 1:V:112:GLN:HG2  | 1:k:149:VAL:CG2  | 2.44                     | 0.47              |
| 1:W:168:TRP:HB2  | 1:W:177:LEU:O    | 2.14                     | 0.47              |
| 1:Y:191:ASN:N    | 1:Y:191:ASN:OD1  | 2.46                     | 0.47              |
| 1:1:145:ARG:NH1  | 1:1:161:GLN:HB3  | 2.29                     | 0.47              |
| 1:4:190:ASN:OD1  | 1:4:190:ASN:N    | 2.47                     | 0.47              |
| 1:a:196:ASN:HD22 | 1:a:196:ASN:C    | 2.20                     | 0.47              |
| 1:d:96:ALA:HB1   | 1:d:169:THR:HB   | 1.96                     | 0.47              |
| 1:k:101:ARG:HE   | 1:k:166:LEU:HD21 | 1.78                     | 0.47              |
| 1:I:116:PRO:HB3  | 1:Y:118:ASN:C    | 2.40                     | 0.47              |
| 1:P:145:ARG:HE   | 1:P:145:ARG:N    | 2.12                     | 0.47              |
| 1:S:98:ILE:HG23  | 1:m:91:ARG:NE    | 2.29                     | 0.47              |
| 1:S:196:ASN:HD22 | 1:S:196:ASN:C    | 2.21                     | 0.47              |
| 1:U:101:ARG:HG2  | 1:U:167:LEU:O    | 2.13                     | 0.47              |
| 1:2:77:TYR:HB3   | 1:2:187:CYS:SG   | 2.54                     | 0.47              |
| 1:4:89:LEU:HD12  | 1:4:92:LEU:HD12  | 1.95                     | 0.47              |
| 1:8:80:VAL:HB    | 1:8:185:LEU:HB2  | 1.97                     | 0.47              |
| 1:8:98:ILE:HG22  | 1:8:99:PHE:CD1   | 2.49                     | 0.47              |
| 1:9:101:ARG:HG2  | 1:9:167:LEU:O    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:165:THR:HG23 | 1:b:166:LEU:N    | 2.27                     | 0.47              |
| 1:d:124:VAL:HG11 | 1:d:138:PHE:CD2  | 2.49                     | 0.47              |
| 1:m:175:GLN:HA   | 1:m:178:THR:HG22 | 1.96                     | 0.47              |
| 1:o:101:ARG:HG2  | 1:o:167:LEU:O    | 2.13                     | 0.47              |
| 1:t:145:ARG:HE   | 1:t:145:ARG:N    | 2.12                     | 0.47              |
| 1:x:101:ARG:HG2  | 1:x:167:LEU:O    | 2.13                     | 0.47              |
| 1:B:112:GLN:HG2  | 1:K:149:VAL:HG23 | 1.96                     | 0.47              |
| 1:B:155:SER:O    | 1:B:156:ARG:HD3  | 2.14                     | 0.47              |
| 1:G:101:ARG:HG2  | 1:G:167:LEU:O    | 2.14                     | 0.47              |
| 1:J:63:ILE:HD11  | 1:J:89:LEU:HD21  | 1.95                     | 0.47              |
| 1:S:60:MET:HE1   | 1:S:110:GLU:OE1  | 2.15                     | 0.47              |
| 1:Y:151:LYS:HD2  | 1:Y:153:TRP:CZ2  | 2.49                     | 0.47              |
| 1:4:107:LEU:O    | 1:4:160:PRO:HD2  | 2.15                     | 0.47              |
| 1:4:151:LYS:HD2  | 1:4:153:TRP:CZ2  | 2.50                     | 0.47              |
| 1:7:113:PRO:HA   | 1:7:197:VAL:HA   | 1.96                     | 0.47              |
| 1:7:139:ASP:O    | 1:9:212:LEU:HD23 | 2.15                     | 0.47              |
| 1:8:100:GLN:HB2  | 1:8:209:VAL:O    | 2.15                     | 0.47              |
| 1:t:63:ILE:HD11  | 1:t:89:LEU:HD21  | 1.97                     | 0.47              |
| 1:B:106:THR:OG1  | 1:B:204:SER:HB3  | 2.15                     | 0.47              |
| 1:G:176:ARG:NH1  | 1:I:168:TRP:CE3  | 2.83                     | 0.47              |
| 1:N:123:TYR:HB2  | 1:N:185:LEU:CD2  | 2.45                     | 0.47              |
| 1:Q:142:GLN:NE2  | 1:p:60:MET:O     | 2.48                     | 0.47              |
| 1:U:152:TRP:HH2  | 1:U:187:CYS:HG   | 1.59                     | 0.47              |
| 1:W:79:VAL:HG23  | 1:W:80:VAL:HG23  | 1.97                     | 0.47              |
| 1:Y:115:CYS:HB2  | 1:Y:116:PRO:HD2  | 1.97                     | 0.47              |
| 1:Y:146:GLY:HA3  | 1:Y:158:VAL:HG23 | 1.96                     | 0.47              |
| 1:0:209:VAL:O    | 1:0:209:VAL:HG23 | 2.14                     | 0.47              |
| 1:4:123:TYR:OH   | 1:4:156:ARG:HB2  | 2.14                     | 0.47              |
| 1:7:175:GLN:HA   | 1:7:178:THR:CG2  | 2.44                     | 0.47              |
| 1:8:146:GLY:O    | 1:8:147:ALA:C    | 2.57                     | 0.47              |
| 1:b:146:GLY:O    | 1:b:147:ALA:C    | 2.57                     | 0.47              |
| 1:g:173:LYS:HD3  | 1:h:173:LYS:O    | 2.15                     | 0.47              |
| 1:i:74:THR:O     | 1:i:75:ASP:C     | 2.58                     | 0.47              |
| 1:i:112:GLN:HG2  | 1:p:149:VAL:CG2  | 2.37                     | 0.47              |
| 1:m:175:GLN:CA   | 1:m:178:THR:HG22 | 2.45                     | 0.47              |
| 1:n:146:GLY:O    | 1:n:147:ALA:O    | 2.33                     | 0.47              |
| 1:s:145:ARG:N    | 1:s:145:ARG:NE   | 2.62                     | 0.47              |
| 1:v:79:VAL:CG2   | 1:v:185:LEU:HD13 | 2.45                     | 0.47              |
| 1:1:107:LEU:HD22 | 1:1:109:PHE:CZ   | 2.50                     | 0.47              |
| 1:2:176:ARG:O    | 1:2:177:LEU:HD13 | 2.14                     | 0.47              |
| 1:3:98:ILE:HG22  | 1:3:99:PHE:CD1   | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:101:ARG:HE   | 1:h:166:LEU:CD2  | 2.18                     | 0.47              |
| 1:k:69:PRO:HD2   | 1:k:72:THR:OG1   | 2.14                     | 0.47              |
| 1:p:163:THR:OG1  | 1:p:165:THR:HG22 | 2.14                     | 0.47              |
| 1:w:63:ILE:HD11  | 1:w:89:LEU:HD21  | 1.97                     | 0.47              |
| 1:l:98:ILE:HG22  | 1:l:99:PHE:CD1   | 2.50                     | 0.47              |
| 1:Q:91:ARG:O     | 1:n:98:ILE:HD11  | 2.15                     | 0.47              |
| 1:S:184:ILE:HG22 | 1:S:186:LEU:HD13 | 1.97                     | 0.47              |
| 1:W:74:THR:O     | 1:W:75:ASP:C     | 2.58                     | 0.47              |
| 1:7:63:ILE:HB    | 1:7:199:VAL:HG23 | 1.96                     | 0.47              |
| 1:d:84:ILE:HB    | 1:d:180:PRO:HD2  | 1.97                     | 0.47              |
| 1:k:54:ASP:OD2   | 1:k:206:ARG:NH1  | 2.48                     | 0.47              |
| 1:m:101:ARG:HE   | 1:m:166:LEU:CD2  | 2.24                     | 0.47              |
| 1:w:122:GLY:N    | 1:w:152:TRP:CE3  | 2.83                     | 0.47              |
| 1:T:69:PRO:HD2   | 1:T:72:THR:OG1   | 2.14                     | 0.47              |
| 1:Y:101:ARG:CZ   | 1:Y:168:TRP:CZ2  | 2.98                     | 0.47              |
| 1:l:145:ARG:N    | 1:l:145:ARG:NE   | 2.63                     | 0.47              |
| 1:d:130:ASP:O    | 1:d:131:PRO:C    | 2.58                     | 0.47              |
| 1:j:145:ARG:N    | 1:j:145:ARG:HE   | 2.12                     | 0.47              |
| 1:j:210:PRO:HG2  | 1:k:145:ARG:NE   | 2.30                     | 0.47              |
| 1:t:212:LEU:HB2  | 1:u:143:ALA:CB   | 2.44                     | 0.47              |
| 1:v:210:PRO:HG2  | 1:w:145:ARG:HD3  | 1.93                     | 0.47              |
| 1:A:145:ARG:N    | 1:A:145:ARG:NE   | 2.63                     | 0.46              |
| 1:F:101:ARG:HG2  | 1:F:167:LEU:O    | 2.15                     | 0.46              |
| 1:P:145:ARG:N    | 1:P:145:ARG:NE   | 2.63                     | 0.46              |
| 1:U:149:VAL:CG2  | 1:k:200:LEU:HD11 | 2.45                     | 0.46              |
| 1:V:138:PHE:CD1  | 1:V:138:PHE:C    | 2.92                     | 0.46              |
| 1:Y:146:GLY:O    | 1:Y:148:VAL:HG13 | 2.16                     | 0.46              |
| 1:Z:131:PRO:HB3  | 1:Z:179:SER:HB3  | 1.97                     | 0.46              |
| 1:a:106:THR:HG23 | 1:a:204:SER:HB3  | 1.97                     | 0.46              |
| 1:b:62:ARG:HD2   | 1:b:198:SER:HB3  | 1.97                     | 0.46              |
| 1:d:168:TRP:CH2  | 1:e:176:ARG:HD2  | 2.51                     | 0.46              |
| 1:h:109:PHE:HB2  | 1:h:158:VAL:HG13 | 1.97                     | 0.46              |
| 1:k:74:THR:O     | 1:k:75:ASP:C     | 2.58                     | 0.46              |
| 1:m:60:MET:HA    | 1:m:201:CYS:O    | 2.14                     | 0.46              |
| 1:m:145:ARG:NE   | 1:o:210:PRO:HB2  | 2.30                     | 0.46              |
| 1:t:80:VAL:O     | 1:t:184:ILE:HA   | 2.15                     | 0.46              |
| 1:v:66:ALA:HB3   | 1:v:197:VAL:HG12 | 1.97                     | 0.46              |
| 1:B:63:ILE:HD11  | 1:B:89:LEU:CD2   | 2.45                     | 0.46              |
| 1:B:150:ALA:O    | 1:E:114:MET:HE2  | 2.15                     | 0.46              |
| 1:C:118:ASN:HB2  | 1:P:118:ASN:HD21 | 1.79                     | 0.46              |
| 1:E:92:LEU:HD11  | 1:E:205:VAL:HG11 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:69:PRO:HD2   | 1:P:72:THR:OG1   | 2.14                     | 0.46              |
| 1:T:98:ILE:HG23  | 1:k:91:ARG:NH1   | 2.31                     | 0.46              |
| 1:3:101:ARG:HG2  | 1:3:167:LEU:O    | 2.15                     | 0.46              |
| 1:7:143:ALA:HB1  | 1:o:91:ARG:HD2   | 1.97                     | 0.46              |
| 1:7:176:ARG:HD2  | 1:9:168:TRP:CZ2  | 2.49                     | 0.46              |
| 1:b:63:ILE:HD11  | 1:b:89:LEU:CD2   | 2.45                     | 0.46              |
| 1:d:79:VAL:HG23  | 1:d:80:VAL:HG23  | 1.97                     | 0.46              |
| 1:g:63:ILE:HD11  | 1:g:89:LEU:HD21  | 1.97                     | 0.46              |
| 1:p:141:LEU:HD21 | 1:p:184:ILE:HB   | 1.96                     | 0.46              |
| 1:v:121:GLY:CA   | 1:v:152:TRP:HE3  | 2.29                     | 0.46              |
| 1:A:98:ILE:HD11  | 1:E:94:HIS:HB2   | 1.98                     | 0.46              |
| 1:T:137:THR:O    | 1:T:138:PHE:C    | 2.58                     | 0.46              |
| 1:Z:123:TYR:CZ   | 1:Z:150:ALA:HB3  | 2.50                     | 0.46              |
| 1:1:123:TYR:HB2  | 1:1:185:LEU:CD2  | 2.45                     | 0.46              |
| 1:e:139:ASP:OD1  | 1:e:139:ASP:N    | 2.49                     | 0.46              |
| 1:h:60:MET:HE3   | 1:h:202:ARG:HB3  | 1.96                     | 0.46              |
| 1:n:96:ALA:HB1   | 1:n:169:THR:HB   | 1.97                     | 0.46              |
| 1:p:63:ILE:HD11  | 1:p:89:LEU:CD2   | 2.45                     | 0.46              |
| 1:E:79:VAL:CG2   | 1:E:185:LEU:HD13 | 2.46                     | 0.46              |
| 1:Q:81:ASP:OD2   | 1:Q:182:ARG:NH2  | 2.49                     | 0.46              |
| 1:2:184:ILE:HG22 | 1:2:186:LEU:CD1  | 2.46                     | 0.46              |
| 1:g:79:VAL:HG22  | 1:g:185:LEU:HB3  | 1.97                     | 0.46              |
| 1:w:184:ILE:HG22 | 1:w:186:LEU:HD13 | 1.98                     | 0.46              |
| 1:C:152:TRP:HH2  | 1:C:187:CYS:HG   | 1.61                     | 0.46              |
| 1:K:106:THR:HG23 | 1:K:204:SER:HB3  | 1.97                     | 0.46              |
| 1:M:121:GLY:HA2  | 1:M:152:TRP:HE3  | 1.81                     | 0.46              |
| 1:O:114:MET:SD   | 1:V:122:GLY:HA3  | 2.54                     | 0.46              |
| 1:Q:130:ASP:HB3  | 1:Q:133:ASP:H    | 1.81                     | 0.46              |
| 1:7:175:GLN:HE21 | 1:7:175:GLN:HB2  | 1.60                     | 0.46              |
| 1:e:61:SER:HB3   | 1:e:90:PRO:HD2   | 1.97                     | 0.46              |
| 1:h:62:ARG:CD    | 1:h:198:SER:HB3  | 2.43                     | 0.46              |
| 1:w:175:GLN:HA   | 1:w:178:THR:CG2  | 2.46                     | 0.46              |
| 1:D:176:ARG:HD2  | 1:F:168:TRP:CZ2  | 2.50                     | 0.46              |
| 1:E:86:PRO:HA    | 1:E:92:LEU:HD23  | 1.97                     | 0.46              |
| 1:E:211:SER:OG   | 1:E:212:LEU:N    | 2.48                     | 0.46              |
| 1:O:128:LEU:HA   | 1:O:129:PRO:HD3  | 1.82                     | 0.46              |
| 1:P:63:ILE:HB    | 1:P:199:VAL:HG22 | 1.97                     | 0.46              |
| 1:P:127:PHE:HB3  | 1:P:160:PRO:HB3  | 1.98                     | 0.46              |
| 1:W:91:ARG:NH1   | 1:w:98:ILE:CG2   | 2.79                     | 0.46              |
| 1:b:73:GLY:O     | 1:b:190:ASN:HB3  | 2.16                     | 0.46              |
| 1:g:175:GLN:CA   | 1:g:178:THR:HG22 | 2.43                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:79:VAL:HG21  | 1:h:185:LEU:HD13 | 1.97                     | 0.46              |
| 1:p:79:VAL:CG2   | 1:p:185:LEU:HD13 | 2.46                     | 0.46              |
| 1:C:99:PHE:HB3   | 1:C:208:SER:O    | 2.16                     | 0.46              |
| 1:H:152:TRP:HH2  | 1:H:187:CYS:SG   | 2.38                     | 0.46              |
| 1:I:101:ARG:HG2  | 1:I:167:LEU:O    | 2.15                     | 0.46              |
| 1:2:67:VAL:O     | 1:2:67:VAL:HG22  | 2.16                     | 0.46              |
| 1:5:141:LEU:O    | 1:5:144:THR:HG23 | 2.15                     | 0.46              |
| 1:7:176:ARG:NH1  | 1:9:170:SER:O    | 2.49                     | 0.46              |
| 1:b:145:ARG:HE   | 1:b:145:ARG:N    | 2.13                     | 0.46              |
| 1:d:74:THR:O     | 1:d:75:ASP:C     | 2.57                     | 0.46              |
| 1:g:92:LEU:HD21  | 1:g:207:LEU:HD21 | 1.98                     | 0.46              |
| 1:k:124:VAL:HG23 | 1:k:149:VAL:HG12 | 1.98                     | 0.46              |
| 1:m:176:ARG:NH2  | 1:o:168:TRP:CZ3  | 2.83                     | 0.46              |
| 1:n:123:TYR:HB2  | 1:n:185:LEU:HD21 | 1.97                     | 0.46              |
| 1:t:63:ILE:HD11  | 1:t:89:LEU:HD23  | 1.97                     | 0.46              |
| 1:t:108:GLU:HB2  | 1:t:202:ARG:HG2  | 1.96                     | 0.46              |
| 1:w:121:GLY:CA   | 1:w:152:TRP:CE3  | 2.96                     | 0.46              |
| 1:J:121:GLY:O    | 1:3:114:MET:HB3  | 2.15                     | 0.46              |
| 1:2:121:GLY:CA   | 1:2:152:TRP:HE3  | 2.28                     | 0.46              |
| 1:g:79:VAL:HG21  | 1:g:185:LEU:HD13 | 1.98                     | 0.46              |
| 1:i:98:ILE:HG23  | 1:r:91:ARG:NE    | 2.31                     | 0.46              |
| 1:k:145:ARG:NH1  | 1:k:161:GLN:HB3  | 2.31                     | 0.46              |
| 1:k:175:GLN:HA   | 1:k:178:THR:HG22 | 1.97                     | 0.46              |
| 1:q:163:THR:OG1  | 1:q:165:THR:HG22 | 2.15                     | 0.46              |
| 1:v:115:CYS:HB2  | 1:v:116:PRO:HD2  | 1.97                     | 0.46              |
| 1:B:177:LEU:O    | 1:B:178:THR:HG22 | 2.16                     | 0.46              |
| 1:F:99:PHE:HB3   | 1:F:208:SER:O    | 2.16                     | 0.46              |
| 1:I:114:MET:HB3  | 1:Y:121:GLY:O    | 2.16                     | 0.46              |
| 1:J:162:TYR:CD1  | 1:J:162:TYR:N    | 2.84                     | 0.46              |
| 1:K:79:VAL:CG2   | 1:K:185:LEU:HD13 | 2.46                     | 0.46              |
| 1:M:184:ILE:HG22 | 1:M:186:LEU:CD1  | 2.45                     | 0.46              |
| 1:Q:184:ILE:HG22 | 1:Q:186:LEU:HD13 | 1.98                     | 0.46              |
| 1:V:101:ARG:HE   | 1:V:166:LEU:HD21 | 1.81                     | 0.46              |
| 1:Y:118:ASN:HB2  | 1:w:118:ASN:ND2  | 2.29                     | 0.46              |
| 1:Z:184:ILE:CG2  | 1:Z:186:LEU:HD13 | 2.46                     | 0.46              |
| 1:6:209:VAL:HG23 | 1:6:209:VAL:O    | 2.15                     | 0.46              |
| 1:e:138:PHE:CE1  | 1:e:142:GLN:HG3  | 2.51                     | 0.46              |
| 1:f:152:TRP:HH2  | 1:f:187:CYS:SG   | 2.39                     | 0.46              |
| 1:t:113:PRO:HA   | 1:t:197:VAL:HA   | 1.98                     | 0.46              |
| 1:B:122:GLY:HA3  | 1:E:114:MET:SD   | 2.56                     | 0.46              |
| 1:G:98:ILE:HD11  | 1:K:91:ARG:O     | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:210:PRO:HB2  | 1:I:145:ARG:NE   | 2.31                     | 0.46              |
| 1:M:77:TYR:CD1   | 1:M:77:TYR:C     | 2.94                     | 0.46              |
| 1:Q:145:ARG:NH1  | 1:Q:161:GLN:HB3  | 2.31                     | 0.46              |
| 1:S:79:VAL:HG23  | 1:S:80:VAL:HG23  | 1.98                     | 0.46              |
| 1:V:121:GLY:HA3  | 1:V:152:TRP:HB2  | 1.98                     | 0.46              |
| 1:O:151:LYS:HD2  | 1:O:153:TRP:CZ2  | 2.52                     | 0.46              |
| 1:1:124:VAL:HG23 | 1:1:149:VAL:HG12 | 1.97                     | 0.46              |
| 1:5:130:ASP:C    | 1:5:132:THR:N    | 2.71                     | 0.46              |
| 1:7:96:ALA:HB1   | 1:7:169:THR:HB   | 1.98                     | 0.46              |
| 1:a:73:GLY:O     | 1:a:190:ASN:HB3  | 2.16                     | 0.46              |
| 1:b:91:ARG:O     | 1:g:98:ILE:HD11  | 2.16                     | 0.46              |
| 1:D:149:VAL:CG2  | 1:U:112:GLN:HG2  | 2.46                     | 0.45              |
| 1:M:162:TYR:O    | 1:M:164:ARG:HG3  | 2.16                     | 0.45              |
| 1:N:152:TRP:HH2  | 1:N:187:CYS:SG   | 2.39                     | 0.45              |
| 1:Q:163:THR:OG1  | 1:Q:165:THR:CG2  | 2.64                     | 0.45              |
| 1:8:145:ARG:N    | 1:8:145:ARG:NE   | 2.64                     | 0.45              |
| 1:l:151:LYS:HD2  | 1:l:153:TRP:CZ2  | 2.52                     | 0.45              |
| 1:p:210:PRO:HG2  | 1:q:145:ARG:NE   | 2.30                     | 0.45              |
| 1:w:168:TRP:HB2  | 1:w:177:LEU:O    | 2.15                     | 0.45              |
| 1:D:61:SER:HB3   | 1:D:90:PRO:HD2   | 1.98                     | 0.45              |
| 1:E:79:VAL:HG22  | 1:E:185:LEU:HB3  | 1.98                     | 0.45              |
| 1:E:146:GLY:O    | 1:E:147:ALA:C    | 2.60                     | 0.45              |
| 1:H:124:VAL:HG13 | 1:H:186:LEU:HB2  | 1.97                     | 0.45              |
| 1:I:122:GLY:CA   | 1:M:114:MET:SD   | 3.05                     | 0.45              |
| 1:1:128:LEU:HD22 | 1:1:128:LEU:H    | 1.81                     | 0.45              |
| 1:7:61:SER:HB3   | 1:7:90:PRO:HD2   | 1.99                     | 0.45              |
| 1:d:83:THR:HA    | 1:d:182:ARG:HB3  | 1.99                     | 0.45              |
| 1:d:145:ARG:HE   | 1:d:145:ARG:N    | 2.14                     | 0.45              |
| 1:g:130:ASP:N    | 1:g:130:ASP:OD1  | 2.49                     | 0.45              |
| 1:q:101:ARG:HE   | 1:q:166:LEU:CD2  | 2.28                     | 0.45              |
| 1:E:74:THR:O     | 1:E:76:GLY:N     | 2.50                     | 0.45              |
| 1:T:175:GLN:HA   | 1:T:178:THR:CG2  | 2.47                     | 0.45              |
| 1:7:173:LYS:O    | 1:9:173:LYS:HD3  | 2.16                     | 0.45              |
| 1:7:176:ARG:CZ   | 1:9:168:TRP:CE3  | 3.00                     | 0.45              |
| 1:a:184:ILE:HG22 | 1:a:186:LEU:CD1  | 2.46                     | 0.45              |
| 1:d:98:ILE:HG22  | 1:d:99:PHE:CE1   | 2.51                     | 0.45              |
| 1:o:128:LEU:HA   | 1:o:129:PRO:HD3  | 1.82                     | 0.45              |
| 1:q:168:TRP:HB2  | 1:q:177:LEU:O    | 2.16                     | 0.45              |
| 1:E:79:VAL:HG21  | 1:E:185:LEU:HD13 | 1.99                     | 0.45              |
| 1:G:109:PHE:HB2  | 1:G:158:VAL:HG22 | 1.98                     | 0.45              |
| 1:G:210:PRO:HG2  | 1:H:145:ARG:HD3  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:168:TRP:CZ3  | 1:L:176:ARG:CZ   | 2.99                     | 0.45              |
| 1:M:121:GLY:CA   | 1:M:152:TRP:HE3  | 2.29                     | 0.45              |
| 1:M:145:ARG:N    | 1:M:145:ARG:NE   | 2.65                     | 0.45              |
| 1:Z:145:ARG:N    | 1:Z:145:ARG:HE   | 2.13                     | 0.45              |
| 1:5:69:PRO:HD2   | 1:5:72:THR:OG1   | 2.15                     | 0.45              |
| 1:8:74:THR:O     | 1:8:76:GLY:N     | 2.48                     | 0.45              |
| 1:8:105:GLU:O    | 1:8:106:THR:HG23 | 2.17                     | 0.45              |
| 1:n:115:CYS:HB2  | 1:n:116:PRO:HD2  | 1.99                     | 0.45              |
| 1:n:168:TRP:HD1  | 1:n:177:LEU:HB3  | 1.81                     | 0.45              |
| 1:o:98:ILE:HG22  | 1:o:99:PHE:CD1   | 2.52                     | 0.45              |
| 1:p:176:ARG:NH1  | 1:r:168:TRP:CE3  | 2.85                     | 0.45              |
| 1:s:73:GLY:O     | 1:s:190:ASN:HA   | 2.17                     | 0.45              |
| 1:t:111:ILE:HG21 | 1:t:123:TYR:CE2  | 2.52                     | 0.45              |
| 1:2:98:ILE:HD11  | 1:q:95:ALA:N     | 2.31                     | 0.45              |
| 1:g:123:TYR:HB2  | 1:g:185:LEU:CD2  | 2.46                     | 0.45              |
| 1:m:184:ILE:CG2  | 1:m:186:LEU:HD13 | 2.45                     | 0.45              |
| 1:t:212:LEU:O    | 1:t:212:LEU:HG   | 2.16                     | 0.45              |
| 1:A:138:PHE:CD1  | 1:A:138:PHE:C    | 2.94                     | 0.45              |
| 1:D:63:ILE:HB    | 1:D:199:VAL:HG22 | 1.98                     | 0.45              |
| 1:V:59:GLY:HA3   | 1:V:203:TRP:CZ2  | 2.52                     | 0.45              |
| 1:V:89:LEU:HD13  | 1:V:203:TRP:CD1  | 2.52                     | 0.45              |
| 1:V:123:TYR:OH   | 1:V:154:GLU:O    | 2.30                     | 0.45              |
| 1:W:73:GLY:O     | 1:W:190:ASN:HB3  | 2.16                     | 0.45              |
| 1:Y:98:ILE:HG23  | 1:v:91:ARG:CZ    | 2.47                     | 0.45              |
| 1:6:114:MET:SD   | 1:j:122:GLY:CA   | 3.04                     | 0.45              |
| 1:8:127:PHE:CZ   | 1:8:181:GLY:HA3  | 2.52                     | 0.45              |
| 1:a:192:THR:HG22 | 1:a:192:THR:O    | 2.16                     | 0.45              |
| 1:b:91:ARG:NH1   | 1:g:98:ILE:HG23  | 2.32                     | 0.45              |
| 1:f:118:ASN:HB2  | 1:v:118:ASN:ND2  | 2.30                     | 0.45              |
| 1:r:98:ILE:HG22  | 1:r:99:PHE:CD1   | 2.52                     | 0.45              |
| 1:C:98:ILE:HG22  | 1:C:99:PHE:CD1   | 2.52                     | 0.45              |
| 1:C:132:THR:HG21 | 1:C:176:ARG:NH2  | 2.32                     | 0.45              |
| 1:G:81:ASP:C     | 1:G:81:ASP:OD1   | 2.60                     | 0.45              |
| 1:K:69:PRO:O     | 1:K:70:ALA:C     | 2.59                     | 0.45              |
| 1:T:130:ASP:OD2  | 1:T:176:ARG:NH2  | 2.50                     | 0.45              |
| 1:2:174:GLU:HB3  | 1:3:174:GLU:OE2  | 2.16                     | 0.45              |
| 1:7:106:THR:HA   | 1:7:162:TYR:OH   | 2.16                     | 0.45              |
| 1:c:151:LYS:HD2  | 1:c:153:TRP:CZ2  | 2.52                     | 0.45              |
| 1:k:166:LEU:O    | 1:k:166:LEU:HD23 | 2.17                     | 0.45              |
| 1:m:62:ARG:HD3   | 1:m:198:SER:HB3  | 1.98                     | 0.45              |
| 1:p:145:ARG:N    | 1:p:145:ARG:NE   | 2.64                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:101:ARG:CZ   | 1:M:168:TRP:CZ2  | 3.00                     | 0.45              |
| 1:M:168:TRP:HZ3  | 1:N:130:ASP:OD1  | 2.00                     | 0.45              |
| 1:P:130:ASP:OD1  | 1:R:168:TRP:HH2  | 2.00                     | 0.45              |
| 1:S:152:TRP:HH2  | 1:S:187:CYS:SG   | 2.39                     | 0.45              |
| 1:V:81:ASP:CG    | 1:V:182:ARG:HH21 | 2.25                     | 0.45              |
| 1:W:55:VAL:HG13  | 1:w:55:VAL:HG13  | 1.99                     | 0.45              |
| 1:Z:100:GLN:HB2  | 1:Z:209:VAL:HG22 | 1.98                     | 0.45              |
| 1:Z:101:ARG:HB2  | 1:Z:208:SER:HB2  | 1.99                     | 0.45              |
| 1:1:89:LEU:HD13  | 1:1:203:TRP:CD1  | 2.51                     | 0.45              |
| 1:7:128:LEU:HD22 | 1:7:128:LEU:H    | 1.81                     | 0.45              |
| 1:b:114:MET:HE2  | 1:h:150:ALA:C    | 2.41                     | 0.45              |
| 1:b:152:TRP:HH2  | 1:b:187:CYS:SG   | 2.38                     | 0.45              |
| 1:e:128:LEU:HA   | 1:e:129:PRO:HD3  | 1.79                     | 0.45              |
| 1:h:130:ASP:C    | 1:h:132:THR:N    | 2.74                     | 0.45              |
| 1:j:130:ASP:N    | 1:j:130:ASP:OD1  | 2.49                     | 0.45              |
| 1:l:98:ILE:HG22  | 1:l:99:PHE:CD1   | 2.52                     | 0.45              |
| 1:m:100:GLN:HG2  | 1:m:211:SER:OG   | 2.17                     | 0.45              |
| 1:p:63:ILE:HD12  | 1:p:88:LEU:HD13  | 1.99                     | 0.45              |
| 1:G:80:VAL:HB    | 1:G:185:LEU:HB2  | 1.99                     | 0.45              |
| 1:G:128:LEU:HA   | 1:G:129:PRO:HD3  | 1.74                     | 0.45              |
| 1:H:79:VAL:CG2   | 1:H:185:LEU:HD13 | 2.47                     | 0.45              |
| 1:M:210:PRO:HG2  | 1:N:145:ARG:CD   | 2.47                     | 0.45              |
| 1:O:98:ILE:HG22  | 1:O:99:PHE:CD1   | 2.52                     | 0.45              |
| 1:R:209:VAL:HG23 | 1:R:209:VAL:O    | 2.16                     | 0.45              |
| 1:V:184:ILE:HG22 | 1:V:186:LEU:CD1  | 2.47                     | 0.45              |
| 1:Y:73:GLY:O     | 1:Y:190:ASN:HB3  | 2.17                     | 0.45              |
| 1:1:128:LEU:HA   | 1:1:129:PRO:HD3  | 1.75                     | 0.45              |
| 1:2:63:ILE:HD11  | 1:2:89:LEU:HD21  | 1.99                     | 0.45              |
| 1:3:150:ALA:C    | 1:q:114:MET:HE2  | 2.42                     | 0.45              |
| 1:7:84:ILE:O     | 1:7:180:PRO:HD2  | 2.17                     | 0.45              |
| 1:h:138:PHE:CE1  | 1:h:142:GLN:HG3  | 2.52                     | 0.45              |
| 1:n:83:THR:HA    | 1:n:182:ARG:HB3  | 1.98                     | 0.45              |
| 1:t:168:TRP:CZ3  | 1:u:176:ARG:CZ   | 3.00                     | 0.45              |
| 1:x:98:ILE:HG22  | 1:x:99:PHE:CD1   | 2.52                     | 0.45              |
| 1:D:98:ILE:HD11  | 1:N:94:HIS:HB2   | 1.99                     | 0.45              |
| 1:F:152:TRP:HH2  | 1:F:187:CYS:SG   | 2.40                     | 0.45              |
| 1:H:171:SER:O    | 1:I:176:ARG:NH1  | 2.49                     | 0.45              |
| 1:K:137:THR:HG23 | 1:K:140:ALA:HB2  | 1.98                     | 0.45              |
| 1:S:74:THR:O     | 1:S:75:ASP:C     | 2.59                     | 0.45              |
| 1:W:121:GLY:CA   | 1:W:152:TRP:CE3  | 2.96                     | 0.45              |
| 1:d:145:ARG:N    | 1:d:145:ARG:NE   | 2.64                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:e:79:VAL:HG23  | 1:e:80:VAL:HG23  | 1.99                     | 0.45              |
| 1:q:104:VAL:HG11 | 1:q:107:LEU:HG   | 1.99                     | 0.45              |
| 1:s:176:ARG:HD2  | 1:u:168:TRP:CZ2  | 2.52                     | 0.45              |
| 1:K:152:TRP:HH2  | 1:K:187:CYS:SG   | 2.40                     | 0.44              |
| 1:M:101:ARG:NH1  | 1:M:168:TRP:CH2  | 2.86                     | 0.44              |
| 1:M:141:LEU:HD21 | 1:M:184:ILE:HB   | 1.99                     | 0.44              |
| 1:W:91:ARG:NH1   | 1:w:98:ILE:HG23  | 2.32                     | 0.44              |
| 1:W:150:ALA:C    | 1:j:114:MET:HE2  | 2.43                     | 0.44              |
| 1:W:165:THR:HG23 | 1:W:166:LEU:N    | 2.32                     | 0.44              |
| 1:a:138:PHE:CD1  | 1:a:138:PHE:C    | 2.95                     | 0.44              |
| 1:k:115:CYS:HB2  | 1:k:116:PRO:HD2  | 1.99                     | 0.44              |
| 1:q:162:TYR:O    | 1:q:164:ARG:HG3  | 2.17                     | 0.44              |
| 1:G:106:THR:HA   | 1:G:162:TYR:OH   | 2.17                     | 0.44              |
| 1:G:145:ARG:NE   | 1:I:210:PRO:HB2  | 2.32                     | 0.44              |
| 1:H:114:MET:HE2  | 1:N:150:ALA:O    | 2.17                     | 0.44              |
| 1:L:98:ILE:HG22  | 1:L:99:PHE:CD1   | 2.52                     | 0.44              |
| 1:O:98:ILE:HG22  | 1:O:99:PHE:CD1   | 2.51                     | 0.44              |
| 1:1:183:LEU:C    | 1:1:183:LEU:HD13 | 2.42                     | 0.44              |
| 1:9:209:VAL:O    | 1:9:209:VAL:HG23 | 2.17                     | 0.44              |
| 1:i:91:ARG:O     | 1:r:98:ILE:HD11  | 2.17                     | 0.44              |
| 1:i:128:LEU:HA   | 1:i:129:PRO:HD3  | 1.81                     | 0.44              |
| 1:n:60:MET:HE2   | 1:n:200:LEU:HB2  | 1.99                     | 0.44              |
| 1:n:151:LYS:NZ   | 1:n:154:GLU:OE1  | 2.46                     | 0.44              |
| 1:q:168:TRP:CZ3  | 1:r:176:ARG:NH2  | 2.85                     | 0.44              |
| 1:s:74:THR:O     | 1:s:76:GLY:N     | 2.50                     | 0.44              |
| 1:v:128:LEU:HA   | 1:v:129:PRO:HD3  | 1.78                     | 0.44              |
| 1:w:211:SER:OG   | 1:w:212:LEU:N    | 2.50                     | 0.44              |
| 1:E:162:TYR:O    | 1:E:164:ARG:HG3  | 2.17                     | 0.44              |
| 1:G:111:ILE:HG21 | 1:G:123:TYR:CE2  | 2.52                     | 0.44              |
| 1:G:121:GLY:CA   | 1:G:152:TRP:CE3  | 2.99                     | 0.44              |
| 1:G:163:THR:C    | 1:G:164:ARG:HG3  | 2.42                     | 0.44              |
| 1:K:130:ASP:HB3  | 1:K:133:ASP:H    | 1.82                     | 0.44              |
| 1:M:145:ARG:N    | 1:M:145:ARG:HE   | 2.16                     | 0.44              |
| 1:W:79:VAL:CG2   | 1:W:185:LEU:HD13 | 2.48                     | 0.44              |
| 1:W:152:TRP:HH2  | 1:W:187:CYS:SG   | 2.40                     | 0.44              |
| 1:Z:60:MET:O     | 1:u:142:GLN:NE2  | 2.50                     | 0.44              |
| 1:Z:168:TRP:CZ3  | 1:O:130:ASP:OD1  | 2.67                     | 0.44              |
| 1:c:209:VAL:HG23 | 1:c:209:VAL:O    | 2.17                     | 0.44              |
| 1:K:210:PRO:HG2  | 1:L:145:ARG:HD2  | 2.00                     | 0.44              |
| 1:Z:55:VAL:HG13  | 1:t:55:VAL:HG13  | 1.99                     | 0.44              |
| 1:8:61:SER:OG    | 1:8:90:PRO:HD2   | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:60:MET:O     | 1:s:142:GLN:NE2  | 2.49                     | 0.44              |
| 1:c:142:GLN:NE2  | 1:g:60:MET:O     | 2.49                     | 0.44              |
| 1:h:202:ARG:HG3  | 1:h:202:ARG:O    | 2.16                     | 0.44              |
| 1:m:176:ARG:NH1  | 1:o:170:SER:O    | 2.45                     | 0.44              |
| 1:w:145:ARG:NE   | 1:w:145:ARG:N    | 2.65                     | 0.44              |
| 1:D:176:ARG:CZ   | 1:F:168:TRP:CZ3  | 3.00                     | 0.44              |
| 1:E:138:PHE:C    | 1:E:138:PHE:CD1  | 2.95                     | 0.44              |
| 1:J:183:LEU:C    | 1:J:183:LEU:HD13 | 2.43                     | 0.44              |
| 1:S:162:TYR:O    | 1:S:164:ARG:HG3  | 2.18                     | 0.44              |
| 1:V:130:ASP:OD1  | 1:X:168:TRP:HH2  | 2.00                     | 0.44              |
| 1:X:132:THR:HG21 | 1:X:176:ARG:NH2  | 2.33                     | 0.44              |
| 1:1:63:ILE:HD11  | 1:1:89:LEU:HD21  | 1.99                     | 0.44              |
| 1:a:74:THR:O     | 1:a:75:ASP:C     | 2.61                     | 0.44              |
| 1:k:128:LEU:HA   | 1:k:129:PRO:HD3  | 1.87                     | 0.44              |
| 1:k:145:ARG:N    | 1:k:145:ARG:NE   | 2.65                     | 0.44              |
| 1:n:105:GLU:O    | 1:n:106:THR:HG23 | 2.16                     | 0.44              |
| 1:v:184:ILE:HG22 | 1:v:186:LEU:HD13 | 1.99                     | 0.44              |
| 1:C:77:TYR:C     | 1:C:77:TYR:CD1   | 2.96                     | 0.44              |
| 1:G:85:VAL:O     | 1:G:86:PRO:C     | 2.58                     | 0.44              |
| 1:Q:63:ILE:HD11  | 1:Q:89:LEU:CD2   | 2.48                     | 0.44              |
| 1:W:162:TYR:O    | 1:W:164:ARG:HG3  | 2.17                     | 0.44              |
| 1:X:99:PHE:HB3   | 1:X:208:SER:O    | 2.18                     | 0.44              |
| 1:X:142:GLN:NE2  | 1:w:60:MET:O     | 2.50                     | 0.44              |
| 1:Y:130:ASP:CG   | 1:0:168:TRP:HH2  | 2.24                     | 0.44              |
| 1:5:63:ILE:HD11  | 1:5:89:LEU:CD2   | 2.48                     | 0.44              |
| 1:7:98:ILE:HG22  | 1:7:99:PHE:CD1   | 2.53                     | 0.44              |
| 1:h:168:TRP:CZ3  | 1:i:130:ASP:CG   | 2.95                     | 0.44              |
| 1:t:125:ALA:O    | 1:t:147:ALA:HA   | 2.18                     | 0.44              |
| 1:w:107:LEU:HD21 | 1:w:201:CYS:SG   | 2.56                     | 0.44              |
| 1:E:73:GLY:O     | 1:E:190:ASN:HB3  | 2.18                     | 0.44              |
| 1:E:123:TYR:HB2  | 1:E:185:LEU:CD2  | 2.48                     | 0.44              |
| 1:G:175:GLN:HA   | 1:G:178:THR:CG2  | 2.48                     | 0.44              |
| 1:K:63:ILE:HD11  | 1:K:201:CYS:HB3  | 1.98                     | 0.44              |
| 1:O:209:VAL:HG23 | 1:O:209:VAL:O    | 2.18                     | 0.44              |
| 1:4:79:VAL:HG21  | 1:4:185:LEU:HD13 | 1.98                     | 0.44              |
| 1:8:92:LEU:HD11  | 1:8:205:VAL:HG11 | 2.00                     | 0.44              |
| 1:8:177:LEU:HD23 | 1:9:174:GLU:HG2  | 2.00                     | 0.44              |
| 1:k:100:GLN:HB2  | 1:k:209:VAL:CG2  | 2.47                     | 0.44              |
| 1:s:109:PHE:HB2  | 1:s:158:VAL:HG13 | 2.00                     | 0.44              |
| 1:u:98:ILE:HG22  | 1:u:99:PHE:CD1   | 2.53                     | 0.44              |
| 1:v:66:ALA:HB3   | 1:v:197:VAL:CG1  | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:100:GLN:HG3  | 1:B:209:VAL:HG23 | 2.00                     | 0.44              |
| 1:B:168:TRP:CZ2  | 1:C:176:ARG:HD2  | 2.53                     | 0.44              |
| 1:F:77:TYR:CD1   | 1:F:77:TYR:C     | 2.96                     | 0.44              |
| 1:G:98:ILE:HG23  | 1:K:91:ARG:CZ    | 2.48                     | 0.44              |
| 1:H:89:LEU:O     | 1:H:90:PRO:C     | 2.61                     | 0.44              |
| 1:Q:168:TRP:CZ3  | 1:R:176:ARG:CZ   | 3.00                     | 0.44              |
| 1:Z:63:ILE:HD11  | 1:Z:89:LEU:HD21  | 1.99                     | 0.44              |
| 1:1:139:ASP:OD1  | 1:1:139:ASP:N    | 2.51                     | 0.44              |
| 1:4:118:ASN:HD21 | 1:l:118:ASN:HB2  | 1.83                     | 0.44              |
| 1:6:98:ILE:HG22  | 1:6:99:PHE:CD1   | 2.52                     | 0.44              |
| 1:7:143:ALA:HB3  | 1:9:212:LEU:HB3  | 2.00                     | 0.44              |
| 1:d:89:LEU:HD13  | 1:d:203:TRP:CD1  | 2.53                     | 0.44              |
| 1:e:74:THR:O     | 1:e:75:ASP:C     | 2.60                     | 0.44              |
| 1:h:124:VAL:HG13 | 1:h:186:LEU:HB2  | 1.99                     | 0.44              |
| 1:h:141:LEU:HD21 | 1:h:184:ILE:HB   | 1.98                     | 0.44              |
| 1:s:108:GLU:HB2  | 1:s:202:ARG:HG2  | 1.99                     | 0.44              |
| 1:D:184:ILE:HG22 | 1:D:186:LEU:CD1  | 2.48                     | 0.44              |
| 1:H:121:GLY:CA   | 1:H:152:TRP:CE3  | 2.96                     | 0.44              |
| 1:M:134:ASN:O    | 1:M:136:HIS:CD2  | 2.70                     | 0.44              |
| 1:N:130:ASP:C    | 1:N:132:THR:N    | 2.75                     | 0.44              |
| 1:O:118:ASN:HB2  | 1:V:118:ASN:ND2  | 2.32                     | 0.44              |
| 1:P:130:ASP:CG   | 1:R:168:TRP:HH2  | 2.26                     | 0.44              |
| 1:Q:89:LEU:HD22  | 1:Q:203:TRP:CD1  | 2.52                     | 0.44              |
| 1:R:98:ILE:HG22  | 1:R:99:PHE:CD1   | 2.53                     | 0.44              |
| 1:V:168:TRP:N    | 1:V:177:LEU:O    | 2.51                     | 0.44              |
| 1:Y:83:THR:HA    | 1:Y:182:ARG:HB3  | 2.00                     | 0.44              |
| 1:1:106:THR:HA   | 1:1:162:TYR:OH   | 2.18                     | 0.44              |
| 1:4:137:THR:HG23 | 1:4:140:ALA:CB   | 2.48                     | 0.44              |
| 1:4:145:ARG:NH1  | 1:4:161:GLN:HB3  | 2.33                     | 0.44              |
| 1:5:112:GLN:HG2  | 1:e:149:VAL:CG2  | 2.48                     | 0.44              |
| 1:7:128:LEU:HA   | 1:7:129:PRO:HD3  | 1.77                     | 0.44              |
| 1:7:143:ALA:CB   | 1:9:212:LEU:CB   | 2.95                     | 0.44              |
| 1:7:146:GLY:O    | 1:7:147:ALA:C    | 2.61                     | 0.44              |
| 1:d:58:SER:O     | 1:d:91:ARG:NH1   | 2.50                     | 0.44              |
| 1:e:121:GLY:HA2  | 1:e:152:TRP:HE3  | 1.83                     | 0.44              |
| 1:e:184:ILE:HG22 | 1:e:186:LEU:HD13 | 1.99                     | 0.44              |
| 1:l:74:THR:O     | 1:l:75:ASP:C     | 2.60                     | 0.44              |
| 1:n:100:GLN:HG2  | 1:n:211:SER:HB2  | 1.99                     | 0.44              |
| 1:p:124:VAL:HG13 | 1:p:186:LEU:HB2  | 1.99                     | 0.44              |
| 1:A:175:GLN:HB2  | 1:A:178:THR:HG23 | 1.99                     | 0.43              |
| 1:C:209:VAL:O    | 1:C:209:VAL:HG23 | 2.17                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:96:ALA:HB1   | 1:E:169:THR:HB   | 2.00                     | 0.43              |
| 1:M:100:GLN:OE1  | 1:N:130:ASP:OD1  | 2.35                     | 0.43              |
| 1:P:210:PRO:HB3  | 1:p:91:ARG:CZ    | 2.48                     | 0.43              |
| 1:R:99:PHE:HB3   | 1:R:208:SER:O    | 2.17                     | 0.43              |
| 1:Z:98:ILE:HG22  | 1:Z:99:PHE:CD1   | 2.52                     | 0.43              |
| 1:2:138:PHE:CD1  | 1:2:138:PHE:C    | 2.95                     | 0.43              |
| 1:4:196:ASN:HD22 | 1:4:196:ASN:C    | 2.26                     | 0.43              |
| 1:6:94:HIS:CB    | 1:l:98:ILE:HD11  | 2.48                     | 0.43              |
| 1:9:91:ARG:CZ    | 1:o:98:ILE:HG23  | 2.48                     | 0.43              |
| 1:c:99:PHE:HB3   | 1:c:208:SER:O    | 2.17                     | 0.43              |
| 1:d:128:LEU:HA   | 1:d:129:PRO:HD3  | 1.77                     | 0.43              |
| 1:f:132:THR:HG21 | 1:f:176:ARG:NH2  | 2.33                     | 0.43              |
| 1:o:130:ASP:N    | 1:o:130:ASP:OD1  | 2.51                     | 0.43              |
| 1:v:63:ILE:HD11  | 1:v:89:LEU:HD21  | 1.99                     | 0.43              |
| 1:B:211:SER:OG   | 1:B:212:LEU:N    | 2.51                     | 0.43              |
| 1:G:89:LEU:HD13  | 1:G:203:TRP:CD1  | 2.52                     | 0.43              |
| 1:N:60:MET:HA    | 1:N:201:CYS:O    | 2.18                     | 0.43              |
| 1:N:65:GLN:HE21  | 1:N:196:ASN:HD21 | 1.66                     | 0.43              |
| 1:Q:63:ILE:HG23  | 1:Q:88:LEU:HD13  | 2.00                     | 0.43              |
| 1:T:79:VAL:CG2   | 1:T:185:LEU:HD13 | 2.49                     | 0.43              |
| 1:T:84:ILE:HB    | 1:T:180:PRO:HD2  | 2.00                     | 0.43              |
| 1:X:145:ARG:NH1  | 1:X:161:GLN:HB3  | 2.33                     | 0.43              |
| 1:Y:61:SER:CB    | 1:Y:90:PRO:HD2   | 2.48                     | 0.43              |
| 1:5:132:THR:OG1  | 1:5:176:ARG:NH2  | 2.51                     | 0.43              |
| 1:c:98:ILE:HG22  | 1:c:99:PHE:CD1   | 2.54                     | 0.43              |
| 1:i:91:ARG:NE    | 1:r:98:ILE:HG23  | 2.33                     | 0.43              |
| 1:m:63:ILE:HB    | 1:m:199:VAL:HG22 | 2.00                     | 0.43              |
| 1:m:128:LEU:HA   | 1:m:129:PRO:HD3  | 1.82                     | 0.43              |
| 1:C:118:ASN:HB2  | 1:P:118:ASN:ND2  | 2.34                     | 0.43              |
| 1:H:138:PHE:CE1  | 1:H:142:GLN:HG3  | 2.53                     | 0.43              |
| 1:S:128:LEU:HA   | 1:S:129:PRO:HD3  | 1.74                     | 0.43              |
| 1:W:91:ARG:O     | 1:w:98:ILE:HD11  | 2.18                     | 0.43              |
| 1:7:92:LEU:O     | 1:7:93:GLY:C     | 2.61                     | 0.43              |
| 1:e:107:LEU:O    | 1:e:160:PRO:HD2  | 2.18                     | 0.43              |
| 1:g:118:ASN:ND2  | 1:r:118:ASN:HB2  | 2.28                     | 0.43              |
| 1:m:111:ILE:HG21 | 1:m:123:TYR:CE2  | 2.54                     | 0.43              |
| 1:m:141:LEU:HD21 | 1:m:184:ILE:HB   | 1.99                     | 0.43              |
| 1:o:151:LYS:HD2  | 1:o:153:TRP:CZ2  | 2.54                     | 0.43              |
| 1:A:96:ALA:C     | 1:A:98:ILE:H     | 2.26                     | 0.43              |
| 1:D:104:VAL:HG21 | 1:D:180:PRO:HG3  | 2.00                     | 0.43              |
| 1:Q:149:VAL:CG2  | 1:p:112:GLN:HG2  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:63:ILE:HD11  | 1:Z:89:LEU:CD2   | 2.48                     | 0.43              |
| 1:0:138:PHE:CD1  | 1:0:138:PHE:C    | 2.96                     | 0.43              |
| 1:d:80:VAL:HB    | 1:d:185:LEU:HB2  | 2.00                     | 0.43              |
| 1:e:101:ARG:NH1  | 1:e:168:TRP:CZ2  | 2.87                     | 0.43              |
| 1:m:175:GLN:HB2  | 1:m:178:THR:CG2  | 2.48                     | 0.43              |
| 1:r:99:PHE:HB3   | 1:r:208:SER:O    | 2.17                     | 0.43              |
| 1:r:151:LYS:HD2  | 1:r:153:TRP:CZ2  | 2.54                     | 0.43              |
| 1:x:63:ILE:HD11  | 1:x:89:LEU:HD11  | 2.00                     | 0.43              |
| 1:I:128:LEU:HA   | 1:I:129:PRO:HD3  | 1.82                     | 0.43              |
| 1:I:138:PHE:CD1  | 1:I:138:PHE:C    | 2.97                     | 0.43              |
| 1:N:100:GLN:HG2  | 1:N:211:SER:HB3  | 1.99                     | 0.43              |
| 1:X:128:LEU:HA   | 1:X:129:PRO:HD3  | 1.82                     | 0.43              |
| 1:2:114:MET:HE2  | 1:r:150:ALA:O    | 2.18                     | 0.43              |
| 1:7:79:VAL:HG22  | 1:7:185:LEU:HB3  | 2.00                     | 0.43              |
| 1:7:114:MET:HE2  | 1:i:150:ALA:O    | 2.18                     | 0.43              |
| 1:8:165:THR:HG23 | 1:8:166:LEU:N    | 2.34                     | 0.43              |
| 1:8:168:TRP:CE2  | 1:9:176:ARG:HD2  | 2.54                     | 0.43              |
| 1:i:99:PHE:HB3   | 1:i:208:SER:O    | 2.17                     | 0.43              |
| 1:k:101:ARG:HG2  | 1:k:167:LEU:O    | 2.18                     | 0.43              |
| 1:p:138:PHE:CD1  | 1:p:138:PHE:C    | 2.96                     | 0.43              |
| 1:A:210:PRO:HG2  | 1:B:145:ARG:HD2  | 1.98                     | 0.43              |
| 1:M:145:ARG:NE   | 1:O:210:PRO:HB2  | 2.33                     | 0.43              |
| 1:Q:100:GLN:HG2  | 1:Q:211:SER:CB   | 2.48                     | 0.43              |
| 1:U:98:ILE:HG22  | 1:U:99:PHE:CD1   | 2.54                     | 0.43              |
| 1:U:149:VAL:HG22 | 1:k:200:LEU:HD11 | 2.01                     | 0.43              |
| 1:W:112:GLN:HG2  | 1:x:149:VAL:CG2  | 2.44                     | 0.43              |
| 1:a:145:ARG:NH1  | 1:a:161:GLN:HB3  | 2.34                     | 0.43              |
| 1:b:85:VAL:O     | 1:b:86:PRO:C     | 2.61                     | 0.43              |
| 1:b:91:ARG:HD2   | 1:g:211:SER:O    | 2.19                     | 0.43              |
| 1:g:63:ILE:CD1   | 1:g:88:LEU:HD22  | 2.48                     | 0.43              |
| 1:h:152:TRP:CD1  | 1:h:195:VAL:HG11 | 2.54                     | 0.43              |
| 1:j:58:SER:O     | 1:j:91:ARG:NH1   | 2.52                     | 0.43              |
| 1:k:84:ILE:O     | 1:k:180:PRO:HD2  | 2.18                     | 0.43              |
| 1:k:178:THR:O    | 1:k:178:THR:OG1  | 2.34                     | 0.43              |
| 1:n:168:TRP:HZ3  | 1:o:130:ASP:OD1  | 2.01                     | 0.43              |
| 1:p:123:TYR:HB2  | 1:p:185:LEU:CD2  | 2.49                     | 0.43              |
| 1:t:175:GLN:HE21 | 1:t:175:GLN:HB2  | 1.58                     | 0.43              |
| 1:A:54:ASP:OD2   | 1:A:206:ARG:NH1  | 2.51                     | 0.43              |
| 1:A:128:LEU:HA   | 1:A:129:PRO:HD3  | 1.85                     | 0.43              |
| 1:A:165:THR:HG23 | 1:A:166:LEU:N    | 2.34                     | 0.43              |
| 1:H:100:GLN:CB   | 1:H:209:VAL:HG22 | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:146:GLY:O    | 1:M:147:ALA:C    | 2.60                     | 0.43              |
| 1:Q:165:THR:O    | 1:Q:167:LEU:HD12 | 2.19                     | 0.43              |
| 1:Z:109:PHE:HA   | 1:Z:200:LEU:O    | 2.19                     | 0.43              |
| 1:Z:149:VAL:CG2  | 1:v:112:GLN:HG2  | 2.47                     | 0.43              |
| 1:1:69:PRO:HG2   | 1:1:72:THR:HG21  | 1.99                     | 0.43              |
| 1:4:184:ILE:HG22 | 1:4:186:LEU:HD13 | 2.00                     | 0.43              |
| 1:6:132:THR:HG21 | 1:6:176:ARG:NH2  | 2.33                     | 0.43              |
| 1:a:142:GLN:NE2  | 1:u:60:MET:O     | 2.50                     | 0.43              |
| 1:d:61:SER:HB3   | 1:d:90:PRO:HD2   | 2.01                     | 0.43              |
| 1:f:99:PHE:HB3   | 1:f:208:SER:O    | 2.18                     | 0.43              |
| 1:f:101:ARG:CG   | 1:f:167:LEU:O    | 2.66                     | 0.43              |
| 1:i:211:SER:OG   | 1:i:212:LEU:N    | 2.50                     | 0.43              |
| 1:m:145:ARG:HD2  | 1:o:210:PRO:HG2  | 2.01                     | 0.43              |
| 1:t:162:TYR:O    | 1:t:164:ARG:HG3  | 2.18                     | 0.43              |
| 1:u:63:ILE:HD11  | 1:u:89:LEU:HD11  | 2.01                     | 0.43              |
| 1:G:104:VAL:HA   | 1:G:205:VAL:HG22 | 2.01                     | 0.43              |
| 1:J:130:ASP:CG   | 1:L:168:TRP:HH2  | 2.26                     | 0.43              |
| 1:J:149:VAL:CG2  | 1:3:200:LEU:HD11 | 2.49                     | 0.43              |
| 1:K:145:ARG:NH1  | 1:K:161:GLN:HB3  | 2.34                     | 0.43              |
| 1:L:132:THR:HG21 | 1:L:176:ARG:NH2  | 2.34                     | 0.43              |
| 1:N:128:LEU:HA   | 1:N:129:PRO:HD3  | 1.76                     | 0.43              |
| 1:X:151:LYS:HD2  | 1:X:153:TRP:CZ2  | 2.54                     | 0.43              |
| 1:Y:130:ASP:CG   | 1:0:168:TRP:CZ3  | 2.97                     | 0.43              |
| 1:Z:62:ARG:NH1   | 1:Z:65:GLN:NE2   | 2.67                     | 0.43              |
| 1:Z:98:ILE:HG23  | 1:t:91:ARG:NH1   | 2.33                     | 0.43              |
| 1:0:108:GLU:HB2  | 1:0:202:ARG:HG2  | 2.00                     | 0.43              |
| 1:8:166:LEU:HD23 | 1:8:166:LEU:O    | 2.18                     | 0.43              |
| 1:9:99:PHE:HB3   | 1:9:208:SER:O    | 2.18                     | 0.43              |
| 1:g:184:ILE:HG22 | 1:g:186:LEU:HD13 | 2.00                     | 0.43              |
| 1:h:210:PRO:HD2  | 1:i:145:ARG:HD2  | 2.00                     | 0.43              |
| 1:k:61:SER:CB    | 1:k:90:PRO:HD2   | 2.48                     | 0.43              |
| 1:n:127:PHE:HB3  | 1:n:160:PRO:HB3  | 2.01                     | 0.43              |
| 1:p:106:THR:HA   | 1:p:162:TYR:OH   | 2.18                     | 0.43              |
| 1:p:175:GLN:HA   | 1:p:178:THR:CG2  | 2.49                     | 0.43              |
| 1:w:124:VAL:CG1  | 1:w:186:LEU:HB2  | 2.48                     | 0.43              |
| 1:A:145:ARG:HD2  | 1:C:210:PRO:HG2  | 2.01                     | 0.43              |
| 1:A:157:THR:HG21 | 1:A:159:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:210:PRO:HG2  | 1:B:145:ARG:NE   | 2.33                     | 0.43              |
| 1:B:61:SER:CB    | 1:B:90:PRO:HD2   | 2.47                     | 0.43              |
| 1:J:128:LEU:H    | 1:J:128:LEU:HD22 | 1.83                     | 0.43              |
| 1:Q:163:THR:OG1  | 1:Q:165:THR:HB   | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:74:THR:O     | 1:V:76:GLY:N     | 2.52                     | 0.43              |
| 1:W:163:THR:OG1  | 1:W:165:THR:HG22 | 2.19                     | 0.43              |
| 1:1:121:GLY:HA3  | 1:1:152:TRP:HB2  | 2.00                     | 0.43              |
| 1:9:151:LYS:HD2  | 1:9:153:TRP:CZ2  | 2.53                     | 0.43              |
| 1:a:124:VAL:HG13 | 1:a:186:LEU:HB2  | 2.01                     | 0.43              |
| 1:a:128:LEU:HA   | 1:a:129:PRO:HD3  | 1.83                     | 0.43              |
| 1:g:130:ASP:CG   | 1:i:168:TRP:HH2  | 2.26                     | 0.43              |
| 1:h:130:ASP:C    | 1:h:132:THR:H    | 2.26                     | 0.43              |
| 1:k:182:ARG:HG3  | 1:k:184:ILE:HD11 | 2.01                     | 0.43              |
| 1:m:63:ILE:HD12  | 1:m:88:LEU:HD13  | 2.01                     | 0.43              |
| 1:q:115:CYS:HB2  | 1:q:116:PRO:HD2  | 2.01                     | 0.43              |
| 1:s:106:THR:HG23 | 1:s:204:SER:HB3  | 1.99                     | 0.43              |
| 1:w:113:PRO:HA   | 1:w:197:VAL:HA   | 2.00                     | 0.43              |
| 1:w:162:TYR:O    | 1:w:164:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:63:ILE:HD11  | 1:B:89:LEU:HD21  | 2.01                     | 0.43              |
| 1:H:138:PHE:CE1  | 1:K:62:ARG:HB2   | 2.54                     | 0.43              |
| 1:I:63:ILE:HD11  | 1:I:89:LEU:HD11  | 2.01                     | 0.43              |
| 1:I:99:PHE:HB3   | 1:I:208:SER:O    | 2.18                     | 0.43              |
| 1:M:196:ASN:C    | 1:M:196:ASN:HD22 | 2.26                     | 0.43              |
| 1:P:137:THR:HG23 | 1:P:140:ALA:HB2  | 2.01                     | 0.43              |
| 1:Q:98:ILE:HG23  | 1:n:91:ARG:HD2   | 2.01                     | 0.43              |
| 1:Q:123:TYR:HB2  | 1:Q:185:LEU:CD2  | 2.49                     | 0.43              |
| 1:R:138:PHE:CD1  | 1:R:138:PHE:C    | 2.96                     | 0.43              |
| 1:T:63:ILE:HD11  | 1:T:89:LEU:CD2   | 2.49                     | 0.43              |
| 1:V:98:ILE:HG22  | 1:V:99:PHE:CE1   | 2.54                     | 0.43              |
| 1:Z:166:LEU:HD23 | 1:Z:166:LEU:C    | 2.44                     | 0.43              |
| 1:3:132:THR:HG21 | 1:3:176:ARG:NH2  | 2.33                     | 0.43              |
| 1:7:200:LEU:HD11 | 1:i:149:VAL:HG22 | 2.01                     | 0.43              |
| 1:9:145:ARG:NH1  | 1:9:161:GLN:HB3  | 2.33                     | 0.43              |
| 1:g:149:VAL:HG22 | 1:r:200:LEU:HD11 | 2.01                     | 0.43              |
| 1:p:212:LEU:O    | 1:p:212:LEU:HG   | 2.19                     | 0.43              |
| 1:C:151:LYS:HD2  | 1:C:153:TRP:CZ2  | 2.53                     | 0.42              |
| 1:F:151:LYS:HD2  | 1:F:153:TRP:CZ2  | 2.54                     | 0.42              |
| 1:K:168:TRP:CH2  | 1:L:176:ARG:HD2  | 2.53                     | 0.42              |
| 1:M:67:VAL:HG13  | 1:M:67:VAL:O     | 2.19                     | 0.42              |
| 1:N:100:GLN:HG2  | 1:N:211:SER:CB   | 2.49                     | 0.42              |
| 1:Q:163:THR:OG1  | 1:Q:165:THR:HG22 | 2.19                     | 0.42              |
| 1:S:123:TYR:CD2  | 1:S:185:LEU:HD21 | 2.54                     | 0.42              |
| 1:Z:165:THR:HG23 | 1:Z:166:LEU:N    | 2.34                     | 0.42              |
| 1:5:149:VAL:O    | 1:5:156:ARG:NH2  | 2.52                     | 0.42              |
| 1:9:211:SER:OG   | 1:9:212:LEU:N    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:145:ARG:N    | 1:b:145:ARG:NE   | 2.67                     | 0.42              |
| 1:l:132:THR:HG21 | 1:l:176:ARG:NH2  | 2.34                     | 0.42              |
| 1:r:209:VAL:O    | 1:r:209:VAL:HG23 | 2.19                     | 0.42              |
| 1:s:130:ASP:C    | 1:s:132:THR:N    | 2.77                     | 0.42              |
| 1:t:145:ARG:N    | 1:t:145:ARG:NE   | 2.66                     | 0.42              |
| 1:v:175:GLN:HA   | 1:v:178:THR:CG2  | 2.49                     | 0.42              |
| 1:x:79:VAL:CG2   | 1:x:185:LEU:HD13 | 2.49                     | 0.42              |
| 1:C:63:ILE:HD11  | 1:C:89:LEU:HD11  | 2.01                     | 0.42              |
| 1:H:130:ASP:HB2  | 1:H:133:ASP:HB2  | 2.01                     | 0.42              |
| 1:Q:168:TRP:CZ3  | 1:R:176:ARG:NH2  | 2.87                     | 0.42              |
| 1:R:63:ILE:HD11  | 1:R:89:LEU:HD11  | 2.01                     | 0.42              |
| 1:U:145:ARG:NH1  | 1:U:161:GLN:HB3  | 2.34                     | 0.42              |
| 1:X:168:TRP:N    | 1:X:177:LEU:O    | 2.52                     | 0.42              |
| 1:9:98:ILE:HG23  | 1:o:91:ARG:CZ    | 2.48                     | 0.42              |
| 1:9:113:PRO:HA   | 1:9:197:VAL:HA   | 2.01                     | 0.42              |
| 1:d:101:ARG:HE   | 1:d:166:LEU:HD21 | 1.84                     | 0.42              |
| 1:e:55:VAL:HG21  | 1:e:99:PHE:CZ    | 2.54                     | 0.42              |
| 1:G:91:ARG:HE    | 1:K:98:ILE:HG23  | 1.83                     | 0.42              |
| 1:M:62:ARG:HD3   | 1:M:198:SER:HB3  | 2.00                     | 0.42              |
| 1:M:63:ILE:HB    | 1:M:199:VAL:CG2  | 2.47                     | 0.42              |
| 1:M:92:LEU:HD11  | 1:M:205:VAL:HG21 | 2.00                     | 0.42              |
| 1:M:107:LEU:O    | 1:M:160:PRO:HD2  | 2.20                     | 0.42              |
| 1:R:108:GLU:HB2  | 1:R:202:ARG:HG2  | 2.01                     | 0.42              |
| 1:R:151:LYS:HD2  | 1:R:153:TRP:CZ2  | 2.54                     | 0.42              |
| 1:R:165:THR:HG23 | 1:R:166:LEU:O    | 2.20                     | 0.42              |
| 1:U:209:VAL:O    | 1:U:209:VAL:CG2  | 2.67                     | 0.42              |
| 1:V:63:ILE:HD11  | 1:V:89:LEU:CD2   | 2.49                     | 0.42              |
| 1:Y:121:GLY:HA3  | 1:Y:152:TRP:HE3  | 1.83                     | 0.42              |
| 1:3:151:LYS:HD2  | 1:3:153:TRP:CZ2  | 2.54                     | 0.42              |
| 1:5:115:CYS:HB2  | 1:5:116:PRO:HD2  | 2.01                     | 0.42              |
| 1:6:151:LYS:HD2  | 1:6:153:TRP:CZ2  | 2.54                     | 0.42              |
| 1:a:130:ASP:C    | 1:a:132:THR:N    | 2.72                     | 0.42              |
| 1:a:168:TRP:N    | 1:a:177:LEU:O    | 2.53                     | 0.42              |
| 1:c:118:ASN:HB2  | 1:s:118:ASN:ND2  | 2.32                     | 0.42              |
| 1:l:128:LEU:HA   | 1:l:129:PRO:HD3  | 1.84                     | 0.42              |
| 1:m:173:LYS:O    | 1:o:173:LYS:HD3  | 2.19                     | 0.42              |
| 1:n:101:ARG:NH1  | 1:n:168:TRP:CZ2  | 2.86                     | 0.42              |
| 1:q:79:VAL:HG23  | 1:q:80:VAL:HG23  | 2.00                     | 0.42              |
| 1:q:168:TRP:CH2  | 1:r:176:ARG:HD2  | 2.54                     | 0.42              |
| 1:v:101:ARG:CZ   | 1:v:168:TRP:CZ2  | 3.01                     | 0.42              |
| 1:x:145:ARG:NH1  | 1:x:161:GLN:HB3  | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:114:MET:SD   | 1:P:122:GLY:CA   | 3.03                     | 0.42              |
| 1:E:125:ALA:O    | 1:E:147:ALA:HA   | 2.19                     | 0.42              |
| 1:E:152:TRP:CD1  | 1:E:195:VAL:HG11 | 2.54                     | 0.42              |
| 1:G:98:ILE:CG2   | 1:K:91:ARG:NH1   | 2.82                     | 0.42              |
| 1:I:162:TYR:O    | 1:I:164:ARG:HG3  | 2.19                     | 0.42              |
| 1:J:58:SER:O     | 1:J:91:ARG:NH1   | 2.51                     | 0.42              |
| 1:R:132:THR:HG21 | 1:R:176:ARG:NH2  | 2.34                     | 0.42              |
| 1:T:152:TRP:CD1  | 1:T:195:VAL:HG11 | 2.53                     | 0.42              |
| 1:W:68:LEU:HA    | 1:W:69:PRO:HD3   | 1.93                     | 0.42              |
| 1:j:123:TYR:CD2  | 1:j:185:LEU:HD21 | 2.55                     | 0.42              |
| 1:l:145:ARG:NH1  | 1:l:161:GLN:HB3  | 2.35                     | 0.42              |
| 1:n:167:LEU:HB3  | 1:n:177:LEU:O    | 2.19                     | 0.42              |
| 1:t:92:LEU:HD13  | 1:t:203:TRP:CZ3  | 2.54                     | 0.42              |
| 1:u:99:PHE:HB3   | 1:u:208:SER:O    | 2.20                     | 0.42              |
| 1:I:152:TRP:HH2  | 1:I:187:CYS:SG   | 2.43                     | 0.42              |
| 1:M:63:ILE:HD11  | 1:M:89:LEU:HD21  | 2.01                     | 0.42              |
| 1:S:98:ILE:HD11  | 1:m:94:HIS:HB2   | 2.02                     | 0.42              |
| 1:W:63:ILE:HA    | 1:W:63:ILE:HD13  | 1.73                     | 0.42              |
| 1:W:168:TRP:CE3  | 1:X:176:ARG:CZ   | 3.02                     | 0.42              |
| 1:X:98:ILE:HG22  | 1:X:99:PHE:CD1   | 2.54                     | 0.42              |
| 1:4:121:GLY:HA3  | 1:4:152:TRP:CE3  | 2.55                     | 0.42              |
| 1:4:203:TRP:CE3  | 1:4:203:TRP:O    | 2.72                     | 0.42              |
| 1:a:130:ASP:OD1  | 1:c:168:TRP:CH2  | 2.72                     | 0.42              |
| 1:f:98:ILE:HD11  | 1:x:94:HIS:HB2   | 2.00                     | 0.42              |
| 1:m:109:PHE:HB2  | 1:m:158:VAL:HG13 | 2.01                     | 0.42              |
| 1:q:113:PRO:HA   | 1:q:197:VAL:HA   | 2.01                     | 0.42              |
| 1:A:79:VAL:CG2   | 1:A:185:LEU:HD13 | 2.49                     | 0.42              |
| 1:A:128:LEU:HD21 | 1:A:184:ILE:HD11 | 2.01                     | 0.42              |
| 1:D:123:TYR:CD2  | 1:D:185:LEU:HD21 | 2.55                     | 0.42              |
| 1:M:112:GLN:OE1  | 1:M:155:SER:OG   | 2.28                     | 0.42              |
| 1:W:122:GLY:HA2  | 1:j:114:MET:SD   | 2.60                     | 0.42              |
| 1:X:77:TYR:C     | 1:X:77:TYR:CD1   | 2.97                     | 0.42              |
| 1:Z:98:ILE:HD11  | 1:t:91:ARG:O     | 2.19                     | 0.42              |
| 1:2:106:THR:HA   | 1:2:162:TYR:OH   | 2.19                     | 0.42              |
| 1:4:101:ARG:CZ   | 1:4:168:TRP:CZ2  | 3.03                     | 0.42              |
| 1:8:124:VAL:HG13 | 1:8:186:LEU:HB2  | 2.01                     | 0.42              |
| 1:b:124:VAL:HG23 | 1:b:149:VAL:HG12 | 2.00                     | 0.42              |
| 1:g:176:ARG:NH1  | 1:i:168:TRP:CE3  | 2.88                     | 0.42              |
| 1:k:167:LEU:O    | 1:k:168:TRP:CD1  | 2.73                     | 0.42              |
| 1:m:138:PHE:C    | 1:m:138:PHE:CD1  | 2.97                     | 0.42              |
| 1:m:163:THR:HA   | 1:o:101:ARG:NH2  | 2.14                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:175:GLN:C    | 1:B:177:LEU:N    | 2.77                     | 0.42              |
| 1:H:67:VAL:O     | 1:H:67:VAL:HG13  | 2.18                     | 0.42              |
| 1:H:210:PRO:HD2  | 1:I:145:ARG:HH11 | 1.84                     | 0.42              |
| 1:K:123:TYR:HB2  | 1:K:185:LEU:CD2  | 2.49                     | 0.42              |
| 1:T:146:GLY:HA3  | 1:T:158:VAL:HG23 | 2.02                     | 0.42              |
| 1:T:162:TYR:O    | 1:T:164:ARG:CG   | 2.67                     | 0.42              |
| 1:U:77:TYR:CD1   | 1:U:77:TYR:C     | 2.97                     | 0.42              |
| 1:2:108:GLU:OE1  | 1:2:202:ARG:NH1  | 2.53                     | 0.42              |
| 1:a:130:ASP:O    | 1:a:131:PRO:C    | 2.59                     | 0.42              |
| 1:c:145:ARG:NH1  | 1:c:161:GLN:HB3  | 2.35                     | 0.42              |
| 1:j:128:LEU:CD2  | 1:j:182:ARG:HG2  | 2.49                     | 0.42              |
| 1:n:165:THR:HG23 | 1:n:166:LEU:N    | 2.34                     | 0.42              |
| 1:x:77:TYR:CD1   | 1:x:77:TYR:C     | 2.97                     | 0.42              |
| 1:F:113:PRO:HA   | 1:F:197:VAL:HA   | 2.01                     | 0.42              |
| 1:K:125:ALA:O    | 1:K:147:ALA:HA   | 2.19                     | 0.42              |
| 1:L:151:LYS:HD2  | 1:L:153:TRP:CZ2  | 2.55                     | 0.42              |
| 1:S:104:VAL:HG21 | 1:S:180:PRO:HG3  | 2.02                     | 0.42              |
| 1:S:130:ASP:C    | 1:S:132:THR:N    | 2.77                     | 0.42              |
| 1:S:141:LEU:HD21 | 1:S:184:ILE:HB   | 2.01                     | 0.42              |
| 1:Z:79:VAL:CG2   | 1:Z:185:LEU:HD13 | 2.50                     | 0.42              |
| 1:Z:79:VAL:HG23  | 1:Z:80:VAL:HG23  | 2.02                     | 0.42              |
| 1:Z:191:ASN:OD1  | 1:Z:191:ASN:N    | 2.51                     | 0.42              |
| 1:2:74:THR:O     | 1:2:75:ASP:C     | 2.63                     | 0.42              |
| 1:c:63:ILE:HD11  | 1:c:89:LEU:HD11  | 2.02                     | 0.42              |
| 1:d:208:SER:O    | 1:d:210:PRO:HD3  | 2.20                     | 0.42              |
| 1:g:184:ILE:HG22 | 1:g:186:LEU:CD1  | 2.50                     | 0.42              |
| 1:h:89:LEU:HB2   | 1:h:92:LEU:HB3   | 2.01                     | 0.42              |
| 1:o:101:ARG:CG   | 1:o:167:LEU:O    | 2.68                     | 0.42              |
| 1:o:166:LEU:HG   | 1:o:167:LEU:N    | 2.35                     | 0.42              |
| 1:t:152:TRP:HH2  | 1:t:187:CYS:HG   | 1.64                     | 0.42              |
| 1:u:168:TRP:N    | 1:u:177:LEU:O    | 2.53                     | 0.42              |
| 1:w:148:VAL:HB   | 1:w:156:ARG:HG2  | 2.01                     | 0.42              |
| 1:x:108:GLU:HB2  | 1:x:202:ARG:HG2  | 2.01                     | 0.42              |
| 1:A:113:PRO:HA   | 1:A:197:VAL:HA   | 2.02                     | 0.42              |
| 1:B:92:LEU:HD11  | 1:B:205:VAL:HG11 | 2.01                     | 0.42              |
| 1:F:108:GLU:HB2  | 1:F:202:ARG:HG2  | 2.02                     | 0.42              |
| 1:H:123:TYR:OH   | 1:H:156:ARG:HB2  | 2.20                     | 0.42              |
| 1:I:151:LYS:HD2  | 1:I:153:TRP:CZ2  | 2.55                     | 0.42              |
| 1:J:118:ASN:C    | 1:3:116:PRO:HB3  | 2.45                     | 0.42              |
| 1:P:112:GLN:HG2  | 1:q:149:VAL:CG2  | 2.46                     | 0.42              |
| 1:R:168:TRP:N    | 1:R:177:LEU:O    | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:123:TYR:HB2  | 1:V:185:LEU:CD2  | 2.50                     | 0.42              |
| 1:O:145:ARG:NH1  | 1:O:161:GLN:HB3  | 2.35                     | 0.42              |
| 1:1:73:GLY:O     | 1:1:190:ASN:HB3  | 2.20                     | 0.42              |
| 1:2:168:TRP:CZ2  | 1:3:176:ARG:HD2  | 2.54                     | 0.42              |
| 1:4:163:THR:HG23 | 1:4:164:ARG:H    | 1.84                     | 0.42              |
| 1:b:58:SER:HA    | 1:b:203:TRP:O    | 2.20                     | 0.42              |
| 1:g:128:LEU:HA   | 1:g:129:PRO:HD3  | 1.79                     | 0.42              |
| 1:h:128:LEU:HA   | 1:h:129:PRO:HD3  | 1.79                     | 0.42              |
| 1:h:184:ILE:HG22 | 1:h:186:LEU:HD13 | 2.02                     | 0.42              |
| 1:i:101:ARG:HE   | 1:i:166:LEU:HD21 | 1.84                     | 0.42              |
| 1:n:145:ARG:NE   | 1:n:145:ARG:H    | 2.15                     | 0.42              |
| 1:r:108:GLU:HB2  | 1:r:202:ARG:HG2  | 2.02                     | 0.42              |
| 1:t:79:VAL:CG2   | 1:t:185:LEU:HD13 | 2.50                     | 0.42              |
| 1:B:73:GLY:O     | 1:B:190:ASN:HB3  | 2.20                     | 0.42              |
| 1:D:131:PRO:HB2  | 1:D:175:GLN:HE21 | 1.84                     | 0.42              |
| 1:F:91:ARG:NE    | 1:U:98:ILE:HG23  | 2.35                     | 0.42              |
| 1:F:98:ILE:HG22  | 1:F:99:PHE:CD1   | 2.55                     | 0.42              |
| 1:O:63:ILE:HD11  | 1:O:89:LEU:HD11  | 2.01                     | 0.42              |
| 1:O:101:ARG:HE   | 1:O:166:LEU:HD21 | 1.85                     | 0.42              |
| 1:P:124:VAL:HG13 | 1:P:186:LEU:HB2  | 2.00                     | 0.42              |
| 1:S:121:GLY:HA3  | 1:S:152:TRP:CE3  | 2.51                     | 0.42              |
| 1:W:146:GLY:O    | 1:W:147:ALA:C    | 2.62                     | 0.42              |
| 1:O:63:ILE:HD11  | 1:O:89:LEU:HD11  | 2.02                     | 0.42              |
| 1:5:113:PRO:HA   | 1:5:197:VAL:HA   | 2.01                     | 0.42              |
| 1:6:99:PHE:HB3   | 1:6:208:SER:O    | 2.20                     | 0.42              |
| 1:c:101:ARG:CG   | 1:c:167:LEU:O    | 2.68                     | 0.42              |
| 1:e:63:ILE:HD11  | 1:e:89:LEU:CD2   | 2.49                     | 0.42              |
| 1:g:63:ILE:HB    | 1:g:199:VAL:HG22 | 2.02                     | 0.42              |
| 1:g:130:ASP:CG   | 1:i:168:TRP:CH2  | 2.98                     | 0.42              |
| 1:j:146:GLY:O    | 1:j:148:VAL:HG13 | 2.20                     | 0.42              |
| 1:l:77:TYR:CD1   | 1:l:77:TYR:C     | 2.98                     | 0.42              |
| 1:m:115:CYS:HB2  | 1:m:116:PRO:HD2  | 2.02                     | 0.42              |
| 1:p:79:VAL:HG21  | 1:p:185:LEU:HD13 | 2.01                     | 0.42              |
| 1:p:137:THR:HG23 | 1:p:140:ALA:CB   | 2.48                     | 0.42              |
| 1:q:168:TRP:CZ2  | 1:r:176:ARG:HD2  | 2.55                     | 0.42              |
| 1:t:152:TRP:HH2  | 1:t:187:CYS:SG   | 2.43                     | 0.42              |
| 1:B:144:THR:C    | 1:B:145:ARG:HE   | 2.27                     | 0.41              |
| 1:G:133:ASP:O    | 1:G:182:ARG:NH1  | 2.53                     | 0.41              |
| 1:I:145:ARG:NH1  | 1:I:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:M:110:GLU:HB3  | 1:M:200:LEU:HB2  | 2.01                     | 0.41              |
| 1:P:127:PHE:CZ   | 1:P:181:GLY:HA3  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:128:LEU:HA   | 1:P:129:PRO:HD3  | 1.85                     | 0.41              |
| 1:Q:100:GLN:HB2  | 1:Q:209:VAL:CG2  | 2.50                     | 0.41              |
| 1:S:145:ARG:NH1  | 1:S:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:T:128:LEU:HA   | 1:T:129:PRO:HD3  | 1.87                     | 0.41              |
| 1:Z:170:SER:O    | 1:O:176:ARG:NH1  | 2.53                     | 0.41              |
| 1:4:137:THR:HG23 | 1:4:140:ALA:HB2  | 2.02                     | 0.41              |
| 1:9:62:ARG:HB2   | 1:m:138:PHE:CE1  | 2.55                     | 0.41              |
| 1:9:114:MET:HB3  | 1:m:121:GLY:O    | 2.19                     | 0.41              |
| 1:c:122:GLY:HA3  | 1:g:114:MET:SD   | 2.60                     | 0.41              |
| 1:v:145:ARG:NH1  | 1:v:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:J:127:PHE:CZ   | 1:J:181:GLY:HA3  | 2.55                     | 0.41              |
| 1:P:61:SER:HB3   | 1:P:90:PRO:HD2   | 2.01                     | 0.41              |
| 1:Q:52:THR:OG1   | 1:Q:53:ASN:N     | 2.51                     | 0.41              |
| 1:Y:124:VAL:HG13 | 1:Y:124:VAL:O    | 2.20                     | 0.41              |
| 1:O:128:LEU:HA   | 1:O:129:PRO:HD3  | 1.84                     | 0.41              |
| 1:7:130:ASP:OD1  | 1:7:130:ASP:N    | 2.54                     | 0.41              |
| 1:i:151:LYS:HD2  | 1:i:153:TRP:CZ2  | 2.55                     | 0.41              |
| 1:r:145:ARG:NH1  | 1:r:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:s:128:LEU:HA   | 1:s:129:PRO:HD3  | 1.73                     | 0.41              |
| 1:x:138:PHE:CD1  | 1:x:138:PHE:C    | 2.98                     | 0.41              |
| 1:G:63:ILE:HD11  | 1:G:89:LEU:CD2   | 2.49                     | 0.41              |
| 1:J:110:GLU:HB3  | 1:J:200:LEU:HB2  | 2.03                     | 0.41              |
| 1:K:100:GLN:OE1  | 1:L:130:ASP:OD1  | 2.38                     | 0.41              |
| 1:M:61:SER:HB3   | 1:M:90:PRO:HD2   | 2.01                     | 0.41              |
| 1:O:79:VAL:CG2   | 1:O:185:LEU:HD13 | 2.51                     | 0.41              |
| 1:O:98:ILE:CD1   | 1:X:95:ALA:HB2   | 2.51                     | 0.41              |
| 1:S:121:GLY:CA   | 1:S:152:TRP:CE3  | 3.03                     | 0.41              |
| 1:S:146:GLY:O    | 1:S:147:ALA:C    | 2.62                     | 0.41              |
| 1:U:113:PRO:HA   | 1:U:197:VAL:HA   | 2.02                     | 0.41              |
| 1:V:130:ASP:HB3  | 1:V:132:THR:OG1  | 2.20                     | 0.41              |
| 1:5:138:PHE:CE2  | 1:8:62:ARG:NH1   | 2.88                     | 0.41              |
| 1:6:77:TYR:CD1   | 1:6:77:TYR:C     | 2.98                     | 0.41              |
| 1:8:89:LEU:HD13  | 1:8:203:TRP:CG   | 2.55                     | 0.41              |
| 1:8:122:GLY:HA3  | 1:h:114:MET:SD   | 2.60                     | 0.41              |
| 1:a:167:LEU:C    | 1:a:168:TRP:CD1  | 2.98                     | 0.41              |
| 1:c:108:GLU:HB2  | 1:c:202:ARG:HG2  | 2.02                     | 0.41              |
| 1:e:77:TYR:CD1   | 1:e:77:TYR:C     | 2.98                     | 0.41              |
| 1:f:128:LEU:HA   | 1:f:129:PRO:HD3  | 1.81                     | 0.41              |
| 1:x:166:LEU:HG   | 1:x:167:LEU:N    | 2.35                     | 0.41              |
| 1:A:62:ARG:HD3   | 1:A:198:SER:HB3  | 2.03                     | 0.41              |
| 1:A:98:ILE:CG2   | 1:E:91:ARG:NH1   | 2.83                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:89:LEU:HD13  | 1:B:203:TRP:CG   | 2.56                     | 0.41              |
| 1:F:145:ARG:NH1  | 1:F:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:G:176:ARG:NH1  | 1:I:170:SER:O    | 2.54                     | 0.41              |
| 1:S:214:ASN:HD21 | 1:T:137:THR:HG21 | 1.86                     | 0.41              |
| 1:U:108:GLU:HB2  | 1:U:202:ARG:HG2  | 2.03                     | 0.41              |
| 1:V:167:LEU:C    | 1:V:168:TRP:CD1  | 2.98                     | 0.41              |
| 1:X:63:ILE:HD11  | 1:X:89:LEU:HD11  | 2.02                     | 0.41              |
| 1:Z:121:GLY:O    | 1:v:114:MET:HB3  | 2.19                     | 0.41              |
| 1:1:79:VAL:HG23  | 1:1:80:VAL:HG23  | 2.02                     | 0.41              |
| 1:5:62:ARG:HB2   | 1:e:138:PHE:CE1  | 2.54                     | 0.41              |
| 1:5:96:ALA:HB1   | 1:5:169:THR:HB   | 2.02                     | 0.41              |
| 1:5:132:THR:HG21 | 1:5:176:ARG:NH2  | 2.35                     | 0.41              |
| 1:b:89:LEU:O     | 1:b:90:PRO:C     | 2.61                     | 0.41              |
| 1:c:79:VAL:CG2   | 1:c:185:LEU:HD13 | 2.51                     | 0.41              |
| 1:d:121:GLY:CA   | 1:d:152:TRP:HE3  | 2.33                     | 0.41              |
| 1:f:145:ARG:NH1  | 1:f:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:B:148:VAL:HG21 | 1:B:156:ARG:HB3  | 2.03                     | 0.41              |
| 1:F:63:ILE:HD11  | 1:F:89:LEU:HD11  | 2.02                     | 0.41              |
| 1:G:163:THR:OG1  | 1:G:165:THR:HG22 | 2.21                     | 0.41              |
| 1:K:107:LEU:HD23 | 1:K:107:LEU:HA   | 1.93                     | 0.41              |
| 1:O:145:ARG:NH1  | 1:O:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:O:151:LYS:HD2  | 1:O:153:TRP:CZ2  | 2.55                     | 0.41              |
| 1:O:168:TRP:HB2  | 1:O:177:LEU:O    | 2.20                     | 0.41              |
| 1:S:138:PHE:CD1  | 1:S:138:PHE:C    | 2.99                     | 0.41              |
| 1:W:175:GLN:HA   | 1:W:178:THR:CG2  | 2.51                     | 0.41              |
| 1:Y:98:ILE:CG2   | 1:v:91:ARG:NH2   | 2.83                     | 0.41              |
| 1:2:96:ALA:HB1   | 1:2:169:THR:HB   | 2.03                     | 0.41              |
| 1:2:168:TRP:CZ3  | 1:3:176:ARG:CZ   | 3.04                     | 0.41              |
| 1:a:113:PRO:HA   | 1:a:197:VAL:HA   | 2.02                     | 0.41              |
| 1:b:61:SER:OG    | 1:b:90:PRO:HD2   | 2.20                     | 0.41              |
| 1:j:55:VAL:HG21  | 1:j:99:PHE:CZ    | 2.55                     | 0.41              |
| 1:j:101:ARG:HG2  | 1:j:167:LEU:O    | 2.21                     | 0.41              |
| 1:o:99:PHE:HB3   | 1:o:208:SER:O    | 2.20                     | 0.41              |
| 1:q:100:GLN:HB2  | 1:q:209:VAL:O    | 2.20                     | 0.41              |
| 1:r:166:LEU:HG   | 1:r:167:LEU:N    | 2.35                     | 0.41              |
| 1:s:192:THR:O    | 1:s:192:THR:CG2  | 2.66                     | 0.41              |
| 1:u:79:VAL:CG2   | 1:u:185:LEU:HD13 | 2.50                     | 0.41              |
| 1:A:140:ALA:O    | 1:A:143:ALA:HB3  | 2.20                     | 0.41              |
| 1:D:146:GLY:O    | 1:D:147:ALA:C    | 2.63                     | 0.41              |
| 1:K:61:SER:O     | 1:K:200:LEU:HA   | 2.21                     | 0.41              |
| 1:O:101:ARG:CG   | 1:O:167:LEU:O    | 2.69                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:130:ASP:OD1  | 1:U:100:GLN:OE1  | 2.38                     | 0.41              |
| 1:7:79:VAL:CG2   | 1:7:185:LEU:HD13 | 2.51                     | 0.41              |
| 1:a:167:LEU:C    | 1:a:168:TRP:HD1  | 2.29                     | 0.41              |
| 1:c:114:MET:HB3  | 1:s:121:GLY:O    | 2.19                     | 0.41              |
| 1:f:63:ILE:HD11  | 1:f:89:LEU:HD11  | 2.03                     | 0.41              |
| 1:n:107:LEU:CD2  | 1:n:201:CYS:SG   | 3.08                     | 0.41              |
| 1:q:121:GLY:CA   | 1:q:152:TRP:CE3  | 3.02                     | 0.41              |
| 1:v:89:LEU:O     | 1:v:90:PRO:C     | 2.64                     | 0.41              |
| 1:v:167:LEU:HD12 | 1:v:167:LEU:N    | 2.36                     | 0.41              |
| 1:w:183:LEU:C    | 1:w:183:LEU:HD13 | 2.46                     | 0.41              |
| 1:H:130:ASP:CB   | 1:H:133:ASP:HB2  | 2.51                     | 0.41              |
| 1:J:151:LYS:HD2  | 1:J:153:TRP:CE2  | 2.55                     | 0.41              |
| 1:J:152:TRP:CZ3  | 1:J:191:ASN:HB3  | 2.55                     | 0.41              |
| 1:L:128:LEU:HA   | 1:L:129:PRO:HD3  | 1.80                     | 0.41              |
| 1:L:145:ARG:NH1  | 1:L:161:GLN:HB3  | 2.36                     | 0.41              |
| 1:O:99:PHE:HB3   | 1:O:208:SER:O    | 2.21                     | 0.41              |
| 1:Q:144:THR:C    | 1:Q:145:ARG:HE   | 2.29                     | 0.41              |
| 1:R:79:VAL:CG2   | 1:R:185:LEU:HD13 | 2.51                     | 0.41              |
| 1:T:145:ARG:NE   | 1:T:145:ARG:N    | 2.69                     | 0.41              |
| 1:4:175:GLN:HB2  | 1:4:178:THR:HG23 | 2.03                     | 0.41              |
| 1:6:145:ARG:NH1  | 1:6:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:9:63:ILE:HD11  | 1:9:89:LEU:HD11  | 2.02                     | 0.41              |
| 1:9:77:TYR:CD1   | 1:9:77:TYR:C     | 2.98                     | 0.41              |
| 1:a:128:LEU:HD22 | 1:a:128:LEU:H    | 1.85                     | 0.41              |
| 1:e:175:GLN:HA   | 1:e:178:THR:HG22 | 2.01                     | 0.41              |
| 1:m:92:LEU:O     | 1:m:93:GLY:C     | 2.64                     | 0.41              |
| 1:m:107:LEU:O    | 1:m:160:PRO:HD2  | 2.21                     | 0.41              |
| 1:o:107:LEU:O    | 1:o:160:PRO:HD2  | 2.21                     | 0.41              |
| 1:p:167:LEU:HD23 | 1:p:179:SER:N    | 2.35                     | 0.41              |
| 1:t:123:TYR:HB2  | 1:t:185:LEU:HD21 | 2.02                     | 0.41              |
| 1:t:168:TRP:CE3  | 1:u:176:ARG:CZ   | 3.03                     | 0.41              |
| 1:u:151:LYS:HD2  | 1:u:153:TRP:CZ2  | 2.56                     | 0.41              |
| 1:v:140:ALA:O    | 1:v:143:ALA:HB3  | 2.20                     | 0.41              |
| 1:B:177:LEU:C    | 1:B:178:THR:HG22 | 2.46                     | 0.41              |
| 1:D:138:PHE:CE2  | 1:U:62:ARG:NH1   | 2.89                     | 0.41              |
| 1:D:163:THR:OG1  | 1:D:165:THR:HG22 | 2.20                     | 0.41              |
| 1:G:130:ASP:N    | 1:G:130:ASP:OD1  | 2.52                     | 0.41              |
| 1:M:210:PRO:HG2  | 1:N:145:ARG:HD2  | 2.03                     | 0.41              |
| 1:W:69:PRO:HD2   | 1:W:72:THR:OG1   | 2.20                     | 0.41              |
| 1:3:145:ARG:NH1  | 1:3:161:GLN:HB3  | 2.35                     | 0.41              |
| 1:5:175:GLN:HA   | 1:5:178:THR:CG2  | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:8:127:PHE:HB3  | 1:8:160:PRO:HB3  | 2.02                     | 0.41              |
| 1:8:212:LEU:HG   | 1:8:212:LEU:O    | 2.21                     | 0.41              |
| 1:j:107:LEU:O    | 1:j:160:PRO:HD2  | 2.20                     | 0.41              |
| 1:m:133:ASP:OD1  | 1:o:213:GLU:OE1  | 2.39                     | 0.41              |
| 1:p:148:VAL:HB   | 1:p:156:ARG:HG2  | 2.02                     | 0.41              |
| 1:t:125:ALA:HA   | 1:t:184:ILE:O    | 2.20                     | 0.41              |
| 1:v:92:LEU:HD11  | 1:v:205:VAL:HG21 | 2.02                     | 0.41              |
| 1:w:168:TRP:HZ3  | 1:x:130:ASP:CG   | 2.28                     | 0.41              |
| 1:B:163:THR:OG1  | 1:B:165:THR:HB   | 2.21                     | 0.41              |
| 1:C:145:ARG:NH1  | 1:C:161:GLN:HB3  | 2.36                     | 0.41              |
| 1:E:121:GLY:CA   | 1:E:152:TRP:HE3  | 2.33                     | 0.41              |
| 1:E:123:TYR:HB2  | 1:E:185:LEU:HD21 | 2.03                     | 0.41              |
| 1:E:145:ARG:N    | 1:E:145:ARG:HE   | 2.19                     | 0.41              |
| 1:E:149:VAL:HG22 | 1:N:112:GLN:HG2  | 1.98                     | 0.41              |
| 1:H:62:ARG:CD    | 1:H:198:SER:HB3  | 2.51                     | 0.41              |
| 1:H:101:ARG:HB2  | 1:H:208:SER:CB   | 2.51                     | 0.41              |
| 1:H:122:GLY:HA2  | 1:H:150:ALA:O    | 2.20                     | 0.41              |
| 1:I:98:ILE:HG12  | 1:O:91:ARG:HG2   | 2.03                     | 0.41              |
| 1:I:101:ARG:HE   | 1:I:166:LEU:HD21 | 1.86                     | 0.41              |
| 1:J:63:ILE:CG1   | 1:J:201:CYS:HB2  | 2.51                     | 0.41              |
| 1:J:79:VAL:HG21  | 1:J:185:LEU:HD13 | 2.02                     | 0.41              |
| 1:J:121:GLY:HA3  | 1:J:152:TRP:CE3  | 2.56                     | 0.41              |
| 1:K:196:ASN:HD22 | 1:K:196:ASN:C    | 2.28                     | 0.41              |
| 1:L:113:PRO:HA   | 1:L:197:VAL:HA   | 2.03                     | 0.41              |
| 1:M:109:PHE:HB2  | 1:M:158:VAL:HG13 | 2.01                     | 0.41              |
| 1:M:122:GLY:HA2  | 1:M:150:ALA:O    | 2.20                     | 0.41              |
| 1:T:61:SER:HB3   | 1:T:90:PRO:HD2   | 2.03                     | 0.41              |
| 1:W:100:GLN:HG2  | 1:W:211:SER:HB2  | 2.02                     | 0.41              |
| 1:W:176:ARG:O    | 1:W:177:LEU:HD13 | 2.21                     | 0.41              |
| 1:Y:63:ILE:HB    | 1:Y:199:VAL:HG22 | 2.03                     | 0.41              |
| 1:Y:168:TRP:N    | 1:Y:177:LEU:O    | 2.53                     | 0.41              |
| 1:Y:170:SER:O    | 1:Z:176:ARG:NH1  | 2.54                     | 0.41              |
| 1:1:121:GLY:CA   | 1:1:152:TRP:HE3  | 2.34                     | 0.41              |
| 1:1:137:THR:O    | 1:1:138:PHE:C    | 2.64                     | 0.41              |
| 1:1:183:LEU:HD13 | 1:1:184:ILE:N    | 2.36                     | 0.41              |
| 1:1:192:THR:O    | 1:1:192:THR:HG22 | 2.19                     | 0.41              |
| 1:5:98:ILE:HG21  | 1:5:98:ILE:HD13  | 1.86                     | 0.41              |
| 1:5:168:TRP:CZ2  | 1:6:176:ARG:HD2  | 2.55                     | 0.41              |
| 1:7:113:PRO:HB3  | 1:7:197:VAL:HG23 | 2.02                     | 0.41              |
| 1:8:61:SER:HB3   | 1:8:90:PRO:HD3   | 2.02                     | 0.41              |
| 1:9:101:ARG:HE   | 1:9:166:LEU:HD21 | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:67:VAL:HG13  | 1:a:67:VAL:O     | 2.21                     | 0.41              |
| 1:b:57:LEU:HD23  | 1:b:57:LEU:HA    | 1.87                     | 0.41              |
| 1:f:138:PHE:CD1  | 1:f:138:PHE:C    | 2.99                     | 0.41              |
| 1:h:83:THR:HA    | 1:h:182:ARG:CB   | 2.51                     | 0.41              |
| 1:i:108:GLU:HB2  | 1:i:202:ARG:HG2  | 2.01                     | 0.41              |
| 1:i:162:TYR:O    | 1:i:164:ARG:HG3  | 2.21                     | 0.41              |
| 1:j:127:PHE:CZ   | 1:j:181:GLY:HA3  | 2.55                     | 0.41              |
| 1:j:210:PRO:CG   | 1:k:145:ARG:HD2  | 2.48                     | 0.41              |
| 1:r:63:ILE:HD11  | 1:r:89:LEU:HD11  | 2.02                     | 0.41              |
| 1:t:212:LEU:HB2  | 1:u:143:ALA:HB2  | 2.02                     | 0.41              |
| 1:u:128:LEU:HA   | 1:u:129:PRO:HD3  | 1.83                     | 0.41              |
| 1:u:209:VAL:CG2  | 1:u:209:VAL:O    | 2.69                     | 0.41              |
| 1:v:63:ILE:HB    | 1:v:199:VAL:HG22 | 2.01                     | 0.41              |
| 1:w:167:LEU:HD23 | 1:w:179:SER:N    | 2.36                     | 0.41              |
| 1:B:91:ARG:HD2   | 1:J:98:ILE:HG23  | 2.02                     | 0.41              |
| 1:G:184:ILE:HG22 | 1:G:186:LEU:HD13 | 2.02                     | 0.41              |
| 1:I:91:ARG:HG2   | 1:O:98:ILE:HG12  | 2.03                     | 0.41              |
| 1:J:62:ARG:HD3   | 1:J:198:SER:HB3  | 2.03                     | 0.41              |
| 1:L:63:ILE:HD11  | 1:L:89:LEU:HD11  | 2.02                     | 0.41              |
| 1:M:83:THR:HA    | 1:M:182:ARG:HB3  | 2.02                     | 0.41              |
| 1:N:163:THR:C    | 1:N:164:ARG:HG3  | 2.46                     | 0.41              |
| 1:Q:149:VAL:HG23 | 1:p:112:GLN:HG2  | 2.02                     | 0.41              |
| 1:T:121:GLY:CA   | 1:T:152:TRP:HE3  | 2.34                     | 0.41              |
| 1:T:146:GLY:O    | 1:T:147:ALA:C    | 2.64                     | 0.41              |
| 1:T:153:TRP:O    | 1:l:151:LYS:HE2  | 2.21                     | 0.41              |
| 1:Y:69:PRO:O     | 1:Y:70:ALA:C     | 2.64                     | 0.41              |
| 1:Y:100:GLN:N    | 1:Y:209:VAL:O    | 2.54                     | 0.41              |
| 1:Y:162:TYR:O    | 1:Y:164:ARG:HG3  | 2.21                     | 0.41              |
| 1:Z:62:ARG:NH1   | 1:Z:65:GLN:HE21  | 2.18                     | 0.41              |
| 1:Z:200:LEU:HD11 | 1:u:149:VAL:CG2  | 2.51                     | 0.41              |
| 1:3:99:PHE:HB3   | 1:3:208:SER:O    | 2.20                     | 0.41              |
| 1:3:128:LEU:HA   | 1:3:129:PRO:HD3  | 1.82                     | 0.41              |
| 1:3:138:PHE:CD1  | 1:3:138:PHE:C    | 2.99                     | 0.41              |
| 1:5:92:LEU:HD11  | 1:5:205:VAL:HG11 | 2.03                     | 0.41              |
| 1:5:168:TRP:HB2  | 1:5:177:LEU:O    | 2.20                     | 0.41              |
| 1:6:101:ARG:CG   | 1:6:167:LEU:O    | 2.68                     | 0.41              |
| 1:9:79:VAL:CG2   | 1:9:185:LEU:HD13 | 2.51                     | 0.41              |
| 1:b:84:ILE:O     | 1:b:180:PRO:HD2  | 2.21                     | 0.41              |
| 1:b:108:GLU:HB2  | 1:b:202:ARG:HG2  | 2.02                     | 0.41              |
| 1:e:100:GLN:HB2  | 1:e:209:VAL:CG2  | 2.51                     | 0.41              |
| 1:f:55:VAL:HG13  | 1:x:55:VAL:HG13  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:98:ILE:HG22  | 1:f:99:PHE:CD1   | 2.55                     | 0.41              |
| 1:i:98:ILE:HD11  | 1:r:91:ARG:O     | 2.21                     | 0.41              |
| 1:j:138:PHE:CD1  | 1:j:138:PHE:C    | 2.98                     | 0.41              |
| 1:j:184:ILE:HG22 | 1:j:186:LEU:HD13 | 2.02                     | 0.41              |
| 1:v:79:VAL:HG21  | 1:v:185:LEU:HD13 | 2.03                     | 0.41              |
| 1:v:184:ILE:HG22 | 1:v:186:LEU:CD1  | 2.51                     | 0.41              |
| 1:D:63:ILE:HD11  | 1:D:89:LEU:HD21  | 2.03                     | 0.40              |
| 1:D:182:ARG:HG3  | 1:D:184:ILE:HD11 | 2.03                     | 0.40              |
| 1:G:139:ASP:O    | 1:I:212:LEU:HD23 | 2.20                     | 0.40              |
| 1:L:101:ARG:CG   | 1:L:167:LEU:O    | 2.69                     | 0.40              |
| 1:L:167:LEU:HB3  | 1:L:168:TRP:H    | 1.78                     | 0.40              |
| 1:P:74:THR:O     | 1:P:75:ASP:C     | 2.64                     | 0.40              |
| 1:P:131:PRO:HA   | 1:P:182:ARG:HD2  | 2.03                     | 0.40              |
| 1:Q:107:LEU:O    | 1:Q:160:PRO:HD2  | 2.21                     | 0.40              |
| 1:R:113:PRO:HA   | 1:R:197:VAL:HA   | 2.03                     | 0.40              |
| 1:U:118:ASN:HD21 | 1:k:118:ASN:HB2  | 1.86                     | 0.40              |
| 1:W:142:GLN:NE2  | 1:j:60:MET:O     | 2.53                     | 0.40              |
| 1:X:108:GLU:HB2  | 1:X:202:ARG:HG2  | 2.03                     | 0.40              |
| 1:Y:114:MET:HG2  | 1:w:151:LYS:HA   | 2.03                     | 0.40              |
| 1:Z:101:ARG:NH1  | 1:Z:168:TRP:CZ2  | 2.90                     | 0.40              |
| 1:0:101:ARG:HE   | 1:0:166:LEU:HD21 | 1.86                     | 0.40              |
| 1:0:130:ASP:OD1  | 1:0:130:ASP:N    | 2.55                     | 0.40              |
| 1:3:63:ILE:HD11  | 1:3:89:LEU:HD11  | 2.02                     | 0.40              |
| 1:4:101:ARG:NE   | 1:4:166:LEU:HD21 | 2.26                     | 0.40              |
| 1:4:121:GLY:HA3  | 1:4:152:TRP:HE3  | 1.86                     | 0.40              |
| 1:6:108:GLU:HB2  | 1:6:202:ARG:HG2  | 2.03                     | 0.40              |
| 1:7:122:GLY:CA   | 1:o:114:MET:SD   | 3.09                     | 0.40              |
| 1:7:149:VAL:CG2  | 1:o:200:LEU:HD11 | 2.51                     | 0.40              |
| 1:b:107:LEU:O    | 1:b:160:PRO:HD2  | 2.21                     | 0.40              |
| 1:e:123:TYR:HB2  | 1:e:185:LEU:CD2  | 2.50                     | 0.40              |
| 1:f:166:LEU:HG   | 1:f:167:LEU:N    | 2.36                     | 0.40              |
| 1:h:168:TRP:CZ3  | 1:i:176:ARG:NH2  | 2.89                     | 0.40              |
| 1:i:79:VAL:CG2   | 1:i:185:LEU:HD13 | 2.51                     | 0.40              |
| 1:j:98:ILE:HD13  | 1:j:98:ILE:HG21  | 1.91                     | 0.40              |
| 1:k:101:ARG:NE   | 1:k:166:LEU:HD21 | 2.36                     | 0.40              |
| 1:m:145:ARG:NH1  | 1:m:161:GLN:HB3  | 2.36                     | 0.40              |
| 1:p:77:TYR:CD1   | 1:p:79:VAL:HG12  | 2.56                     | 0.40              |
| 1:q:130:ASP:OD2  | 1:q:132:THR:OG1  | 2.39                     | 0.40              |
| 1:s:167:LEU:C    | 1:s:168:TRP:CD1  | 2.99                     | 0.40              |
| 1:w:107:LEU:HD23 | 1:w:107:LEU:HA   | 1.89                     | 0.40              |
| 1:C:168:TRP:N    | 1:C:177:LEU:O    | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:104:VAL:CG1  | 1:D:107:LEU:HG   | 2.51                     | 0.40              |
| 1:E:63:ILE:HD13  | 1:E:63:ILE:HA    | 1.91                     | 0.40              |
| 1:F:166:LEU:HG   | 1:F:167:LEU:N    | 2.36                     | 0.40              |
| 1:N:121:GLY:HA3  | 1:N:152:TRP:HE3  | 1.86                     | 0.40              |
| 1:O:162:TYR:O    | 1:O:164:ARG:HG3  | 2.20                     | 0.40              |
| 1:Q:98:ILE:HG22  | 1:Q:99:PHE:CD1   | 2.56                     | 0.40              |
| 1:S:127:PHE:CZ   | 1:S:181:GLY:HA3  | 2.56                     | 0.40              |
| 1:V:168:TRP:CZ3  | 1:W:176:ARG:CZ   | 3.04                     | 0.40              |
| 1:Z:100:GLN:OE1  | 1:0:130:ASP:OD1  | 2.38                     | 0.40              |
| 1:2:128:LEU:HA   | 1:2:129:PRO:HD3  | 1.79                     | 0.40              |
| 1:6:165:THR:HG23 | 1:6:166:LEU:O    | 2.22                     | 0.40              |
| 1:7:168:TRP:HZ3  | 1:8:130:ASP:CG   | 2.28                     | 0.40              |
| 1:9:113:PRO:O    | 1:m:151:LYS:HE3  | 2.22                     | 0.40              |
| 1:9:166:LEU:HG   | 1:9:167:LEU:N    | 2.36                     | 0.40              |
| 1:a:101:ARG:NE   | 1:a:166:LEU:HD21 | 2.32                     | 0.40              |
| 1:b:98:ILE:HG22  | 1:b:99:PHE:CD1   | 2.57                     | 0.40              |
| 1:f:209:VAL:O    | 1:f:209:VAL:HG23 | 2.19                     | 0.40              |
| 1:h:98:ILE:HD13  | 1:h:98:ILE:HG21  | 1.78                     | 0.40              |
| 1:i:101:ARG:CG   | 1:i:167:LEU:O    | 2.69                     | 0.40              |
| 1:o:145:ARG:NH1  | 1:o:161:GLN:HB3  | 2.36                     | 0.40              |
| 1:q:63:ILE:CG2   | 1:q:82:ALA:CB    | 3.00                     | 0.40              |
| 1:q:86:PRO:HA    | 1:q:92:LEU:HD23  | 2.03                     | 0.40              |
| 1:q:130:ASP:HB3  | 1:q:133:ASP:H    | 1.86                     | 0.40              |
| 1:v:79:VAL:HG22  | 1:v:185:LEU:HB3  | 2.03                     | 0.40              |
| 1:w:88:LEU:HD23  | 1:w:88:LEU:HA    | 1.96                     | 0.40              |
| 1:x:168:TRP:N    | 1:x:177:LEU:O    | 2.54                     | 0.40              |
| 1:B:91:ARG:NH1   | 1:J:210:PRO:HB3  | 2.36                     | 0.40              |
| 1:B:109:PHE:CD2  | 1:B:183:LEU:HD23 | 2.57                     | 0.40              |
| 1:G:98:ILE:HG23  | 1:K:91:ARG:HD2   | 2.04                     | 0.40              |
| 1:H:152:TRP:HH2  | 1:H:187:CYS:HG   | 1.65                     | 0.40              |
| 1:H:162:TYR:O    | 1:H:164:ARG:HG3  | 2.21                     | 0.40              |
| 1:H:168:TRP:CZ3  | 1:I:130:ASP:OD1  | 2.74                     | 0.40              |
| 1:I:114:MET:SD   | 1:Y:122:GLY:HA2  | 2.62                     | 0.40              |
| 1:J:163:THR:HG23 | 1:J:164:ARG:N    | 2.37                     | 0.40              |
| 1:N:100:GLN:NE2  | 1:N:213:GLU:OE2  | 2.54                     | 0.40              |
| 1:O:166:LEU:HG   | 1:O:167:LEU:N    | 2.36                     | 0.40              |
| 1:P:196:ASN:HD22 | 1:P:196:ASN:C    | 2.30                     | 0.40              |
| 1:Q:163:THR:C    | 1:Q:165:THR:N    | 2.79                     | 0.40              |
| 1:T:210:PRO:HB2  | 1:U:145:ARG:HD3  | 2.03                     | 0.40              |
| 1:V:128:LEU:HA   | 1:V:129:PRO:HD3  | 1.78                     | 0.40              |
| 1:b:212:LEU:HG   | 1:b:212:LEU:O    | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:e:69:PRO:HD2   | 1:e:72:THR:OG1   | 2.22                     | 0.40              |
| 1:f:151:LYS:HD2  | 1:f:153:TRP:CZ2  | 2.56                     | 0.40              |
| 1:i:81:ASP:OD1   | 1:i:81:ASP:C     | 2.65                     | 0.40              |
| 1:i:145:ARG:NH1  | 1:i:161:GLN:HB3  | 2.35                     | 0.40              |
| 1:j:123:TYR:HA   | 1:j:186:LEU:O    | 2.21                     | 0.40              |
| 1:m:73:GLY:O     | 1:m:190:ASN:HB3  | 2.21                     | 0.40              |
| 1:r:101:ARG:CG   | 1:r:167:LEU:O    | 2.69                     | 0.40              |
| 1:s:168:TRP:CZ3  | 1:t:176:ARG:HD2  | 2.57                     | 0.40              |
| 1:t:100:GLN:HB2  | 1:t:209:VAL:CG2  | 2.49                     | 0.40              |
| 1:D:109:PHE:HB2  | 1:D:158:VAL:HG22 | 2.04                     | 0.40              |
| 1:D:138:PHE:CD1  | 1:D:138:PHE:C    | 2.99                     | 0.40              |
| 1:H:74:THR:O     | 1:H:76:GLY:N     | 2.54                     | 0.40              |
| 1:H:112:GLN:HG2  | 1:N:149:VAL:HG22 | 2.03                     | 0.40              |
| 1:H:210:PRO:HB2  | 1:I:145:ARG:CD   | 2.51                     | 0.40              |
| 1:L:168:TRP:N    | 1:L:177:LEU:O    | 2.55                     | 0.40              |
| 1:Q:98:ILE:O     | 1:Q:211:SER:N    | 2.54                     | 0.40              |
| 1:Q:128:LEU:HA   | 1:Q:129:PRO:HD3  | 1.78                     | 0.40              |
| 1:U:63:ILE:HD11  | 1:U:89:LEU:HD11  | 2.03                     | 0.40              |
| 1:U:211:SER:OG   | 1:U:212:LEU:N    | 2.54                     | 0.40              |
| 1:V:167:LEU:HB3  | 1:V:168:TRP:H    | 1.77                     | 0.40              |
| 1:Y:151:LYS:HD2  | 1:Y:153:TRP:CE2  | 2.56                     | 0.40              |
| 1:7:132:THR:OG1  | 1:7:176:ARG:NH2  | 2.54                     | 0.40              |
| 1:8:100:GLN:HG2  | 1:8:211:SER:CB   | 2.52                     | 0.40              |
| 1:f:168:TRP:HB2  | 1:f:177:LEU:O    | 2.22                     | 0.40              |
| 1:g:162:TYR:O    | 1:g:164:ARG:HG3  | 2.20                     | 0.40              |
| 1:i:107:LEU:O    | 1:i:160:PRO:HD2  | 2.21                     | 0.40              |
| 1:i:138:PHE:CD1  | 1:i:138:PHE:C    | 2.99                     | 0.40              |
| 1:j:60:MET:HE1   | 1:j:202:ARG:NH2  | 2.37                     | 0.40              |
| 1:j:128:LEU:HD22 | 1:j:128:LEU:H    | 1.86                     | 0.40              |
| 1:l:165:THR:HG23 | 1:l:166:LEU:O    | 2.21                     | 0.40              |
| 1:r:138:PHE:CD1  | 1:r:138:PHE:C    | 2.99                     | 0.40              |
| 1:s:79:VAL:HG21  | 1:s:185:LEU:HD13 | 2.03                     | 0.40              |
| 1:B:87:ASP:OD1   | 1:B:87:ASP:N     | 2.55                     | 0.40              |
| 1:B:100:GLN:HB2  | 1:B:209:VAL:CG2  | 2.52                     | 0.40              |
| 1:B:128:LEU:HA   | 1:B:129:PRO:HD3  | 1.95                     | 0.40              |
| 1:E:184:ILE:HG22 | 1:E:186:LEU:HD13 | 2.03                     | 0.40              |
| 1:J:188:VAL:C    | 1:J:189:GLY:O    | 2.64                     | 0.40              |
| 1:N:79:VAL:HG22  | 1:N:185:LEU:HB3  | 2.04                     | 0.40              |
| 1:O:113:PRO:HA   | 1:O:197:VAL:HA   | 2.03                     | 0.40              |
| 1:P:98:ILE:HD13  | 1:P:98:ILE:HG21  | 1.88                     | 0.40              |
| 1:R:69:PRO:O     | 1:R:72:THR:HG23  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:145:ARG:NH1  | 1:R:161:GLN:HB3  | 2.36                     | 0.40              |
| 1:T:101:ARG:HH21 | 1:T:166:LEU:HD22 | 1.87                     | 0.40              |
| 1:Z:63:ILE:HA    | 1:Z:63:ILE:HD13  | 1.83                     | 0.40              |
| 1:O:79:VAL:CG2   | 1:O:185:LEU:HD13 | 2.52                     | 0.40              |
| 1:2:151:LYS:HD2  | 1:2:153:TRP:CZ2  | 2.57                     | 0.40              |
| 1:a:163:THR:HG22 | 1:a:180:PRO:CB   | 2.51                     | 0.40              |
| 1:l:108:GLU:HB2  | 1:l:202:ARG:HG2  | 2.03                     | 0.40              |
| 1:l:209:VAL:CG2  | 1:l:209:VAL:O    | 2.69                     | 0.40              |
| 1:p:151:LYS:HD2  | 1:p:153:TRP:CE2  | 2.57                     | 0.40              |
| 1:q:68:LEU:HA    | 1:q:69:PRO:HD3   | 1.93                     | 0.40              |
| 1:r:77:TYR:CD1   | 1:r:77:TYR:C     | 3.00                     | 0.40              |
| 1:x:209:VAL:O    | 1:x:209:VAL:HG23 | 2.22                     | 0.40              |

All (1) 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:N:77:TYR:OH | 1:3:134:ASN:OD1[3_654] | 1.87                     | 0.33              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | 0     | 161/183 (88%) | 151 (94%) | 9 (6%)   | 1 (1%)   | 21          | 52 |
| 1   | 1     | 161/183 (88%) | 142 (88%) | 17 (11%) | 2 (1%)   | 10          | 37 |
| 1   | 2     | 161/183 (88%) | 136 (84%) | 22 (14%) | 3 (2%)   | 6           | 27 |
| 1   | 3     | 161/183 (88%) | 151 (94%) | 9 (6%)   | 1 (1%)   | 21          | 52 |
| 1   | 4     | 161/183 (88%) | 141 (88%) | 18 (11%) | 2 (1%)   | 10          | 37 |
| 1   | 5     | 161/183 (88%) | 148 (92%) | 9 (6%)   | 4 (2%)   | 4           | 21 |
| 1   | 6     | 161/183 (88%) | 152 (94%) | 8 (5%)   | 1 (1%)   | 21          | 52 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | 7     | 161/183 (88%) | 141 (88%) | 18 (11%) | 2 (1%)   | 10          | 37  |
| 1   | 8     | 161/183 (88%) | 145 (90%) | 12 (8%)  | 4 (2%)   | 4           | 21  |
| 1   | 9     | 161/183 (88%) | 150 (93%) | 10 (6%)  | 1 (1%)   | 21          | 52  |
| 1   | A     | 161/183 (88%) | 148 (92%) | 11 (7%)  | 2 (1%)   | 10          | 37  |
| 1   | B     | 161/183 (88%) | 142 (88%) | 16 (10%) | 3 (2%)   | 6           | 27  |
| 1   | C     | 161/183 (88%) | 151 (94%) | 9 (6%)   | 1 (1%)   | 21          | 52  |
| 1   | D     | 161/183 (88%) | 149 (92%) | 10 (6%)  | 2 (1%)   | 10          | 37  |
| 1   | E     | 161/183 (88%) | 147 (91%) | 12 (8%)  | 2 (1%)   | 10          | 37  |
| 1   | F     | 161/183 (88%) | 151 (94%) | 9 (6%)   | 1 (1%)   | 21          | 52  |
| 1   | G     | 161/183 (88%) | 144 (89%) | 16 (10%) | 1 (1%)   | 21          | 52  |
| 1   | H     | 161/183 (88%) | 143 (89%) | 15 (9%)  | 3 (2%)   | 6           | 27  |
| 1   | I     | 161/183 (88%) | 151 (94%) | 9 (6%)   | 1 (1%)   | 21          | 52  |
| 1   | J     | 161/183 (88%) | 145 (90%) | 15 (9%)  | 1 (1%)   | 21          | 52  |
| 1   | K     | 161/183 (88%) | 142 (88%) | 16 (10%) | 3 (2%)   | 6           | 27  |
| 1   | L     | 161/183 (88%) | 151 (94%) | 9 (6%)   | 1 (1%)   | 21          | 52  |
| 1   | M     | 161/183 (88%) | 141 (88%) | 16 (10%) | 4 (2%)   | 4           | 21  |
| 1   | N     | 161/183 (88%) | 143 (89%) | 18 (11%) | 0        | 100         | 100 |
| 1   | O     | 161/183 (88%) | 150 (93%) | 10 (6%)  | 1 (1%)   | 21          | 52  |
| 1   | P     | 161/183 (88%) | 139 (86%) | 20 (12%) | 2 (1%)   | 10          | 37  |
| 1   | Q     | 161/183 (88%) | 145 (90%) | 15 (9%)  | 1 (1%)   | 21          | 52  |
| 1   | R     | 161/183 (88%) | 150 (93%) | 10 (6%)  | 1 (1%)   | 21          | 52  |
| 1   | S     | 161/183 (88%) | 146 (91%) | 13 (8%)  | 2 (1%)   | 10          | 37  |
| 1   | T     | 161/183 (88%) | 146 (91%) | 15 (9%)  | 0        | 100         | 100 |
| 1   | U     | 161/183 (88%) | 150 (93%) | 10 (6%)  | 1 (1%)   | 21          | 52  |
| 1   | V     | 161/183 (88%) | 145 (90%) | 14 (9%)  | 2 (1%)   | 10          | 37  |
| 1   | W     | 161/183 (88%) | 142 (88%) | 17 (11%) | 2 (1%)   | 10          | 37  |
| 1   | X     | 161/183 (88%) | 150 (93%) | 10 (6%)  | 1 (1%)   | 21          | 52  |
| 1   | Y     | 161/183 (88%) | 147 (91%) | 13 (8%)  | 1 (1%)   | 21          | 52  |
| 1   | Z     | 161/183 (88%) | 143 (89%) | 15 (9%)  | 3 (2%)   | 6           | 27  |
| 1   | a     | 161/183 (88%) | 140 (87%) | 20 (12%) | 1 (1%)   | 21          | 52  |
| 1   | b     | 161/183 (88%) | 141 (88%) | 17 (11%) | 3 (2%)   | 6           | 27  |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | c     | 161/183 (88%)    | 151 (94%)  | 9 (6%)   | 1 (1%)   | 21          | 52 |
| 1   | d     | 161/183 (88%)    | 148 (92%)  | 12 (8%)  | 1 (1%)   | 21          | 52 |
| 1   | e     | 161/183 (88%)    | 143 (89%)  | 17 (11%) | 1 (1%)   | 21          | 52 |
| 1   | f     | 161/183 (88%)    | 151 (94%)  | 9 (6%)   | 1 (1%)   | 21          | 52 |
| 1   | g     | 161/183 (88%)    | 146 (91%)  | 14 (9%)  | 1 (1%)   | 21          | 52 |
| 1   | h     | 161/183 (88%)    | 145 (90%)  | 15 (9%)  | 1 (1%)   | 21          | 52 |
| 1   | i     | 161/183 (88%)    | 150 (93%)  | 10 (6%)  | 1 (1%)   | 21          | 52 |
| 1   | j     | 161/183 (88%)    | 146 (91%)  | 13 (8%)  | 2 (1%)   | 10          | 37 |
| 1   | k     | 161/183 (88%)    | 143 (89%)  | 17 (11%) | 1 (1%)   | 21          | 52 |
| 1   | l     | 161/183 (88%)    | 150 (93%)  | 10 (6%)  | 1 (1%)   | 21          | 52 |
| 1   | m     | 161/183 (88%)    | 144 (89%)  | 16 (10%) | 1 (1%)   | 21          | 52 |
| 1   | n     | 161/183 (88%)    | 146 (91%)  | 13 (8%)  | 2 (1%)   | 10          | 37 |
| 1   | o     | 161/183 (88%)    | 150 (93%)  | 10 (6%)  | 1 (1%)   | 21          | 52 |
| 1   | p     | 161/183 (88%)    | 144 (89%)  | 15 (9%)  | 2 (1%)   | 10          | 37 |
| 1   | q     | 161/183 (88%)    | 145 (90%)  | 15 (9%)  | 1 (1%)   | 21          | 52 |
| 1   | r     | 161/183 (88%)    | 151 (94%)  | 9 (6%)   | 1 (1%)   | 21          | 52 |
| 1   | s     | 161/183 (88%)    | 134 (83%)  | 26 (16%) | 1 (1%)   | 21          | 52 |
| 1   | t     | 161/183 (88%)    | 147 (91%)  | 12 (8%)  | 2 (1%)   | 10          | 37 |
| 1   | u     | 161/183 (88%)    | 151 (94%)  | 9 (6%)   | 1 (1%)   | 21          | 52 |
| 1   | v     | 161/183 (88%)    | 143 (89%)  | 16 (10%) | 2 (1%)   | 10          | 37 |
| 1   | w     | 161/183 (88%)    | 146 (91%)  | 14 (9%)  | 1 (1%)   | 21          | 52 |
| 1   | x     | 161/183 (88%)    | 150 (93%)  | 10 (6%)  | 1 (1%)   | 21          | 52 |
| All | All   | 9660/10980 (88%) | 8763 (91%) | 803 (8%) | 94 (1%)  | 12          | 41 |

All (94) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 178 | THR  |
| 1   | C     | 209 | VAL  |
| 1   | H     | 70  | ALA  |
| 1   | K     | 70  | ALA  |
| 1   | W     | 70  | ALA  |
| 1   | Z     | 70  | ALA  |
| 1   | 5     | 70  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7     | 147 | ALA  |
| 1   | 8     | 121 | GLY  |
| 1   | b     | 70  | ALA  |
| 1   | b     | 75  | ASP  |
| 1   | j     | 70  | ALA  |
| 1   | j     | 178 | THR  |
| 1   | l     | 209 | VAL  |
| 1   | n     | 147 | ALA  |
| 1   | q     | 70  | ALA  |
| 1   | s     | 75  | ASP  |
| 1   | t     | 70  | ALA  |
| 1   | t     | 147 | ALA  |
| 1   | x     | 209 | VAL  |
| 1   | B     | 70  | ALA  |
| 1   | B     | 178 | THR  |
| 1   | D     | 147 | ALA  |
| 1   | F     | 209 | VAL  |
| 1   | G     | 121 | GLY  |
| 1   | H     | 75  | ASP  |
| 1   | I     | 209 | VAL  |
| 1   | J     | 147 | ALA  |
| 1   | L     | 209 | VAL  |
| 1   | M     | 135 | ASP  |
| 1   | O     | 209 | VAL  |
| 1   | P     | 171 | SER  |
| 1   | P     | 178 | THR  |
| 1   | R     | 209 | VAL  |
| 1   | S     | 147 | ALA  |
| 1   | U     | 209 | VAL  |
| 1   | X     | 209 | VAL  |
| 1   | Y     | 70  | ALA  |
| 1   | 0     | 209 | VAL  |
| 1   | 2     | 147 | ALA  |
| 1   | 3     | 209 | VAL  |
| 1   | 5     | 147 | ALA  |
| 1   | 6     | 209 | VAL  |
| 1   | 9     | 209 | VAL  |
| 1   | a     | 70  | ALA  |
| 1   | b     | 147 | ALA  |
| 1   | c     | 209 | VAL  |
| 1   | f     | 209 | VAL  |
| 1   | g     | 70  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | i     | 209 | VAL  |
| 1   | k     | 178 | THR  |
| 1   | o     | 209 | VAL  |
| 1   | p     | 75  | ASP  |
| 1   | r     | 209 | VAL  |
| 1   | u     | 209 | VAL  |
| 1   | v     | 75  | ASP  |
| 1   | w     | 75  | ASP  |
| 1   | D     | 70  | ALA  |
| 1   | E     | 75  | ASP  |
| 1   | M     | 75  | ASP  |
| 1   | V     | 75  | ASP  |
| 1   | 4     | 147 | ALA  |
| 1   | 8     | 147 | ALA  |
| 1   | E     | 70  | ALA  |
| 1   | H     | 147 | ALA  |
| 1   | K     | 147 | ALA  |
| 1   | M     | 70  | ALA  |
| 1   | V     | 147 | ALA  |
| 1   | Z     | 75  | ASP  |
| 1   | 1     | 97  | ARG  |
| 1   | 2     | 70  | ALA  |
| 1   | 7     | 75  | ASP  |
| 1   | 8     | 75  | ASP  |
| 1   | K     | 129 | PRO  |
| 1   | S     | 70  | ALA  |
| 1   | 5     | 75  | ASP  |
| 1   | 8     | 70  | ALA  |
| 1   | e     | 70  | ALA  |
| 1   | v     | 147 | ALA  |
| 1   | 4     | 129 | PRO  |
| 1   | h     | 70  | ALA  |
| 1   | n     | 75  | ASP  |
| 1   | 5     | 86  | PRO  |
| 1   | B     | 189 | GLY  |
| 1   | W     | 189 | GLY  |
| 1   | A     | 90  | PRO  |
| 1   | Z     | 113 | PRO  |
| 1   | d     | 131 | PRO  |
| 1   | m     | 93  | GLY  |
| 1   | M     | 90  | PRO  |
| 1   | Q     | 121 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 121 | GLY  |
| 1   | 2     | 71  | GLY  |
| 1   | p     | 71  | GLY  |

### 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   | 0     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |
| 1   | 1     | 138/153 (90%) | 103 (75%) | 35 (25%) | 0           | 2 |
| 1   | 2     | 138/153 (90%) | 109 (79%) | 29 (21%) | 1           | 5 |
| 1   | 3     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |
| 1   | 4     | 138/153 (90%) | 103 (75%) | 35 (25%) | 0           | 2 |
| 1   | 5     | 138/153 (90%) | 111 (80%) | 27 (20%) | 1           | 6 |
| 1   | 6     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |
| 1   | 7     | 138/153 (90%) | 105 (76%) | 33 (24%) | 1           | 3 |
| 1   | 8     | 138/153 (90%) | 109 (79%) | 29 (21%) | 1           | 5 |
| 1   | 9     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |
| 1   | A     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |
| 1   | B     | 138/153 (90%) | 106 (77%) | 32 (23%) | 1           | 4 |
| 1   | C     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |
| 1   | D     | 138/153 (90%) | 106 (77%) | 32 (23%) | 1           | 4 |
| 1   | E     | 138/153 (90%) | 103 (75%) | 35 (25%) | 0           | 2 |
| 1   | F     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |
| 1   | G     | 138/153 (90%) | 100 (72%) | 38 (28%) | 0           | 1 |
| 1   | H     | 138/153 (90%) | 105 (76%) | 33 (24%) | 1           | 3 |
| 1   | I     | 138/153 (90%) | 106 (77%) | 32 (23%) | 1           | 4 |
| 1   | J     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |
| 1   | K     | 138/153 (90%) | 109 (79%) | 29 (21%) | 1           | 5 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |   |  |
|-----|-------|---------------|-----------|----------|-------------|---|--|
| 1   | L     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |  |
| 1   | M     | 138/153 (90%) | 105 (76%) | 33 (24%) | 1           | 3 |  |
| 1   | N     | 138/153 (90%) | 106 (77%) | 32 (23%) | 1           | 4 |  |
| 1   | O     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | P     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | Q     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | R     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |  |
| 1   | S     | 138/153 (90%) | 106 (77%) | 32 (23%) | 1           | 4 |  |
| 1   | T     | 138/153 (90%) | 99 (72%)  | 39 (28%) | 0           | 1 |  |
| 1   | U     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | V     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | W     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | X     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |  |
| 1   | Y     | 138/153 (90%) | 109 (79%) | 29 (21%) | 1           | 5 |  |
| 1   | Z     | 138/153 (90%) | 104 (75%) | 34 (25%) | 1           | 3 |  |
| 1   | a     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | b     | 138/153 (90%) | 110 (80%) | 28 (20%) | 1           | 5 |  |
| 1   | c     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |  |
| 1   | d     | 138/153 (90%) | 104 (75%) | 34 (25%) | 1           | 3 |  |
| 1   | e     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |  |
| 1   | f     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |  |
| 1   | g     | 138/153 (90%) | 104 (75%) | 34 (25%) | 1           | 3 |  |
| 1   | h     | 138/153 (90%) | 104 (75%) | 34 (25%) | 1           | 3 |  |
| 1   | i     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | j     | 138/153 (90%) | 109 (79%) | 29 (21%) | 1           | 5 |  |
| 1   | k     | 138/153 (90%) | 109 (79%) | 29 (21%) | 1           | 5 |  |
| 1   | l     | 138/153 (90%) | 107 (78%) | 31 (22%) | 1           | 4 |  |
| 1   | m     | 138/153 (90%) | 101 (73%) | 37 (27%) | 0           | 2 |  |
| 1   | n     | 138/153 (90%) | 108 (78%) | 30 (22%) | 1           | 5 |  |
| 1   | o     | 138/153 (90%) | 106 (77%) | 32 (23%) | 1           | 4 |  |
| 1   | p     | 138/153 (90%) | 104 (75%) | 34 (25%) | 1           | 3 |  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |   |
|-----|-------|-----------------|------------|------------|-------------|---|
| 1   | q     | 138/153 (90%)   | 110 (80%)  | 28 (20%)   | 1           | 5 |
| 1   | r     | 138/153 (90%)   | 107 (78%)  | 31 (22%)   | 1           | 4 |
| 1   | s     | 138/153 (90%)   | 109 (79%)  | 29 (21%)   | 1           | 5 |
| 1   | t     | 138/153 (90%)   | 107 (78%)  | 31 (22%)   | 1           | 4 |
| 1   | u     | 138/153 (90%)   | 107 (78%)  | 31 (22%)   | 1           | 4 |
| 1   | v     | 138/153 (90%)   | 107 (78%)  | 31 (22%)   | 1           | 4 |
| 1   | w     | 138/153 (90%)   | 109 (79%)  | 29 (21%)   | 1           | 5 |
| 1   | x     | 138/153 (90%)   | 108 (78%)  | 30 (22%)   | 1           | 5 |
| All | All   | 8280/9180 (90%) | 6397 (77%) | 1883 (23%) | 1           | 4 |

All (1883) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 52  | THR  |
| 1   | A     | 57  | LEU  |
| 1   | A     | 61  | SER  |
| 1   | A     | 62  | ARG  |
| 1   | A     | 64  | SER  |
| 1   | A     | 74  | THR  |
| 1   | A     | 79  | VAL  |
| 1   | A     | 88  | LEU  |
| 1   | A     | 92  | LEU  |
| 1   | A     | 101 | ARG  |
| 1   | A     | 105 | GLU  |
| 1   | A     | 118 | ASN  |
| 1   | A     | 128 | LEU  |
| 1   | A     | 130 | ASP  |
| 1   | A     | 142 | GLN  |
| 1   | A     | 145 | ARG  |
| 1   | A     | 151 | LYS  |
| 1   | A     | 152 | TRP  |
| 1   | A     | 155 | SER  |
| 1   | A     | 158 | VAL  |
| 1   | A     | 159 | ARG  |
| 1   | A     | 165 | THR  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 185 | LEU  |
| 1   | A     | 190 | ASN  |
| 1   | A     | 193 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 196 | ASN  |
| 1   | A     | 199 | VAL  |
| 1   | A     | 201 | CYS  |
| 1   | A     | 202 | ARG  |
| 1   | A     | 205 | VAL  |
| 1   | B     | 57  | LEU  |
| 1   | B     | 60  | MET  |
| 1   | B     | 72  | THR  |
| 1   | B     | 74  | THR  |
| 1   | B     | 79  | VAL  |
| 1   | B     | 100 | GLN  |
| 1   | B     | 107 | LEU  |
| 1   | B     | 124 | VAL  |
| 1   | B     | 128 | LEU  |
| 1   | B     | 133 | ASP  |
| 1   | B     | 134 | ASN  |
| 1   | B     | 137 | THR  |
| 1   | B     | 142 | GLN  |
| 1   | B     | 145 | ARG  |
| 1   | B     | 148 | VAL  |
| 1   | B     | 149 | VAL  |
| 1   | B     | 152 | TRP  |
| 1   | B     | 156 | ARG  |
| 1   | B     | 158 | VAL  |
| 1   | B     | 164 | ARG  |
| 1   | B     | 165 | THR  |
| 1   | B     | 170 | SER  |
| 1   | B     | 178 | THR  |
| 1   | B     | 179 | SER  |
| 1   | B     | 185 | LEU  |
| 1   | B     | 186 | LEU  |
| 1   | B     | 190 | ASN  |
| 1   | B     | 193 | ASP  |
| 1   | B     | 199 | VAL  |
| 1   | B     | 202 | ARG  |
| 1   | B     | 205 | VAL  |
| 1   | B     | 211 | SER  |
| 1   | C     | 57  | LEU  |
| 1   | C     | 72  | THR  |
| 1   | C     | 74  | THR  |
| 1   | C     | 87  | ASP  |
| 1   | C     | 88  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 89  | LEU  |
| 1   | C     | 92  | LEU  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 128 | LEU  |
| 1   | C     | 137 | THR  |
| 1   | C     | 142 | GLN  |
| 1   | C     | 145 | ARG  |
| 1   | C     | 149 | VAL  |
| 1   | C     | 151 | LYS  |
| 1   | C     | 152 | TRP  |
| 1   | C     | 158 | VAL  |
| 1   | C     | 164 | ARG  |
| 1   | C     | 165 | THR  |
| 1   | C     | 167 | LEU  |
| 1   | C     | 170 | SER  |
| 1   | C     | 185 | LEU  |
| 1   | C     | 193 | ASP  |
| 1   | C     | 196 | ASN  |
| 1   | C     | 198 | SER  |
| 1   | C     | 199 | VAL  |
| 1   | C     | 202 | ARG  |
| 1   | C     | 205 | VAL  |
| 1   | C     | 208 | SER  |
| 1   | C     | 209 | VAL  |
| 1   | C     | 211 | SER  |
| 1   | C     | 213 | GLU  |
| 1   | D     | 57  | LEU  |
| 1   | D     | 58  | SER  |
| 1   | D     | 62  | ARG  |
| 1   | D     | 74  | THR  |
| 1   | D     | 79  | VAL  |
| 1   | D     | 88  | LEU  |
| 1   | D     | 92  | LEU  |
| 1   | D     | 101 | ARG  |
| 1   | D     | 106 | THR  |
| 1   | D     | 112 | GLN  |
| 1   | D     | 128 | LEU  |
| 1   | D     | 137 | THR  |
| 1   | D     | 142 | GLN  |
| 1   | D     | 145 | ARG  |
| 1   | D     | 149 | VAL  |
| 1   | D     | 151 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 152 | TRP  |
| 1   | D     | 154 | GLU  |
| 1   | D     | 156 | ARG  |
| 1   | D     | 158 | VAL  |
| 1   | D     | 164 | ARG  |
| 1   | D     | 165 | THR  |
| 1   | D     | 176 | ARG  |
| 1   | D     | 177 | LEU  |
| 1   | D     | 185 | LEU  |
| 1   | D     | 190 | ASN  |
| 1   | D     | 193 | ASP  |
| 1   | D     | 196 | ASN  |
| 1   | D     | 199 | VAL  |
| 1   | D     | 202 | ARG  |
| 1   | D     | 204 | SER  |
| 1   | D     | 213 | GLU  |
| 1   | E     | 57  | LEU  |
| 1   | E     | 64  | SER  |
| 1   | E     | 67  | VAL  |
| 1   | E     | 74  | THR  |
| 1   | E     | 75  | ASP  |
| 1   | E     | 98  | ILE  |
| 1   | E     | 105 | GLU  |
| 1   | E     | 128 | LEU  |
| 1   | E     | 137 | THR  |
| 1   | E     | 142 | GLN  |
| 1   | E     | 145 | ARG  |
| 1   | E     | 149 | VAL  |
| 1   | E     | 151 | LYS  |
| 1   | E     | 152 | TRP  |
| 1   | E     | 156 | ARG  |
| 1   | E     | 158 | VAL  |
| 1   | E     | 161 | GLN  |
| 1   | E     | 162 | TYR  |
| 1   | E     | 164 | ARG  |
| 1   | E     | 177 | LEU  |
| 1   | E     | 178 | THR  |
| 1   | E     | 185 | LEU  |
| 1   | E     | 192 | THR  |
| 1   | E     | 193 | ASP  |
| 1   | E     | 196 | ASN  |
| 1   | E     | 198 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 199 | VAL  |
| 1   | E     | 200 | LEU  |
| 1   | E     | 202 | ARG  |
| 1   | E     | 204 | SER  |
| 1   | E     | 205 | VAL  |
| 1   | E     | 207 | LEU  |
| 1   | E     | 209 | VAL  |
| 1   | E     | 211 | SER  |
| 1   | E     | 213 | GLU  |
| 1   | F     | 57  | LEU  |
| 1   | F     | 72  | THR  |
| 1   | F     | 74  | THR  |
| 1   | F     | 87  | ASP  |
| 1   | F     | 88  | LEU  |
| 1   | F     | 89  | LEU  |
| 1   | F     | 92  | LEU  |
| 1   | F     | 118 | ASN  |
| 1   | F     | 128 | LEU  |
| 1   | F     | 137 | THR  |
| 1   | F     | 142 | GLN  |
| 1   | F     | 145 | ARG  |
| 1   | F     | 149 | VAL  |
| 1   | F     | 151 | LYS  |
| 1   | F     | 152 | TRP  |
| 1   | F     | 158 | VAL  |
| 1   | F     | 164 | ARG  |
| 1   | F     | 165 | THR  |
| 1   | F     | 167 | LEU  |
| 1   | F     | 170 | SER  |
| 1   | F     | 185 | LEU  |
| 1   | F     | 193 | ASP  |
| 1   | F     | 196 | ASN  |
| 1   | F     | 198 | SER  |
| 1   | F     | 199 | VAL  |
| 1   | F     | 202 | ARG  |
| 1   | F     | 205 | VAL  |
| 1   | F     | 208 | SER  |
| 1   | F     | 209 | VAL  |
| 1   | F     | 211 | SER  |
| 1   | F     | 213 | GLU  |
| 1   | G     | 57  | LEU  |
| 1   | G     | 61  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 62  | ARG  |
| 1   | G     | 68  | LEU  |
| 1   | G     | 74  | THR  |
| 1   | G     | 75  | ASP  |
| 1   | G     | 79  | VAL  |
| 1   | G     | 88  | LEU  |
| 1   | G     | 92  | LEU  |
| 1   | G     | 101 | ARG  |
| 1   | G     | 105 | GLU  |
| 1   | G     | 118 | ASN  |
| 1   | G     | 128 | LEU  |
| 1   | G     | 130 | ASP  |
| 1   | G     | 135 | ASP  |
| 1   | G     | 142 | GLN  |
| 1   | G     | 145 | ARG  |
| 1   | G     | 149 | VAL  |
| 1   | G     | 151 | LYS  |
| 1   | G     | 152 | TRP  |
| 1   | G     | 156 | ARG  |
| 1   | G     | 158 | VAL  |
| 1   | G     | 164 | ARG  |
| 1   | G     | 165 | THR  |
| 1   | G     | 175 | GLN  |
| 1   | G     | 176 | ARG  |
| 1   | G     | 177 | LEU  |
| 1   | G     | 178 | THR  |
| 1   | G     | 185 | LEU  |
| 1   | G     | 186 | LEU  |
| 1   | G     | 190 | ASN  |
| 1   | G     | 193 | ASP  |
| 1   | G     | 196 | ASN  |
| 1   | G     | 199 | VAL  |
| 1   | G     | 202 | ARG  |
| 1   | G     | 205 | VAL  |
| 1   | G     | 208 | SER  |
| 1   | G     | 213 | GLU  |
| 1   | H     | 61  | SER  |
| 1   | H     | 74  | THR  |
| 1   | H     | 79  | VAL  |
| 1   | H     | 105 | GLU  |
| 1   | H     | 107 | LEU  |
| 1   | H     | 124 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 128 | LEU  |
| 1   | H     | 130 | ASP  |
| 1   | H     | 133 | ASP  |
| 1   | H     | 134 | ASN  |
| 1   | H     | 137 | THR  |
| 1   | H     | 142 | GLN  |
| 1   | H     | 145 | ARG  |
| 1   | H     | 149 | VAL  |
| 1   | H     | 152 | TRP  |
| 1   | H     | 155 | SER  |
| 1   | H     | 158 | VAL  |
| 1   | H     | 161 | GLN  |
| 1   | H     | 164 | ARG  |
| 1   | H     | 175 | GLN  |
| 1   | H     | 176 | ARG  |
| 1   | H     | 177 | LEU  |
| 1   | H     | 178 | THR  |
| 1   | H     | 185 | LEU  |
| 1   | H     | 186 | LEU  |
| 1   | H     | 190 | ASN  |
| 1   | H     | 192 | THR  |
| 1   | H     | 196 | ASN  |
| 1   | H     | 199 | VAL  |
| 1   | H     | 202 | ARG  |
| 1   | H     | 205 | VAL  |
| 1   | H     | 209 | VAL  |
| 1   | H     | 211 | SER  |
| 1   | I     | 57  | LEU  |
| 1   | I     | 72  | THR  |
| 1   | I     | 74  | THR  |
| 1   | I     | 87  | ASP  |
| 1   | I     | 88  | LEU  |
| 1   | I     | 89  | LEU  |
| 1   | I     | 92  | LEU  |
| 1   | I     | 118 | ASN  |
| 1   | I     | 128 | LEU  |
| 1   | I     | 137 | THR  |
| 1   | I     | 142 | GLN  |
| 1   | I     | 145 | ARG  |
| 1   | I     | 149 | VAL  |
| 1   | I     | 151 | LYS  |
| 1   | I     | 152 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 158 | VAL  |
| 1   | I     | 164 | ARG  |
| 1   | I     | 165 | THR  |
| 1   | I     | 167 | LEU  |
| 1   | I     | 170 | SER  |
| 1   | I     | 177 | LEU  |
| 1   | I     | 185 | LEU  |
| 1   | I     | 193 | ASP  |
| 1   | I     | 196 | ASN  |
| 1   | I     | 198 | SER  |
| 1   | I     | 199 | VAL  |
| 1   | I     | 202 | ARG  |
| 1   | I     | 205 | VAL  |
| 1   | I     | 208 | SER  |
| 1   | I     | 209 | VAL  |
| 1   | I     | 211 | SER  |
| 1   | I     | 213 | GLU  |
| 1   | J     | 57  | LEU  |
| 1   | J     | 62  | ARG  |
| 1   | J     | 64  | SER  |
| 1   | J     | 74  | THR  |
| 1   | J     | 87  | ASP  |
| 1   | J     | 88  | LEU  |
| 1   | J     | 92  | LEU  |
| 1   | J     | 98  | ILE  |
| 1   | J     | 101 | ARG  |
| 1   | J     | 105 | GLU  |
| 1   | J     | 107 | LEU  |
| 1   | J     | 128 | LEU  |
| 1   | J     | 130 | ASP  |
| 1   | J     | 142 | GLN  |
| 1   | J     | 145 | ARG  |
| 1   | J     | 151 | LYS  |
| 1   | J     | 152 | TRP  |
| 1   | J     | 158 | VAL  |
| 1   | J     | 159 | ARG  |
| 1   | J     | 165 | THR  |
| 1   | J     | 166 | LEU  |
| 1   | J     | 177 | LEU  |
| 1   | J     | 178 | THR  |
| 1   | J     | 185 | LEU  |
| 1   | J     | 186 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 190 | ASN  |
| 1   | J     | 193 | ASP  |
| 1   | J     | 198 | SER  |
| 1   | J     | 199 | VAL  |
| 1   | J     | 205 | VAL  |
| 1   | J     | 206 | ARG  |
| 1   | K     | 57  | LEU  |
| 1   | K     | 67  | VAL  |
| 1   | K     | 74  | THR  |
| 1   | K     | 106 | THR  |
| 1   | K     | 124 | VAL  |
| 1   | K     | 128 | LEU  |
| 1   | K     | 134 | ASN  |
| 1   | K     | 137 | THR  |
| 1   | K     | 145 | ARG  |
| 1   | K     | 149 | VAL  |
| 1   | K     | 152 | TRP  |
| 1   | K     | 156 | ARG  |
| 1   | K     | 158 | VAL  |
| 1   | K     | 164 | ARG  |
| 1   | K     | 170 | SER  |
| 1   | K     | 171 | SER  |
| 1   | K     | 178 | THR  |
| 1   | K     | 185 | LEU  |
| 1   | K     | 186 | LEU  |
| 1   | K     | 190 | ASN  |
| 1   | K     | 192 | THR  |
| 1   | K     | 196 | ASN  |
| 1   | K     | 199 | VAL  |
| 1   | K     | 202 | ARG  |
| 1   | K     | 205 | VAL  |
| 1   | K     | 206 | ARG  |
| 1   | K     | 210 | PRO  |
| 1   | K     | 211 | SER  |
| 1   | K     | 213 | GLU  |
| 1   | L     | 57  | LEU  |
| 1   | L     | 72  | THR  |
| 1   | L     | 74  | THR  |
| 1   | L     | 87  | ASP  |
| 1   | L     | 88  | LEU  |
| 1   | L     | 89  | LEU  |
| 1   | L     | 92  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 118 | ASN  |
| 1   | L     | 128 | LEU  |
| 1   | L     | 137 | THR  |
| 1   | L     | 142 | GLN  |
| 1   | L     | 145 | ARG  |
| 1   | L     | 149 | VAL  |
| 1   | L     | 151 | LYS  |
| 1   | L     | 152 | TRP  |
| 1   | L     | 158 | VAL  |
| 1   | L     | 164 | ARG  |
| 1   | L     | 165 | THR  |
| 1   | L     | 167 | LEU  |
| 1   | L     | 170 | SER  |
| 1   | L     | 185 | LEU  |
| 1   | L     | 193 | ASP  |
| 1   | L     | 196 | ASN  |
| 1   | L     | 198 | SER  |
| 1   | L     | 199 | VAL  |
| 1   | L     | 202 | ARG  |
| 1   | L     | 205 | VAL  |
| 1   | L     | 208 | SER  |
| 1   | L     | 209 | VAL  |
| 1   | L     | 211 | SER  |
| 1   | L     | 213 | GLU  |
| 1   | M     | 57  | LEU  |
| 1   | M     | 62  | ARG  |
| 1   | M     | 68  | LEU  |
| 1   | M     | 74  | THR  |
| 1   | M     | 79  | VAL  |
| 1   | M     | 81  | ASP  |
| 1   | M     | 92  | LEU  |
| 1   | M     | 98  | ILE  |
| 1   | M     | 101 | ARG  |
| 1   | M     | 105 | GLU  |
| 1   | M     | 106 | THR  |
| 1   | M     | 107 | LEU  |
| 1   | M     | 118 | ASN  |
| 1   | M     | 128 | LEU  |
| 1   | M     | 130 | ASP  |
| 1   | M     | 135 | ASP  |
| 1   | M     | 137 | THR  |
| 1   | M     | 145 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 151 | LYS  |
| 1   | M     | 152 | TRP  |
| 1   | M     | 158 | VAL  |
| 1   | M     | 164 | ARG  |
| 1   | M     | 165 | THR  |
| 1   | M     | 175 | GLN  |
| 1   | M     | 176 | ARG  |
| 1   | M     | 177 | LEU  |
| 1   | M     | 185 | LEU  |
| 1   | M     | 190 | ASN  |
| 1   | M     | 196 | ASN  |
| 1   | M     | 199 | VAL  |
| 1   | M     | 202 | ARG  |
| 1   | M     | 205 | VAL  |
| 1   | M     | 213 | GLU  |
| 1   | N     | 57  | LEU  |
| 1   | N     | 72  | THR  |
| 1   | N     | 74  | THR  |
| 1   | N     | 79  | VAL  |
| 1   | N     | 105 | GLU  |
| 1   | N     | 128 | LEU  |
| 1   | N     | 133 | ASP  |
| 1   | N     | 137 | THR  |
| 1   | N     | 142 | GLN  |
| 1   | N     | 145 | ARG  |
| 1   | N     | 149 | VAL  |
| 1   | N     | 152 | TRP  |
| 1   | N     | 156 | ARG  |
| 1   | N     | 158 | VAL  |
| 1   | N     | 164 | ARG  |
| 1   | N     | 165 | THR  |
| 1   | N     | 170 | SER  |
| 1   | N     | 175 | GLN  |
| 1   | N     | 176 | ARG  |
| 1   | N     | 177 | LEU  |
| 1   | N     | 178 | THR  |
| 1   | N     | 179 | SER  |
| 1   | N     | 185 | LEU  |
| 1   | N     | 186 | LEU  |
| 1   | N     | 192 | THR  |
| 1   | N     | 198 | SER  |
| 1   | N     | 199 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 200 | LEU  |
| 1   | N     | 202 | ARG  |
| 1   | N     | 205 | VAL  |
| 1   | N     | 209 | VAL  |
| 1   | N     | 213 | GLU  |
| 1   | O     | 57  | LEU  |
| 1   | O     | 72  | THR  |
| 1   | O     | 74  | THR  |
| 1   | O     | 87  | ASP  |
| 1   | O     | 88  | LEU  |
| 1   | O     | 89  | LEU  |
| 1   | O     | 92  | LEU  |
| 1   | O     | 118 | ASN  |
| 1   | O     | 128 | LEU  |
| 1   | O     | 137 | THR  |
| 1   | O     | 142 | GLN  |
| 1   | O     | 145 | ARG  |
| 1   | O     | 149 | VAL  |
| 1   | O     | 151 | LYS  |
| 1   | O     | 152 | TRP  |
| 1   | O     | 158 | VAL  |
| 1   | O     | 164 | ARG  |
| 1   | O     | 165 | THR  |
| 1   | O     | 167 | LEU  |
| 1   | O     | 170 | SER  |
| 1   | O     | 185 | LEU  |
| 1   | O     | 193 | ASP  |
| 1   | O     | 196 | ASN  |
| 1   | O     | 198 | SER  |
| 1   | O     | 199 | VAL  |
| 1   | O     | 202 | ARG  |
| 1   | O     | 208 | SER  |
| 1   | O     | 209 | VAL  |
| 1   | O     | 211 | SER  |
| 1   | O     | 213 | GLU  |
| 1   | P     | 53  | ASN  |
| 1   | P     | 57  | LEU  |
| 1   | P     | 62  | ARG  |
| 1   | P     | 64  | SER  |
| 1   | P     | 74  | THR  |
| 1   | P     | 79  | VAL  |
| 1   | P     | 88  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 92  | LEU  |
| 1   | P     | 101 | ARG  |
| 1   | P     | 105 | GLU  |
| 1   | P     | 106 | THR  |
| 1   | P     | 107 | LEU  |
| 1   | P     | 128 | LEU  |
| 1   | P     | 137 | THR  |
| 1   | P     | 142 | GLN  |
| 1   | P     | 145 | ARG  |
| 1   | P     | 151 | LYS  |
| 1   | P     | 152 | TRP  |
| 1   | P     | 156 | ARG  |
| 1   | P     | 158 | VAL  |
| 1   | P     | 165 | THR  |
| 1   | P     | 170 | SER  |
| 1   | P     | 177 | LEU  |
| 1   | P     | 178 | THR  |
| 1   | P     | 185 | LEU  |
| 1   | P     | 190 | ASN  |
| 1   | P     | 196 | ASN  |
| 1   | P     | 199 | VAL  |
| 1   | P     | 202 | ARG  |
| 1   | P     | 205 | VAL  |
| 1   | Q     | 57  | LEU  |
| 1   | Q     | 72  | THR  |
| 1   | Q     | 74  | THR  |
| 1   | Q     | 87  | ASP  |
| 1   | Q     | 105 | GLU  |
| 1   | Q     | 107 | LEU  |
| 1   | Q     | 128 | LEU  |
| 1   | Q     | 134 | ASN  |
| 1   | Q     | 137 | THR  |
| 1   | Q     | 142 | GLN  |
| 1   | Q     | 145 | ARG  |
| 1   | Q     | 149 | VAL  |
| 1   | Q     | 152 | TRP  |
| 1   | Q     | 156 | ARG  |
| 1   | Q     | 158 | VAL  |
| 1   | Q     | 164 | ARG  |
| 1   | Q     | 165 | THR  |
| 1   | Q     | 170 | SER  |
| 1   | Q     | 177 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 178 | THR  |
| 1   | Q     | 185 | LEU  |
| 1   | Q     | 190 | ASN  |
| 1   | Q     | 192 | THR  |
| 1   | Q     | 193 | ASP  |
| 1   | Q     | 196 | ASN  |
| 1   | Q     | 198 | SER  |
| 1   | Q     | 199 | VAL  |
| 1   | Q     | 202 | ARG  |
| 1   | Q     | 205 | VAL  |
| 1   | Q     | 211 | SER  |
| 1   | R     | 57  | LEU  |
| 1   | R     | 72  | THR  |
| 1   | R     | 74  | THR  |
| 1   | R     | 87  | ASP  |
| 1   | R     | 88  | LEU  |
| 1   | R     | 89  | LEU  |
| 1   | R     | 92  | LEU  |
| 1   | R     | 118 | ASN  |
| 1   | R     | 128 | LEU  |
| 1   | R     | 137 | THR  |
| 1   | R     | 142 | GLN  |
| 1   | R     | 145 | ARG  |
| 1   | R     | 149 | VAL  |
| 1   | R     | 151 | LYS  |
| 1   | R     | 152 | TRP  |
| 1   | R     | 158 | VAL  |
| 1   | R     | 164 | ARG  |
| 1   | R     | 165 | THR  |
| 1   | R     | 167 | LEU  |
| 1   | R     | 170 | SER  |
| 1   | R     | 185 | LEU  |
| 1   | R     | 193 | ASP  |
| 1   | R     | 196 | ASN  |
| 1   | R     | 198 | SER  |
| 1   | R     | 199 | VAL  |
| 1   | R     | 202 | ARG  |
| 1   | R     | 205 | VAL  |
| 1   | R     | 208 | SER  |
| 1   | R     | 209 | VAL  |
| 1   | R     | 211 | SER  |
| 1   | R     | 213 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 57  | LEU  |
| 1   | S     | 62  | ARG  |
| 1   | S     | 74  | THR  |
| 1   | S     | 79  | VAL  |
| 1   | S     | 88  | LEU  |
| 1   | S     | 92  | LEU  |
| 1   | S     | 101 | ARG  |
| 1   | S     | 105 | GLU  |
| 1   | S     | 106 | THR  |
| 1   | S     | 112 | GLN  |
| 1   | S     | 118 | ASN  |
| 1   | S     | 128 | LEU  |
| 1   | S     | 130 | ASP  |
| 1   | S     | 135 | ASP  |
| 1   | S     | 137 | THR  |
| 1   | S     | 142 | GLN  |
| 1   | S     | 145 | ARG  |
| 1   | S     | 151 | LYS  |
| 1   | S     | 152 | TRP  |
| 1   | S     | 156 | ARG  |
| 1   | S     | 158 | VAL  |
| 1   | S     | 159 | ARG  |
| 1   | S     | 175 | GLN  |
| 1   | S     | 176 | ARG  |
| 1   | S     | 177 | LEU  |
| 1   | S     | 185 | LEU  |
| 1   | S     | 190 | ASN  |
| 1   | S     | 196 | ASN  |
| 1   | S     | 199 | VAL  |
| 1   | S     | 202 | ARG  |
| 1   | S     | 205 | VAL  |
| 1   | S     | 208 | SER  |
| 1   | T     | 57  | LEU  |
| 1   | T     | 58  | SER  |
| 1   | T     | 64  | SER  |
| 1   | T     | 67  | VAL  |
| 1   | T     | 68  | LEU  |
| 1   | T     | 74  | THR  |
| 1   | T     | 79  | VAL  |
| 1   | T     | 88  | LEU  |
| 1   | T     | 98  | ILE  |
| 1   | T     | 105 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 128 | LEU  |
| 1   | T     | 133 | ASP  |
| 1   | T     | 137 | THR  |
| 1   | T     | 142 | GLN  |
| 1   | T     | 145 | ARG  |
| 1   | T     | 149 | VAL  |
| 1   | T     | 151 | LYS  |
| 1   | T     | 152 | TRP  |
| 1   | T     | 156 | ARG  |
| 1   | T     | 158 | VAL  |
| 1   | T     | 164 | ARG  |
| 1   | T     | 165 | THR  |
| 1   | T     | 170 | SER  |
| 1   | T     | 176 | ARG  |
| 1   | T     | 177 | LEU  |
| 1   | T     | 178 | THR  |
| 1   | T     | 185 | LEU  |
| 1   | T     | 190 | ASN  |
| 1   | T     | 192 | THR  |
| 1   | T     | 193 | ASP  |
| 1   | T     | 196 | ASN  |
| 1   | T     | 198 | SER  |
| 1   | T     | 199 | VAL  |
| 1   | T     | 202 | ARG  |
| 1   | T     | 204 | SER  |
| 1   | T     | 205 | VAL  |
| 1   | T     | 209 | VAL  |
| 1   | T     | 211 | SER  |
| 1   | T     | 213 | GLU  |
| 1   | U     | 57  | LEU  |
| 1   | U     | 72  | THR  |
| 1   | U     | 74  | THR  |
| 1   | U     | 87  | ASP  |
| 1   | U     | 88  | LEU  |
| 1   | U     | 89  | LEU  |
| 1   | U     | 92  | LEU  |
| 1   | U     | 118 | ASN  |
| 1   | U     | 128 | LEU  |
| 1   | U     | 137 | THR  |
| 1   | U     | 142 | GLN  |
| 1   | U     | 145 | ARG  |
| 1   | U     | 149 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | U     | 151 | LYS  |
| 1   | U     | 152 | TRP  |
| 1   | U     | 158 | VAL  |
| 1   | U     | 164 | ARG  |
| 1   | U     | 165 | THR  |
| 1   | U     | 167 | LEU  |
| 1   | U     | 170 | SER  |
| 1   | U     | 185 | LEU  |
| 1   | U     | 196 | ASN  |
| 1   | U     | 198 | SER  |
| 1   | U     | 199 | VAL  |
| 1   | U     | 202 | ARG  |
| 1   | U     | 205 | VAL  |
| 1   | U     | 208 | SER  |
| 1   | U     | 209 | VAL  |
| 1   | U     | 211 | SER  |
| 1   | U     | 213 | GLU  |
| 1   | V     | 57  | LEU  |
| 1   | V     | 61  | SER  |
| 1   | V     | 62  | ARG  |
| 1   | V     | 74  | THR  |
| 1   | V     | 79  | VAL  |
| 1   | V     | 87  | ASP  |
| 1   | V     | 88  | LEU  |
| 1   | V     | 92  | LEU  |
| 1   | V     | 101 | ARG  |
| 1   | V     | 106 | THR  |
| 1   | V     | 128 | LEU  |
| 1   | V     | 137 | THR  |
| 1   | V     | 145 | ARG  |
| 1   | V     | 151 | LYS  |
| 1   | V     | 152 | TRP  |
| 1   | V     | 158 | VAL  |
| 1   | V     | 165 | THR  |
| 1   | V     | 170 | SER  |
| 1   | V     | 177 | LEU  |
| 1   | V     | 178 | THR  |
| 1   | V     | 185 | LEU  |
| 1   | V     | 190 | ASN  |
| 1   | V     | 196 | ASN  |
| 1   | V     | 199 | VAL  |
| 1   | V     | 202 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | V     | 204 | SER  |
| 1   | V     | 205 | VAL  |
| 1   | V     | 206 | ARG  |
| 1   | V     | 209 | VAL  |
| 1   | V     | 211 | SER  |
| 1   | W     | 57  | LEU  |
| 1   | W     | 67  | VAL  |
| 1   | W     | 74  | THR  |
| 1   | W     | 79  | VAL  |
| 1   | W     | 92  | LEU  |
| 1   | W     | 105 | GLU  |
| 1   | W     | 107 | LEU  |
| 1   | W     | 128 | LEU  |
| 1   | W     | 137 | THR  |
| 1   | W     | 142 | GLN  |
| 1   | W     | 145 | ARG  |
| 1   | W     | 149 | VAL  |
| 1   | W     | 151 | LYS  |
| 1   | W     | 152 | TRP  |
| 1   | W     | 156 | ARG  |
| 1   | W     | 158 | VAL  |
| 1   | W     | 164 | ARG  |
| 1   | W     | 170 | SER  |
| 1   | W     | 177 | LEU  |
| 1   | W     | 178 | THR  |
| 1   | W     | 185 | LEU  |
| 1   | W     | 193 | ASP  |
| 1   | W     | 196 | ASN  |
| 1   | W     | 197 | VAL  |
| 1   | W     | 199 | VAL  |
| 1   | W     | 202 | ARG  |
| 1   | W     | 205 | VAL  |
| 1   | W     | 210 | PRO  |
| 1   | W     | 211 | SER  |
| 1   | W     | 213 | GLU  |
| 1   | X     | 57  | LEU  |
| 1   | X     | 72  | THR  |
| 1   | X     | 74  | THR  |
| 1   | X     | 87  | ASP  |
| 1   | X     | 88  | LEU  |
| 1   | X     | 89  | LEU  |
| 1   | X     | 92  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 118 | ASN  |
| 1   | X     | 128 | LEU  |
| 1   | X     | 137 | THR  |
| 1   | X     | 142 | GLN  |
| 1   | X     | 145 | ARG  |
| 1   | X     | 149 | VAL  |
| 1   | X     | 151 | LYS  |
| 1   | X     | 152 | TRP  |
| 1   | X     | 158 | VAL  |
| 1   | X     | 164 | ARG  |
| 1   | X     | 165 | THR  |
| 1   | X     | 167 | LEU  |
| 1   | X     | 170 | SER  |
| 1   | X     | 185 | LEU  |
| 1   | X     | 193 | ASP  |
| 1   | X     | 196 | ASN  |
| 1   | X     | 198 | SER  |
| 1   | X     | 199 | VAL  |
| 1   | X     | 202 | ARG  |
| 1   | X     | 205 | VAL  |
| 1   | X     | 208 | SER  |
| 1   | X     | 209 | VAL  |
| 1   | X     | 211 | SER  |
| 1   | X     | 213 | GLU  |
| 1   | Y     | 57  | LEU  |
| 1   | Y     | 62  | ARG  |
| 1   | Y     | 67  | VAL  |
| 1   | Y     | 74  | THR  |
| 1   | Y     | 79  | VAL  |
| 1   | Y     | 88  | LEU  |
| 1   | Y     | 92  | LEU  |
| 1   | Y     | 101 | ARG  |
| 1   | Y     | 105 | GLU  |
| 1   | Y     | 107 | LEU  |
| 1   | Y     | 128 | LEU  |
| 1   | Y     | 130 | ASP  |
| 1   | Y     | 135 | ASP  |
| 1   | Y     | 142 | GLN  |
| 1   | Y     | 145 | ARG  |
| 1   | Y     | 151 | LYS  |
| 1   | Y     | 152 | TRP  |
| 1   | Y     | 158 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 165 | THR  |
| 1   | Y     | 175 | GLN  |
| 1   | Y     | 176 | ARG  |
| 1   | Y     | 177 | LEU  |
| 1   | Y     | 178 | THR  |
| 1   | Y     | 185 | LEU  |
| 1   | Y     | 190 | ASN  |
| 1   | Y     | 199 | VAL  |
| 1   | Y     | 202 | ARG  |
| 1   | Y     | 205 | VAL  |
| 1   | Y     | 208 | SER  |
| 1   | Z     | 57  | LEU  |
| 1   | Z     | 58  | SER  |
| 1   | Z     | 64  | SER  |
| 1   | Z     | 67  | VAL  |
| 1   | Z     | 74  | THR  |
| 1   | Z     | 75  | ASP  |
| 1   | Z     | 79  | VAL  |
| 1   | Z     | 107 | LEU  |
| 1   | Z     | 128 | LEU  |
| 1   | Z     | 130 | ASP  |
| 1   | Z     | 133 | ASP  |
| 1   | Z     | 134 | ASN  |
| 1   | Z     | 137 | THR  |
| 1   | Z     | 142 | GLN  |
| 1   | Z     | 145 | ARG  |
| 1   | Z     | 149 | VAL  |
| 1   | Z     | 151 | LYS  |
| 1   | Z     | 152 | TRP  |
| 1   | Z     | 156 | ARG  |
| 1   | Z     | 158 | VAL  |
| 1   | Z     | 164 | ARG  |
| 1   | Z     | 165 | THR  |
| 1   | Z     | 175 | GLN  |
| 1   | Z     | 177 | LEU  |
| 1   | Z     | 178 | THR  |
| 1   | Z     | 185 | LEU  |
| 1   | Z     | 186 | LEU  |
| 1   | Z     | 190 | ASN  |
| 1   | Z     | 193 | ASP  |
| 1   | Z     | 196 | ASN  |
| 1   | Z     | 199 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Z     | 202 | ARG  |
| 1   | Z     | 205 | VAL  |
| 1   | Z     | 211 | SER  |
| 1   | 0     | 57  | LEU  |
| 1   | 0     | 72  | THR  |
| 1   | 0     | 74  | THR  |
| 1   | 0     | 87  | ASP  |
| 1   | 0     | 88  | LEU  |
| 1   | 0     | 89  | LEU  |
| 1   | 0     | 92  | LEU  |
| 1   | 0     | 118 | ASN  |
| 1   | 0     | 128 | LEU  |
| 1   | 0     | 137 | THR  |
| 1   | 0     | 142 | GLN  |
| 1   | 0     | 145 | ARG  |
| 1   | 0     | 149 | VAL  |
| 1   | 0     | 151 | LYS  |
| 1   | 0     | 152 | TRP  |
| 1   | 0     | 158 | VAL  |
| 1   | 0     | 164 | ARG  |
| 1   | 0     | 165 | THR  |
| 1   | 0     | 167 | LEU  |
| 1   | 0     | 170 | SER  |
| 1   | 0     | 185 | LEU  |
| 1   | 0     | 196 | ASN  |
| 1   | 0     | 198 | SER  |
| 1   | 0     | 199 | VAL  |
| 1   | 0     | 202 | ARG  |
| 1   | 0     | 205 | VAL  |
| 1   | 0     | 208 | SER  |
| 1   | 0     | 209 | VAL  |
| 1   | 0     | 211 | SER  |
| 1   | 0     | 213 | GLU  |
| 1   | 1     | 57  | LEU  |
| 1   | 1     | 62  | ARG  |
| 1   | 1     | 64  | SER  |
| 1   | 1     | 72  | THR  |
| 1   | 1     | 74  | THR  |
| 1   | 1     | 79  | VAL  |
| 1   | 1     | 92  | LEU  |
| 1   | 1     | 101 | ARG  |
| 1   | 1     | 105 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 128 | LEU  |
| 1   | 1     | 130 | ASP  |
| 1   | 1     | 134 | ASN  |
| 1   | 1     | 137 | THR  |
| 1   | 1     | 141 | LEU  |
| 1   | 1     | 145 | ARG  |
| 1   | 1     | 149 | VAL  |
| 1   | 1     | 151 | LYS  |
| 1   | 1     | 152 | TRP  |
| 1   | 1     | 155 | SER  |
| 1   | 1     | 156 | ARG  |
| 1   | 1     | 158 | VAL  |
| 1   | 1     | 159 | ARG  |
| 1   | 1     | 165 | THR  |
| 1   | 1     | 166 | LEU  |
| 1   | 1     | 185 | LEU  |
| 1   | 1     | 186 | LEU  |
| 1   | 1     | 190 | ASN  |
| 1   | 1     | 193 | ASP  |
| 1   | 1     | 196 | ASN  |
| 1   | 1     | 198 | SER  |
| 1   | 1     | 199 | VAL  |
| 1   | 1     | 202 | ARG  |
| 1   | 1     | 205 | VAL  |
| 1   | 1     | 208 | SER  |
| 1   | 1     | 213 | GLU  |
| 1   | 2     | 57  | LEU  |
| 1   | 2     | 67  | VAL  |
| 1   | 2     | 72  | THR  |
| 1   | 2     | 74  | THR  |
| 1   | 2     | 79  | VAL  |
| 1   | 2     | 110 | GLU  |
| 1   | 2     | 124 | VAL  |
| 1   | 2     | 128 | LEU  |
| 1   | 2     | 130 | ASP  |
| 1   | 2     | 134 | ASN  |
| 1   | 2     | 142 | GLN  |
| 1   | 2     | 145 | ARG  |
| 1   | 2     | 149 | VAL  |
| 1   | 2     | 152 | TRP  |
| 1   | 2     | 158 | VAL  |
| 1   | 2     | 164 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 165 | THR  |
| 1   | 2     | 175 | GLN  |
| 1   | 2     | 177 | LEU  |
| 1   | 2     | 178 | THR  |
| 1   | 2     | 185 | LEU  |
| 1   | 2     | 190 | ASN  |
| 1   | 2     | 193 | ASP  |
| 1   | 2     | 196 | ASN  |
| 1   | 2     | 199 | VAL  |
| 1   | 2     | 202 | ARG  |
| 1   | 2     | 205 | VAL  |
| 1   | 2     | 211 | SER  |
| 1   | 2     | 213 | GLU  |
| 1   | 3     | 57  | LEU  |
| 1   | 3     | 72  | THR  |
| 1   | 3     | 74  | THR  |
| 1   | 3     | 87  | ASP  |
| 1   | 3     | 88  | LEU  |
| 1   | 3     | 89  | LEU  |
| 1   | 3     | 92  | LEU  |
| 1   | 3     | 118 | ASN  |
| 1   | 3     | 128 | LEU  |
| 1   | 3     | 137 | THR  |
| 1   | 3     | 142 | GLN  |
| 1   | 3     | 145 | ARG  |
| 1   | 3     | 149 | VAL  |
| 1   | 3     | 151 | LYS  |
| 1   | 3     | 152 | TRP  |
| 1   | 3     | 158 | VAL  |
| 1   | 3     | 164 | ARG  |
| 1   | 3     | 165 | THR  |
| 1   | 3     | 167 | LEU  |
| 1   | 3     | 170 | SER  |
| 1   | 3     | 185 | LEU  |
| 1   | 3     | 193 | ASP  |
| 1   | 3     | 196 | ASN  |
| 1   | 3     | 198 | SER  |
| 1   | 3     | 199 | VAL  |
| 1   | 3     | 202 | ARG  |
| 1   | 3     | 205 | VAL  |
| 1   | 3     | 208 | SER  |
| 1   | 3     | 209 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3     | 211 | SER  |
| 1   | 3     | 213 | GLU  |
| 1   | 4     | 57  | LEU  |
| 1   | 4     | 61  | SER  |
| 1   | 4     | 62  | ARG  |
| 1   | 4     | 64  | SER  |
| 1   | 4     | 67  | VAL  |
| 1   | 4     | 74  | THR  |
| 1   | 4     | 79  | VAL  |
| 1   | 4     | 81  | ASP  |
| 1   | 4     | 88  | LEU  |
| 1   | 4     | 92  | LEU  |
| 1   | 4     | 101 | ARG  |
| 1   | 4     | 106 | THR  |
| 1   | 4     | 107 | LEU  |
| 1   | 4     | 128 | LEU  |
| 1   | 4     | 130 | ASP  |
| 1   | 4     | 137 | THR  |
| 1   | 4     | 139 | ASP  |
| 1   | 4     | 145 | ARG  |
| 1   | 4     | 151 | LYS  |
| 1   | 4     | 152 | TRP  |
| 1   | 4     | 158 | VAL  |
| 1   | 4     | 159 | ARG  |
| 1   | 4     | 164 | ARG  |
| 1   | 4     | 165 | THR  |
| 1   | 4     | 171 | SER  |
| 1   | 4     | 178 | THR  |
| 1   | 4     | 185 | LEU  |
| 1   | 4     | 186 | LEU  |
| 1   | 4     | 190 | ASN  |
| 1   | 4     | 193 | ASP  |
| 1   | 4     | 196 | ASN  |
| 1   | 4     | 199 | VAL  |
| 1   | 4     | 202 | ARG  |
| 1   | 4     | 205 | VAL  |
| 1   | 4     | 206 | ARG  |
| 1   | 5     | 57  | LEU  |
| 1   | 5     | 74  | THR  |
| 1   | 5     | 107 | LEU  |
| 1   | 5     | 128 | LEU  |
| 1   | 5     | 134 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5     | 137 | THR  |
| 1   | 5     | 145 | ARG  |
| 1   | 5     | 149 | VAL  |
| 1   | 5     | 151 | LYS  |
| 1   | 5     | 152 | TRP  |
| 1   | 5     | 156 | ARG  |
| 1   | 5     | 158 | VAL  |
| 1   | 5     | 162 | TYR  |
| 1   | 5     | 164 | ARG  |
| 1   | 5     | 171 | SER  |
| 1   | 5     | 178 | THR  |
| 1   | 5     | 185 | LEU  |
| 1   | 5     | 190 | ASN  |
| 1   | 5     | 192 | THR  |
| 1   | 5     | 193 | ASP  |
| 1   | 5     | 196 | ASN  |
| 1   | 5     | 198 | SER  |
| 1   | 5     | 199 | VAL  |
| 1   | 5     | 202 | ARG  |
| 1   | 5     | 205 | VAL  |
| 1   | 5     | 211 | SER  |
| 1   | 5     | 213 | GLU  |
| 1   | 6     | 57  | LEU  |
| 1   | 6     | 72  | THR  |
| 1   | 6     | 74  | THR  |
| 1   | 6     | 87  | ASP  |
| 1   | 6     | 88  | LEU  |
| 1   | 6     | 89  | LEU  |
| 1   | 6     | 92  | LEU  |
| 1   | 6     | 118 | ASN  |
| 1   | 6     | 128 | LEU  |
| 1   | 6     | 137 | THR  |
| 1   | 6     | 142 | GLN  |
| 1   | 6     | 145 | ARG  |
| 1   | 6     | 149 | VAL  |
| 1   | 6     | 151 | LYS  |
| 1   | 6     | 152 | TRP  |
| 1   | 6     | 158 | VAL  |
| 1   | 6     | 164 | ARG  |
| 1   | 6     | 165 | THR  |
| 1   | 6     | 167 | LEU  |
| 1   | 6     | 170 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 185 | LEU  |
| 1   | 6     | 193 | ASP  |
| 1   | 6     | 196 | ASN  |
| 1   | 6     | 198 | SER  |
| 1   | 6     | 199 | VAL  |
| 1   | 6     | 202 | ARG  |
| 1   | 6     | 205 | VAL  |
| 1   | 6     | 208 | SER  |
| 1   | 6     | 209 | VAL  |
| 1   | 6     | 211 | SER  |
| 1   | 6     | 213 | GLU  |
| 1   | 7     | 57  | LEU  |
| 1   | 7     | 72  | THR  |
| 1   | 7     | 74  | THR  |
| 1   | 7     | 79  | VAL  |
| 1   | 7     | 88  | LEU  |
| 1   | 7     | 92  | LEU  |
| 1   | 7     | 101 | ARG  |
| 1   | 7     | 106 | THR  |
| 1   | 7     | 128 | LEU  |
| 1   | 7     | 130 | ASP  |
| 1   | 7     | 137 | THR  |
| 1   | 7     | 141 | LEU  |
| 1   | 7     | 142 | GLN  |
| 1   | 7     | 145 | ARG  |
| 1   | 7     | 151 | LYS  |
| 1   | 7     | 152 | TRP  |
| 1   | 7     | 155 | SER  |
| 1   | 7     | 158 | VAL  |
| 1   | 7     | 164 | ARG  |
| 1   | 7     | 165 | THR  |
| 1   | 7     | 166 | LEU  |
| 1   | 7     | 170 | SER  |
| 1   | 7     | 175 | GLN  |
| 1   | 7     | 176 | ARG  |
| 1   | 7     | 177 | LEU  |
| 1   | 7     | 178 | THR  |
| 1   | 7     | 185 | LEU  |
| 1   | 7     | 190 | ASN  |
| 1   | 7     | 196 | ASN  |
| 1   | 7     | 199 | VAL  |
| 1   | 7     | 202 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7     | 204 | SER  |
| 1   | 7     | 205 | VAL  |
| 1   | 8     | 57  | LEU  |
| 1   | 8     | 67  | VAL  |
| 1   | 8     | 74  | THR  |
| 1   | 8     | 79  | VAL  |
| 1   | 8     | 105 | GLU  |
| 1   | 8     | 106 | THR  |
| 1   | 8     | 128 | LEU  |
| 1   | 8     | 134 | ASN  |
| 1   | 8     | 137 | THR  |
| 1   | 8     | 142 | GLN  |
| 1   | 8     | 145 | ARG  |
| 1   | 8     | 149 | VAL  |
| 1   | 8     | 152 | TRP  |
| 1   | 8     | 156 | ARG  |
| 1   | 8     | 158 | VAL  |
| 1   | 8     | 164 | ARG  |
| 1   | 8     | 165 | THR  |
| 1   | 8     | 175 | GLN  |
| 1   | 8     | 176 | ARG  |
| 1   | 8     | 177 | LEU  |
| 1   | 8     | 178 | THR  |
| 1   | 8     | 185 | LEU  |
| 1   | 8     | 190 | ASN  |
| 1   | 8     | 196 | ASN  |
| 1   | 8     | 199 | VAL  |
| 1   | 8     | 202 | ARG  |
| 1   | 8     | 205 | VAL  |
| 1   | 8     | 208 | SER  |
| 1   | 8     | 211 | SER  |
| 1   | 9     | 57  | LEU  |
| 1   | 9     | 72  | THR  |
| 1   | 9     | 74  | THR  |
| 1   | 9     | 87  | ASP  |
| 1   | 9     | 88  | LEU  |
| 1   | 9     | 89  | LEU  |
| 1   | 9     | 92  | LEU  |
| 1   | 9     | 118 | ASN  |
| 1   | 9     | 128 | LEU  |
| 1   | 9     | 137 | THR  |
| 1   | 9     | 142 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 9     | 145 | ARG  |
| 1   | 9     | 149 | VAL  |
| 1   | 9     | 151 | LYS  |
| 1   | 9     | 152 | TRP  |
| 1   | 9     | 158 | VAL  |
| 1   | 9     | 164 | ARG  |
| 1   | 9     | 165 | THR  |
| 1   | 9     | 167 | LEU  |
| 1   | 9     | 170 | SER  |
| 1   | 9     | 185 | LEU  |
| 1   | 9     | 193 | ASP  |
| 1   | 9     | 196 | ASN  |
| 1   | 9     | 198 | SER  |
| 1   | 9     | 199 | VAL  |
| 1   | 9     | 202 | ARG  |
| 1   | 9     | 205 | VAL  |
| 1   | 9     | 208 | SER  |
| 1   | 9     | 209 | VAL  |
| 1   | 9     | 211 | SER  |
| 1   | 9     | 213 | GLU  |
| 1   | a     | 57  | LEU  |
| 1   | a     | 72  | THR  |
| 1   | a     | 74  | THR  |
| 1   | a     | 88  | LEU  |
| 1   | a     | 92  | LEU  |
| 1   | a     | 101 | ARG  |
| 1   | a     | 105 | GLU  |
| 1   | a     | 106 | THR  |
| 1   | a     | 128 | LEU  |
| 1   | a     | 142 | GLN  |
| 1   | a     | 144 | THR  |
| 1   | a     | 145 | ARG  |
| 1   | a     | 149 | VAL  |
| 1   | a     | 151 | LYS  |
| 1   | a     | 152 | TRP  |
| 1   | a     | 156 | ARG  |
| 1   | a     | 158 | VAL  |
| 1   | a     | 159 | ARG  |
| 1   | a     | 170 | SER  |
| 1   | a     | 171 | SER  |
| 1   | a     | 175 | GLN  |
| 1   | a     | 177 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 178 | THR  |
| 1   | a     | 185 | LEU  |
| 1   | a     | 186 | LEU  |
| 1   | a     | 190 | ASN  |
| 1   | a     | 196 | ASN  |
| 1   | a     | 199 | VAL  |
| 1   | a     | 202 | ARG  |
| 1   | a     | 205 | VAL  |
| 1   | b     | 64  | SER  |
| 1   | b     | 74  | THR  |
| 1   | b     | 107 | LEU  |
| 1   | b     | 128 | LEU  |
| 1   | b     | 137 | THR  |
| 1   | b     | 142 | GLN  |
| 1   | b     | 144 | THR  |
| 1   | b     | 145 | ARG  |
| 1   | b     | 149 | VAL  |
| 1   | b     | 152 | TRP  |
| 1   | b     | 154 | GLU  |
| 1   | b     | 155 | SER  |
| 1   | b     | 156 | ARG  |
| 1   | b     | 158 | VAL  |
| 1   | b     | 164 | ARG  |
| 1   | b     | 165 | THR  |
| 1   | b     | 170 | SER  |
| 1   | b     | 175 | GLN  |
| 1   | b     | 178 | THR  |
| 1   | b     | 185 | LEU  |
| 1   | b     | 192 | THR  |
| 1   | b     | 196 | ASN  |
| 1   | b     | 198 | SER  |
| 1   | b     | 199 | VAL  |
| 1   | b     | 202 | ARG  |
| 1   | b     | 209 | VAL  |
| 1   | b     | 211 | SER  |
| 1   | b     | 213 | GLU  |
| 1   | c     | 57  | LEU  |
| 1   | c     | 72  | THR  |
| 1   | c     | 74  | THR  |
| 1   | c     | 87  | ASP  |
| 1   | c     | 88  | LEU  |
| 1   | c     | 89  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | c     | 92  | LEU  |
| 1   | c     | 118 | ASN  |
| 1   | c     | 128 | LEU  |
| 1   | c     | 137 | THR  |
| 1   | c     | 142 | GLN  |
| 1   | c     | 145 | ARG  |
| 1   | c     | 149 | VAL  |
| 1   | c     | 151 | LYS  |
| 1   | c     | 152 | TRP  |
| 1   | c     | 158 | VAL  |
| 1   | c     | 164 | ARG  |
| 1   | c     | 165 | THR  |
| 1   | c     | 167 | LEU  |
| 1   | c     | 170 | SER  |
| 1   | c     | 185 | LEU  |
| 1   | c     | 193 | ASP  |
| 1   | c     | 196 | ASN  |
| 1   | c     | 198 | SER  |
| 1   | c     | 199 | VAL  |
| 1   | c     | 202 | ARG  |
| 1   | c     | 205 | VAL  |
| 1   | c     | 208 | SER  |
| 1   | c     | 209 | VAL  |
| 1   | c     | 211 | SER  |
| 1   | c     | 213 | GLU  |
| 1   | d     | 57  | LEU  |
| 1   | d     | 62  | ARG  |
| 1   | d     | 64  | SER  |
| 1   | d     | 74  | THR  |
| 1   | d     | 79  | VAL  |
| 1   | d     | 87  | ASP  |
| 1   | d     | 88  | LEU  |
| 1   | d     | 92  | LEU  |
| 1   | d     | 100 | GLN  |
| 1   | d     | 101 | ARG  |
| 1   | d     | 106 | THR  |
| 1   | d     | 107 | LEU  |
| 1   | d     | 118 | ASN  |
| 1   | d     | 128 | LEU  |
| 1   | d     | 130 | ASP  |
| 1   | d     | 137 | THR  |
| 1   | d     | 142 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | d     | 145 | ARG  |
| 1   | d     | 149 | VAL  |
| 1   | d     | 152 | TRP  |
| 1   | d     | 154 | GLU  |
| 1   | d     | 156 | ARG  |
| 1   | d     | 158 | VAL  |
| 1   | d     | 165 | THR  |
| 1   | d     | 171 | SER  |
| 1   | d     | 175 | GLN  |
| 1   | d     | 178 | THR  |
| 1   | d     | 185 | LEU  |
| 1   | d     | 190 | ASN  |
| 1   | d     | 196 | ASN  |
| 1   | d     | 198 | SER  |
| 1   | d     | 199 | VAL  |
| 1   | d     | 202 | ARG  |
| 1   | d     | 205 | VAL  |
| 1   | e     | 57  | LEU  |
| 1   | e     | 64  | SER  |
| 1   | e     | 67  | VAL  |
| 1   | e     | 74  | THR  |
| 1   | e     | 79  | VAL  |
| 1   | e     | 100 | GLN  |
| 1   | e     | 105 | GLU  |
| 1   | e     | 128 | LEU  |
| 1   | e     | 134 | ASN  |
| 1   | e     | 137 | THR  |
| 1   | e     | 145 | ARG  |
| 1   | e     | 149 | VAL  |
| 1   | e     | 152 | TRP  |
| 1   | e     | 155 | SER  |
| 1   | e     | 156 | ARG  |
| 1   | e     | 158 | VAL  |
| 1   | e     | 164 | ARG  |
| 1   | e     | 170 | SER  |
| 1   | e     | 175 | GLN  |
| 1   | e     | 178 | THR  |
| 1   | e     | 185 | LEU  |
| 1   | e     | 186 | LEU  |
| 1   | e     | 190 | ASN  |
| 1   | e     | 192 | THR  |
| 1   | e     | 193 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | e     | 196 | ASN  |
| 1   | e     | 198 | SER  |
| 1   | e     | 199 | VAL  |
| 1   | e     | 202 | ARG  |
| 1   | e     | 205 | VAL  |
| 1   | e     | 213 | GLU  |
| 1   | f     | 57  | LEU  |
| 1   | f     | 72  | THR  |
| 1   | f     | 74  | THR  |
| 1   | f     | 87  | ASP  |
| 1   | f     | 88  | LEU  |
| 1   | f     | 89  | LEU  |
| 1   | f     | 92  | LEU  |
| 1   | f     | 118 | ASN  |
| 1   | f     | 128 | LEU  |
| 1   | f     | 137 | THR  |
| 1   | f     | 142 | GLN  |
| 1   | f     | 145 | ARG  |
| 1   | f     | 149 | VAL  |
| 1   | f     | 151 | LYS  |
| 1   | f     | 152 | TRP  |
| 1   | f     | 158 | VAL  |
| 1   | f     | 164 | ARG  |
| 1   | f     | 165 | THR  |
| 1   | f     | 167 | LEU  |
| 1   | f     | 170 | SER  |
| 1   | f     | 185 | LEU  |
| 1   | f     | 193 | ASP  |
| 1   | f     | 196 | ASN  |
| 1   | f     | 198 | SER  |
| 1   | f     | 199 | VAL  |
| 1   | f     | 202 | ARG  |
| 1   | f     | 205 | VAL  |
| 1   | f     | 208 | SER  |
| 1   | f     | 209 | VAL  |
| 1   | f     | 211 | SER  |
| 1   | f     | 213 | GLU  |
| 1   | g     | 52  | THR  |
| 1   | g     | 57  | LEU  |
| 1   | g     | 62  | ARG  |
| 1   | g     | 64  | SER  |
| 1   | g     | 74  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | g     | 75  | ASP  |
| 1   | g     | 79  | VAL  |
| 1   | g     | 88  | LEU  |
| 1   | g     | 92  | LEU  |
| 1   | g     | 101 | ARG  |
| 1   | g     | 105 | GLU  |
| 1   | g     | 128 | LEU  |
| 1   | g     | 130 | ASP  |
| 1   | g     | 137 | THR  |
| 1   | g     | 142 | GLN  |
| 1   | g     | 145 | ARG  |
| 1   | g     | 149 | VAL  |
| 1   | g     | 151 | LYS  |
| 1   | g     | 152 | TRP  |
| 1   | g     | 156 | ARG  |
| 1   | g     | 158 | VAL  |
| 1   | g     | 164 | ARG  |
| 1   | g     | 165 | THR  |
| 1   | g     | 170 | SER  |
| 1   | g     | 175 | GLN  |
| 1   | g     | 176 | ARG  |
| 1   | g     | 177 | LEU  |
| 1   | g     | 185 | LEU  |
| 1   | g     | 190 | ASN  |
| 1   | g     | 193 | ASP  |
| 1   | g     | 196 | ASN  |
| 1   | g     | 199 | VAL  |
| 1   | g     | 202 | ARG  |
| 1   | g     | 205 | VAL  |
| 1   | h     | 57  | LEU  |
| 1   | h     | 72  | THR  |
| 1   | h     | 74  | THR  |
| 1   | h     | 79  | VAL  |
| 1   | h     | 98  | ILE  |
| 1   | h     | 101 | ARG  |
| 1   | h     | 128 | LEU  |
| 1   | h     | 130 | ASP  |
| 1   | h     | 133 | ASP  |
| 1   | h     | 134 | ASN  |
| 1   | h     | 135 | ASP  |
| 1   | h     | 137 | THR  |
| 1   | h     | 142 | GLN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | h     | 145 | ARG  |
| 1   | h     | 149 | VAL  |
| 1   | h     | 152 | TRP  |
| 1   | h     | 158 | VAL  |
| 1   | h     | 161 | GLN  |
| 1   | h     | 164 | ARG  |
| 1   | h     | 165 | THR  |
| 1   | h     | 176 | ARG  |
| 1   | h     | 177 | LEU  |
| 1   | h     | 178 | THR  |
| 1   | h     | 185 | LEU  |
| 1   | h     | 186 | LEU  |
| 1   | h     | 190 | ASN  |
| 1   | h     | 192 | THR  |
| 1   | h     | 196 | ASN  |
| 1   | h     | 198 | SER  |
| 1   | h     | 199 | VAL  |
| 1   | h     | 202 | ARG  |
| 1   | h     | 205 | VAL  |
| 1   | h     | 209 | VAL  |
| 1   | h     | 211 | SER  |
| 1   | i     | 57  | LEU  |
| 1   | i     | 72  | THR  |
| 1   | i     | 74  | THR  |
| 1   | i     | 87  | ASP  |
| 1   | i     | 88  | LEU  |
| 1   | i     | 89  | LEU  |
| 1   | i     | 92  | LEU  |
| 1   | i     | 118 | ASN  |
| 1   | i     | 128 | LEU  |
| 1   | i     | 137 | THR  |
| 1   | i     | 142 | GLN  |
| 1   | i     | 145 | ARG  |
| 1   | i     | 151 | LYS  |
| 1   | i     | 152 | TRP  |
| 1   | i     | 158 | VAL  |
| 1   | i     | 164 | ARG  |
| 1   | i     | 165 | THR  |
| 1   | i     | 167 | LEU  |
| 1   | i     | 170 | SER  |
| 1   | i     | 185 | LEU  |
| 1   | i     | 193 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | i     | 196 | ASN  |
| 1   | i     | 198 | SER  |
| 1   | i     | 199 | VAL  |
| 1   | i     | 202 | ARG  |
| 1   | i     | 205 | VAL  |
| 1   | i     | 208 | SER  |
| 1   | i     | 209 | VAL  |
| 1   | i     | 211 | SER  |
| 1   | i     | 213 | GLU  |
| 1   | j     | 57  | LEU  |
| 1   | j     | 62  | ARG  |
| 1   | j     | 72  | THR  |
| 1   | j     | 74  | THR  |
| 1   | j     | 79  | VAL  |
| 1   | j     | 88  | LEU  |
| 1   | j     | 92  | LEU  |
| 1   | j     | 100 | GLN  |
| 1   | j     | 101 | ARG  |
| 1   | j     | 105 | GLU  |
| 1   | j     | 128 | LEU  |
| 1   | j     | 130 | ASP  |
| 1   | j     | 133 | ASP  |
| 1   | j     | 144 | THR  |
| 1   | j     | 145 | ARG  |
| 1   | j     | 149 | VAL  |
| 1   | j     | 151 | LYS  |
| 1   | j     | 152 | TRP  |
| 1   | j     | 155 | SER  |
| 1   | j     | 156 | ARG  |
| 1   | j     | 158 | VAL  |
| 1   | j     | 165 | THR  |
| 1   | j     | 166 | LEU  |
| 1   | j     | 185 | LEU  |
| 1   | j     | 186 | LEU  |
| 1   | j     | 198 | SER  |
| 1   | j     | 199 | VAL  |
| 1   | j     | 202 | ARG  |
| 1   | j     | 205 | VAL  |
| 1   | k     | 57  | LEU  |
| 1   | k     | 61  | SER  |
| 1   | k     | 72  | THR  |
| 1   | k     | 74  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | k     | 79  | VAL  |
| 1   | k     | 100 | GLN  |
| 1   | k     | 105 | GLU  |
| 1   | k     | 128 | LEU  |
| 1   | k     | 142 | GLN  |
| 1   | k     | 145 | ARG  |
| 1   | k     | 149 | VAL  |
| 1   | k     | 152 | TRP  |
| 1   | k     | 158 | VAL  |
| 1   | k     | 164 | ARG  |
| 1   | k     | 165 | THR  |
| 1   | k     | 170 | SER  |
| 1   | k     | 175 | GLN  |
| 1   | k     | 178 | THR  |
| 1   | k     | 185 | LEU  |
| 1   | k     | 190 | ASN  |
| 1   | k     | 192 | THR  |
| 1   | k     | 193 | ASP  |
| 1   | k     | 196 | ASN  |
| 1   | k     | 198 | SER  |
| 1   | k     | 199 | VAL  |
| 1   | k     | 202 | ARG  |
| 1   | k     | 205 | VAL  |
| 1   | k     | 211 | SER  |
| 1   | k     | 213 | GLU  |
| 1   | l     | 57  | LEU  |
| 1   | l     | 72  | THR  |
| 1   | l     | 74  | THR  |
| 1   | l     | 87  | ASP  |
| 1   | l     | 88  | LEU  |
| 1   | l     | 89  | LEU  |
| 1   | l     | 92  | LEU  |
| 1   | l     | 118 | ASN  |
| 1   | l     | 128 | LEU  |
| 1   | l     | 137 | THR  |
| 1   | l     | 142 | GLN  |
| 1   | l     | 145 | ARG  |
| 1   | l     | 149 | VAL  |
| 1   | l     | 151 | LYS  |
| 1   | l     | 152 | TRP  |
| 1   | l     | 158 | VAL  |
| 1   | l     | 164 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | l     | 165 | THR  |
| 1   | l     | 167 | LEU  |
| 1   | l     | 170 | SER  |
| 1   | l     | 185 | LEU  |
| 1   | l     | 193 | ASP  |
| 1   | l     | 196 | ASN  |
| 1   | l     | 198 | SER  |
| 1   | l     | 199 | VAL  |
| 1   | l     | 202 | ARG  |
| 1   | l     | 205 | VAL  |
| 1   | l     | 208 | SER  |
| 1   | l     | 209 | VAL  |
| 1   | l     | 211 | SER  |
| 1   | l     | 213 | GLU  |
| 1   | m     | 57  | LEU  |
| 1   | m     | 58  | SER  |
| 1   | m     | 62  | ARG  |
| 1   | m     | 72  | THR  |
| 1   | m     | 74  | THR  |
| 1   | m     | 79  | VAL  |
| 1   | m     | 87  | ASP  |
| 1   | m     | 88  | LEU  |
| 1   | m     | 92  | LEU  |
| 1   | m     | 101 | ARG  |
| 1   | m     | 105 | GLU  |
| 1   | m     | 118 | ASN  |
| 1   | m     | 128 | LEU  |
| 1   | m     | 130 | ASP  |
| 1   | m     | 135 | ASP  |
| 1   | m     | 137 | THR  |
| 1   | m     | 142 | GLN  |
| 1   | m     | 145 | ARG  |
| 1   | m     | 149 | VAL  |
| 1   | m     | 151 | LYS  |
| 1   | m     | 152 | TRP  |
| 1   | m     | 156 | ARG  |
| 1   | m     | 158 | VAL  |
| 1   | m     | 165 | THR  |
| 1   | m     | 176 | ARG  |
| 1   | m     | 177 | LEU  |
| 1   | m     | 179 | SER  |
| 1   | m     | 185 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | m     | 186 | LEU  |
| 1   | m     | 193 | ASP  |
| 1   | m     | 196 | ASN  |
| 1   | m     | 198 | SER  |
| 1   | m     | 199 | VAL  |
| 1   | m     | 202 | ARG  |
| 1   | m     | 205 | VAL  |
| 1   | m     | 206 | ARG  |
| 1   | m     | 213 | GLU  |
| 1   | n     | 57  | LEU  |
| 1   | n     | 72  | THR  |
| 1   | n     | 74  | THR  |
| 1   | n     | 79  | VAL  |
| 1   | n     | 91  | ARG  |
| 1   | n     | 105 | GLU  |
| 1   | n     | 128 | LEU  |
| 1   | n     | 130 | ASP  |
| 1   | n     | 133 | ASP  |
| 1   | n     | 134 | ASN  |
| 1   | n     | 137 | THR  |
| 1   | n     | 142 | GLN  |
| 1   | n     | 145 | ARG  |
| 1   | n     | 149 | VAL  |
| 1   | n     | 152 | TRP  |
| 1   | n     | 156 | ARG  |
| 1   | n     | 158 | VAL  |
| 1   | n     | 161 | GLN  |
| 1   | n     | 164 | ARG  |
| 1   | n     | 176 | ARG  |
| 1   | n     | 177 | LEU  |
| 1   | n     | 178 | THR  |
| 1   | n     | 185 | LEU  |
| 1   | n     | 190 | ASN  |
| 1   | n     | 192 | THR  |
| 1   | n     | 193 | ASP  |
| 1   | n     | 199 | VAL  |
| 1   | n     | 202 | ARG  |
| 1   | n     | 210 | PRO  |
| 1   | n     | 211 | SER  |
| 1   | o     | 57  | LEU  |
| 1   | o     | 72  | THR  |
| 1   | o     | 74  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | o     | 87  | ASP  |
| 1   | o     | 88  | LEU  |
| 1   | o     | 89  | LEU  |
| 1   | o     | 92  | LEU  |
| 1   | o     | 118 | ASN  |
| 1   | o     | 128 | LEU  |
| 1   | o     | 130 | ASP  |
| 1   | o     | 137 | THR  |
| 1   | o     | 142 | GLN  |
| 1   | o     | 145 | ARG  |
| 1   | o     | 149 | VAL  |
| 1   | o     | 151 | LYS  |
| 1   | o     | 152 | TRP  |
| 1   | o     | 158 | VAL  |
| 1   | o     | 164 | ARG  |
| 1   | o     | 165 | THR  |
| 1   | o     | 167 | LEU  |
| 1   | o     | 170 | SER  |
| 1   | o     | 185 | LEU  |
| 1   | o     | 193 | ASP  |
| 1   | o     | 196 | ASN  |
| 1   | o     | 198 | SER  |
| 1   | o     | 199 | VAL  |
| 1   | o     | 202 | ARG  |
| 1   | o     | 205 | VAL  |
| 1   | o     | 208 | SER  |
| 1   | o     | 209 | VAL  |
| 1   | o     | 211 | SER  |
| 1   | o     | 213 | GLU  |
| 1   | p     | 57  | LEU  |
| 1   | p     | 61  | SER  |
| 1   | p     | 62  | ARG  |
| 1   | p     | 67  | VAL  |
| 1   | p     | 74  | THR  |
| 1   | p     | 79  | VAL  |
| 1   | p     | 87  | ASP  |
| 1   | p     | 88  | LEU  |
| 1   | p     | 92  | LEU  |
| 1   | p     | 101 | ARG  |
| 1   | p     | 106 | THR  |
| 1   | p     | 107 | LEU  |
| 1   | p     | 118 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | p     | 128 | LEU  |
| 1   | p     | 130 | ASP  |
| 1   | p     | 137 | THR  |
| 1   | p     | 142 | GLN  |
| 1   | p     | 145 | ARG  |
| 1   | p     | 151 | LYS  |
| 1   | p     | 152 | TRP  |
| 1   | p     | 156 | ARG  |
| 1   | p     | 158 | VAL  |
| 1   | p     | 165 | THR  |
| 1   | p     | 176 | ARG  |
| 1   | p     | 177 | LEU  |
| 1   | p     | 178 | THR  |
| 1   | p     | 185 | LEU  |
| 1   | p     | 186 | LEU  |
| 1   | p     | 190 | ASN  |
| 1   | p     | 193 | ASP  |
| 1   | p     | 196 | ASN  |
| 1   | p     | 199 | VAL  |
| 1   | p     | 202 | ARG  |
| 1   | p     | 205 | VAL  |
| 1   | q     | 52  | THR  |
| 1   | q     | 57  | LEU  |
| 1   | q     | 67  | VAL  |
| 1   | q     | 74  | THR  |
| 1   | q     | 79  | VAL  |
| 1   | q     | 128 | LEU  |
| 1   | q     | 130 | ASP  |
| 1   | q     | 134 | ASN  |
| 1   | q     | 135 | ASP  |
| 1   | q     | 137 | THR  |
| 1   | q     | 142 | GLN  |
| 1   | q     | 145 | ARG  |
| 1   | q     | 149 | VAL  |
| 1   | q     | 152 | TRP  |
| 1   | q     | 156 | ARG  |
| 1   | q     | 158 | VAL  |
| 1   | q     | 164 | ARG  |
| 1   | q     | 165 | THR  |
| 1   | q     | 170 | SER  |
| 1   | q     | 176 | ARG  |
| 1   | q     | 178 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | q     | 185 | LEU  |
| 1   | q     | 193 | ASP  |
| 1   | q     | 199 | VAL  |
| 1   | q     | 202 | ARG  |
| 1   | q     | 205 | VAL  |
| 1   | q     | 210 | PRO  |
| 1   | q     | 213 | GLU  |
| 1   | r     | 57  | LEU  |
| 1   | r     | 72  | THR  |
| 1   | r     | 74  | THR  |
| 1   | r     | 87  | ASP  |
| 1   | r     | 88  | LEU  |
| 1   | r     | 89  | LEU  |
| 1   | r     | 92  | LEU  |
| 1   | r     | 118 | ASN  |
| 1   | r     | 128 | LEU  |
| 1   | r     | 137 | THR  |
| 1   | r     | 142 | GLN  |
| 1   | r     | 145 | ARG  |
| 1   | r     | 149 | VAL  |
| 1   | r     | 151 | LYS  |
| 1   | r     | 152 | TRP  |
| 1   | r     | 158 | VAL  |
| 1   | r     | 164 | ARG  |
| 1   | r     | 165 | THR  |
| 1   | r     | 167 | LEU  |
| 1   | r     | 170 | SER  |
| 1   | r     | 185 | LEU  |
| 1   | r     | 193 | ASP  |
| 1   | r     | 196 | ASN  |
| 1   | r     | 198 | SER  |
| 1   | r     | 199 | VAL  |
| 1   | r     | 202 | ARG  |
| 1   | r     | 205 | VAL  |
| 1   | r     | 208 | SER  |
| 1   | r     | 209 | VAL  |
| 1   | r     | 211 | SER  |
| 1   | r     | 213 | GLU  |
| 1   | s     | 57  | LEU  |
| 1   | s     | 72  | THR  |
| 1   | s     | 74  | THR  |
| 1   | s     | 75  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | s     | 88  | LEU  |
| 1   | s     | 92  | LEU  |
| 1   | s     | 101 | ARG  |
| 1   | s     | 105 | GLU  |
| 1   | s     | 106 | THR  |
| 1   | s     | 128 | LEU  |
| 1   | s     | 130 | ASP  |
| 1   | s     | 137 | THR  |
| 1   | s     | 142 | GLN  |
| 1   | s     | 145 | ARG  |
| 1   | s     | 151 | LYS  |
| 1   | s     | 152 | TRP  |
| 1   | s     | 156 | ARG  |
| 1   | s     | 158 | VAL  |
| 1   | s     | 159 | ARG  |
| 1   | s     | 170 | SER  |
| 1   | s     | 171 | SER  |
| 1   | s     | 177 | LEU  |
| 1   | s     | 185 | LEU  |
| 1   | s     | 190 | ASN  |
| 1   | s     | 193 | ASP  |
| 1   | s     | 196 | ASN  |
| 1   | s     | 199 | VAL  |
| 1   | s     | 202 | ARG  |
| 1   | s     | 205 | VAL  |
| 1   | t     | 57  | LEU  |
| 1   | t     | 64  | SER  |
| 1   | t     | 74  | THR  |
| 1   | t     | 128 | LEU  |
| 1   | t     | 130 | ASP  |
| 1   | t     | 134 | ASN  |
| 1   | t     | 137 | THR  |
| 1   | t     | 144 | THR  |
| 1   | t     | 145 | ARG  |
| 1   | t     | 149 | VAL  |
| 1   | t     | 152 | TRP  |
| 1   | t     | 156 | ARG  |
| 1   | t     | 158 | VAL  |
| 1   | t     | 164 | ARG  |
| 1   | t     | 165 | THR  |
| 1   | t     | 170 | SER  |
| 1   | t     | 175 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | t     | 177 | LEU  |
| 1   | t     | 178 | THR  |
| 1   | t     | 185 | LEU  |
| 1   | t     | 190 | ASN  |
| 1   | t     | 192 | THR  |
| 1   | t     | 193 | ASP  |
| 1   | t     | 196 | ASN  |
| 1   | t     | 198 | SER  |
| 1   | t     | 199 | VAL  |
| 1   | t     | 200 | LEU  |
| 1   | t     | 201 | CYS  |
| 1   | t     | 202 | ARG  |
| 1   | t     | 209 | VAL  |
| 1   | t     | 211 | SER  |
| 1   | u     | 57  | LEU  |
| 1   | u     | 72  | THR  |
| 1   | u     | 74  | THR  |
| 1   | u     | 87  | ASP  |
| 1   | u     | 88  | LEU  |
| 1   | u     | 89  | LEU  |
| 1   | u     | 92  | LEU  |
| 1   | u     | 118 | ASN  |
| 1   | u     | 128 | LEU  |
| 1   | u     | 137 | THR  |
| 1   | u     | 142 | GLN  |
| 1   | u     | 145 | ARG  |
| 1   | u     | 149 | VAL  |
| 1   | u     | 151 | LYS  |
| 1   | u     | 152 | TRP  |
| 1   | u     | 158 | VAL  |
| 1   | u     | 164 | ARG  |
| 1   | u     | 165 | THR  |
| 1   | u     | 167 | LEU  |
| 1   | u     | 170 | SER  |
| 1   | u     | 185 | LEU  |
| 1   | u     | 193 | ASP  |
| 1   | u     | 196 | ASN  |
| 1   | u     | 198 | SER  |
| 1   | u     | 199 | VAL  |
| 1   | u     | 202 | ARG  |
| 1   | u     | 205 | VAL  |
| 1   | u     | 208 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | u     | 209 | VAL  |
| 1   | u     | 211 | SER  |
| 1   | u     | 213 | GLU  |
| 1   | v     | 57  | LEU  |
| 1   | v     | 61  | SER  |
| 1   | v     | 62  | ARG  |
| 1   | v     | 74  | THR  |
| 1   | v     | 79  | VAL  |
| 1   | v     | 88  | LEU  |
| 1   | v     | 92  | LEU  |
| 1   | v     | 101 | ARG  |
| 1   | v     | 106 | THR  |
| 1   | v     | 124 | VAL  |
| 1   | v     | 128 | LEU  |
| 1   | v     | 130 | ASP  |
| 1   | v     | 137 | THR  |
| 1   | v     | 145 | ARG  |
| 1   | v     | 149 | VAL  |
| 1   | v     | 151 | LYS  |
| 1   | v     | 152 | TRP  |
| 1   | v     | 158 | VAL  |
| 1   | v     | 165 | THR  |
| 1   | v     | 170 | SER  |
| 1   | v     | 171 | SER  |
| 1   | v     | 177 | LEU  |
| 1   | v     | 178 | THR  |
| 1   | v     | 185 | LEU  |
| 1   | v     | 190 | ASN  |
| 1   | v     | 196 | ASN  |
| 1   | v     | 198 | SER  |
| 1   | v     | 199 | VAL  |
| 1   | v     | 202 | ARG  |
| 1   | v     | 205 | VAL  |
| 1   | v     | 213 | GLU  |
| 1   | w     | 57  | LEU  |
| 1   | w     | 67  | VAL  |
| 1   | w     | 74  | THR  |
| 1   | w     | 87  | ASP  |
| 1   | w     | 101 | ARG  |
| 1   | w     | 107 | LEU  |
| 1   | w     | 114 | MET  |
| 1   | w     | 128 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | w     | 130 | ASP  |
| 1   | w     | 134 | ASN  |
| 1   | w     | 137 | THR  |
| 1   | w     | 142 | GLN  |
| 1   | w     | 145 | ARG  |
| 1   | w     | 149 | VAL  |
| 1   | w     | 152 | TRP  |
| 1   | w     | 156 | ARG  |
| 1   | w     | 158 | VAL  |
| 1   | w     | 164 | ARG  |
| 1   | w     | 170 | SER  |
| 1   | w     | 178 | THR  |
| 1   | w     | 185 | LEU  |
| 1   | w     | 186 | LEU  |
| 1   | w     | 190 | ASN  |
| 1   | w     | 199 | VAL  |
| 1   | w     | 202 | ARG  |
| 1   | w     | 205 | VAL  |
| 1   | w     | 210 | PRO  |
| 1   | w     | 211 | SER  |
| 1   | w     | 213 | GLU  |
| 1   | x     | 57  | LEU  |
| 1   | x     | 72  | THR  |
| 1   | x     | 74  | THR  |
| 1   | x     | 87  | ASP  |
| 1   | x     | 88  | LEU  |
| 1   | x     | 89  | LEU  |
| 1   | x     | 92  | LEU  |
| 1   | x     | 118 | ASN  |
| 1   | x     | 128 | LEU  |
| 1   | x     | 137 | THR  |
| 1   | x     | 142 | GLN  |
| 1   | x     | 145 | ARG  |
| 1   | x     | 149 | VAL  |
| 1   | x     | 151 | LYS  |
| 1   | x     | 152 | TRP  |
| 1   | x     | 158 | VAL  |
| 1   | x     | 164 | ARG  |
| 1   | x     | 165 | THR  |
| 1   | x     | 167 | LEU  |
| 1   | x     | 170 | SER  |
| 1   | x     | 185 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | x     | 196 | ASN  |
| 1   | x     | 198 | SER  |
| 1   | x     | 199 | VAL  |
| 1   | x     | 202 | ARG  |
| 1   | x     | 205 | VAL  |
| 1   | x     | 208 | SER  |
| 1   | x     | 209 | VAL  |
| 1   | x     | 211 | SER  |
| 1   | x     | 213 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (266) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 65  | GLN  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 175 | GLN  |
| 1   | B     | 94  | HIS  |
| 1   | B     | 142 | GLN  |
| 1   | B     | 161 | GLN  |
| 1   | B     | 214 | ASN  |
| 1   | C     | 65  | GLN  |
| 1   | C     | 161 | GLN  |
| 1   | C     | 175 | GLN  |
| 1   | D     | 65  | GLN  |
| 1   | D     | 118 | ASN  |
| 1   | D     | 136 | HIS  |
| 1   | D     | 142 | GLN  |
| 1   | D     | 175 | GLN  |
| 1   | D     | 196 | ASN  |
| 1   | E     | 94  | HIS  |
| 1   | E     | 100 | GLN  |
| 1   | E     | 142 | GLN  |
| 1   | E     | 161 | GLN  |
| 1   | E     | 175 | GLN  |
| 1   | E     | 190 | ASN  |
| 1   | E     | 196 | ASN  |
| 1   | F     | 65  | GLN  |
| 1   | F     | 118 | ASN  |
| 1   | F     | 161 | GLN  |
| 1   | F     | 175 | GLN  |
| 1   | G     | 65  | GLN  |
| 1   | G     | 100 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 118 | ASN  |
| 1   | G     | 175 | GLN  |
| 1   | G     | 196 | ASN  |
| 1   | H     | 118 | ASN  |
| 1   | H     | 161 | GLN  |
| 1   | H     | 175 | GLN  |
| 1   | H     | 196 | ASN  |
| 1   | I     | 65  | GLN  |
| 1   | I     | 94  | HIS  |
| 1   | I     | 142 | GLN  |
| 1   | I     | 175 | GLN  |
| 1   | J     | 65  | GLN  |
| 1   | J     | 112 | GLN  |
| 1   | J     | 118 | ASN  |
| 1   | J     | 142 | GLN  |
| 1   | J     | 175 | GLN  |
| 1   | K     | 65  | GLN  |
| 1   | K     | 175 | GLN  |
| 1   | K     | 196 | ASN  |
| 1   | L     | 65  | GLN  |
| 1   | L     | 94  | HIS  |
| 1   | L     | 175 | GLN  |
| 1   | M     | 100 | GLN  |
| 1   | M     | 136 | HIS  |
| 1   | M     | 175 | GLN  |
| 1   | M     | 196 | ASN  |
| 1   | N     | 65  | GLN  |
| 1   | N     | 134 | ASN  |
| 1   | N     | 136 | HIS  |
| 1   | N     | 142 | GLN  |
| 1   | N     | 161 | GLN  |
| 1   | N     | 175 | GLN  |
| 1   | O     | 65  | GLN  |
| 1   | O     | 100 | GLN  |
| 1   | O     | 142 | GLN  |
| 1   | O     | 161 | GLN  |
| 1   | O     | 175 | GLN  |
| 1   | P     | 65  | GLN  |
| 1   | P     | 94  | HIS  |
| 1   | P     | 118 | ASN  |
| 1   | P     | 175 | GLN  |
| 1   | P     | 196 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 65  | GLN  |
| 1   | Q     | 118 | ASN  |
| 1   | Q     | 142 | GLN  |
| 1   | Q     | 161 | GLN  |
| 1   | R     | 65  | GLN  |
| 1   | R     | 100 | GLN  |
| 1   | R     | 118 | ASN  |
| 1   | R     | 161 | GLN  |
| 1   | S     | 94  | HIS  |
| 1   | S     | 100 | GLN  |
| 1   | S     | 142 | GLN  |
| 1   | S     | 175 | GLN  |
| 1   | T     | 65  | GLN  |
| 1   | T     | 94  | HIS  |
| 1   | T     | 134 | ASN  |
| 1   | T     | 142 | GLN  |
| 1   | T     | 161 | GLN  |
| 1   | T     | 175 | GLN  |
| 1   | T     | 214 | ASN  |
| 1   | U     | 65  | GLN  |
| 1   | U     | 100 | GLN  |
| 1   | U     | 118 | ASN  |
| 1   | U     | 161 | GLN  |
| 1   | U     | 175 | GLN  |
| 1   | V     | 56  | HIS  |
| 1   | V     | 65  | GLN  |
| 1   | V     | 118 | ASN  |
| 1   | V     | 196 | ASN  |
| 1   | W     | 118 | ASN  |
| 1   | W     | 142 | GLN  |
| 1   | X     | 65  | GLN  |
| 1   | X     | 94  | HIS  |
| 1   | X     | 118 | ASN  |
| 1   | X     | 136 | HIS  |
| 1   | X     | 175 | GLN  |
| 1   | Y     | 65  | GLN  |
| 1   | Y     | 118 | ASN  |
| 1   | Y     | 175 | GLN  |
| 1   | Y     | 196 | ASN  |
| 1   | Z     | 65  | GLN  |
| 1   | Z     | 118 | ASN  |
| 1   | Z     | 142 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Z     | 161 | GLN  |
| 1   | Z     | 175 | GLN  |
| 1   | 0     | 65  | GLN  |
| 1   | 0     | 94  | HIS  |
| 1   | 0     | 100 | GLN  |
| 1   | 0     | 142 | GLN  |
| 1   | 0     | 161 | GLN  |
| 1   | 0     | 175 | GLN  |
| 1   | 1     | 65  | GLN  |
| 1   | 1     | 118 | ASN  |
| 1   | 1     | 161 | GLN  |
| 1   | 1     | 175 | GLN  |
| 1   | 1     | 196 | ASN  |
| 1   | 2     | 65  | GLN  |
| 1   | 2     | 136 | HIS  |
| 1   | 2     | 161 | GLN  |
| 1   | 2     | 175 | GLN  |
| 1   | 3     | 65  | GLN  |
| 1   | 3     | 94  | HIS  |
| 1   | 3     | 100 | GLN  |
| 1   | 3     | 161 | GLN  |
| 1   | 3     | 175 | GLN  |
| 1   | 4     | 65  | GLN  |
| 1   | 4     | 94  | HIS  |
| 1   | 4     | 100 | GLN  |
| 1   | 4     | 118 | ASN  |
| 1   | 4     | 196 | ASN  |
| 1   | 5     | 65  | GLN  |
| 1   | 5     | 142 | GLN  |
| 1   | 5     | 161 | GLN  |
| 1   | 6     | 65  | GLN  |
| 1   | 6     | 100 | GLN  |
| 1   | 6     | 118 | ASN  |
| 1   | 6     | 142 | GLN  |
| 1   | 6     | 161 | GLN  |
| 1   | 6     | 175 | GLN  |
| 1   | 7     | 65  | GLN  |
| 1   | 7     | 100 | GLN  |
| 1   | 7     | 112 | GLN  |
| 1   | 7     | 118 | ASN  |
| 1   | 7     | 161 | GLN  |
| 1   | 7     | 175 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7     | 196 | ASN  |
| 1   | 8     | 65  | GLN  |
| 1   | 8     | 142 | GLN  |
| 1   | 8     | 161 | GLN  |
| 1   | 8     | 175 | GLN  |
| 1   | 8     | 196 | ASN  |
| 1   | 8     | 214 | ASN  |
| 1   | 9     | 65  | GLN  |
| 1   | 9     | 94  | HIS  |
| 1   | 9     | 161 | GLN  |
| 1   | 9     | 175 | GLN  |
| 1   | a     | 65  | GLN  |
| 1   | a     | 94  | HIS  |
| 1   | a     | 118 | ASN  |
| 1   | a     | 134 | ASN  |
| 1   | a     | 175 | GLN  |
| 1   | a     | 190 | ASN  |
| 1   | b     | 56  | HIS  |
| 1   | b     | 100 | GLN  |
| 1   | b     | 112 | GLN  |
| 1   | b     | 118 | ASN  |
| 1   | b     | 175 | GLN  |
| 1   | c     | 65  | GLN  |
| 1   | c     | 94  | HIS  |
| 1   | c     | 161 | GLN  |
| 1   | c     | 175 | GLN  |
| 1   | d     | 65  | GLN  |
| 1   | d     | 161 | GLN  |
| 1   | d     | 175 | GLN  |
| 1   | d     | 196 | ASN  |
| 1   | e     | 94  | HIS  |
| 1   | e     | 142 | GLN  |
| 1   | e     | 175 | GLN  |
| 1   | e     | 214 | ASN  |
| 1   | f     | 65  | GLN  |
| 1   | f     | 94  | HIS  |
| 1   | f     | 142 | GLN  |
| 1   | f     | 161 | GLN  |
| 1   | f     | 175 | GLN  |
| 1   | g     | 65  | GLN  |
| 1   | g     | 118 | ASN  |
| 1   | g     | 161 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | g     | 175 | GLN  |
| 1   | g     | 196 | ASN  |
| 1   | h     | 65  | GLN  |
| 1   | h     | 161 | GLN  |
| 1   | h     | 175 | GLN  |
| 1   | h     | 196 | ASN  |
| 1   | i     | 65  | GLN  |
| 1   | i     | 100 | GLN  |
| 1   | i     | 142 | GLN  |
| 1   | i     | 175 | GLN  |
| 1   | j     | 65  | GLN  |
| 1   | j     | 94  | HIS  |
| 1   | j     | 100 | GLN  |
| 1   | j     | 112 | GLN  |
| 1   | k     | 161 | GLN  |
| 1   | k     | 214 | ASN  |
| 1   | l     | 65  | GLN  |
| 1   | l     | 100 | GLN  |
| 1   | l     | 175 | GLN  |
| 1   | m     | 142 | GLN  |
| 1   | m     | 175 | GLN  |
| 1   | m     | 196 | ASN  |
| 1   | n     | 94  | HIS  |
| 1   | n     | 142 | GLN  |
| 1   | n     | 161 | GLN  |
| 1   | n     | 175 | GLN  |
| 1   | n     | 190 | ASN  |
| 1   | o     | 65  | GLN  |
| 1   | o     | 94  | HIS  |
| 1   | o     | 100 | GLN  |
| 1   | p     | 65  | GLN  |
| 1   | p     | 142 | GLN  |
| 1   | q     | 65  | GLN  |
| 1   | q     | 100 | GLN  |
| 1   | q     | 175 | GLN  |
| 1   | r     | 65  | GLN  |
| 1   | r     | 94  | HIS  |
| 1   | r     | 100 | GLN  |
| 1   | r     | 161 | GLN  |
| 1   | r     | 175 | GLN  |
| 1   | s     | 65  | GLN  |
| 1   | s     | 100 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | s     | 118 | ASN  |
| 1   | s     | 134 | ASN  |
| 1   | s     | 161 | GLN  |
| 1   | s     | 175 | GLN  |
| 1   | s     | 196 | ASN  |
| 1   | t     | 161 | GLN  |
| 1   | t     | 175 | GLN  |
| 1   | t     | 196 | ASN  |
| 1   | t     | 214 | ASN  |
| 1   | u     | 65  | GLN  |
| 1   | u     | 94  | HIS  |
| 1   | u     | 161 | GLN  |
| 1   | u     | 175 | GLN  |
| 1   | v     | 56  | HIS  |
| 1   | v     | 65  | GLN  |
| 1   | v     | 118 | ASN  |
| 1   | v     | 161 | GLN  |
| 1   | v     | 175 | GLN  |
| 1   | v     | 196 | ASN  |
| 1   | w     | 94  | HIS  |
| 1   | w     | 136 | HIS  |
| 1   | w     | 161 | GLN  |
| 1   | x     | 65  | GLN  |
| 1   | x     | 94  | HIS  |
| 1   | x     | 100 | GLN  |
| 1   | x     | 118 | ASN  |
| 1   | x     | 175 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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   | 0     | 163/183 (89%) | -1.67  | 0 100 100 | 28, 44, 82, 144       | 0     |
| 1   | 1     | 163/183 (89%) | -1.62  | 0 100 100 | 30, 49, 106, 153      | 0     |
| 1   | 2     | 163/183 (89%) | -1.60  | 0 100 100 | 36, 55, 110, 160      | 0     |
| 1   | 3     | 163/183 (89%) | -1.62  | 0 100 100 | 26, 45, 109, 163      | 0     |
| 1   | 4     | 163/183 (89%) | -1.62  | 0 100 100 | 30, 52, 109, 171      | 0     |
| 1   | 5     | 163/183 (89%) | -1.63  | 0 100 100 | 30, 51, 104, 156      | 0     |
| 1   | 6     | 163/183 (89%) | -1.53  | 0 100 100 | 32, 56, 122, 194      | 0     |
| 1   | 7     | 163/183 (89%) | -1.70  | 0 100 100 | 26, 41, 72, 127       | 0     |
| 1   | 8     | 163/183 (89%) | -1.66  | 0 100 100 | 26, 42, 76, 120       | 0     |
| 1   | 9     | 163/183 (89%) | -1.68  | 0 100 100 | 25, 43, 86, 112       | 0     |
| 1   | A     | 163/183 (89%) | -1.66  | 0 100 100 | 31, 47, 89, 132       | 0     |
| 1   | B     | 163/183 (89%) | -1.66  | 0 100 100 | 29, 47, 101, 189      | 0     |
| 1   | C     | 163/183 (89%) | -1.60  | 0 100 100 | 26, 50, 111, 183      | 0     |
| 1   | D     | 163/183 (89%) | -1.72  | 0 100 100 | 32, 46, 81, 112       | 0     |
| 1   | E     | 163/183 (89%) | -1.68  | 0 100 100 | 24, 43, 79, 126       | 0     |
| 1   | F     | 163/183 (89%) | -1.60  | 0 100 100 | 32, 53, 101, 137      | 0     |
| 1   | G     | 163/183 (89%) | -1.71  | 0 100 100 | 25, 42, 74, 114       | 0     |
| 1   | H     | 163/183 (89%) | -1.70  | 0 100 100 | 26, 41, 76, 105       | 0     |
| 1   | I     | 163/183 (89%) | -1.64  | 0 100 100 | 27, 44, 81, 118       | 0     |
| 1   | J     | 163/183 (89%) | -1.59  | 0 100 100 | 27, 52, 110, 177      | 0     |
| 1   | K     | 163/183 (89%) | -1.59  | 0 100 100 | 26, 53, 106, 171      | 0     |
| 1   | L     | 163/183 (89%) | -1.60  | 0 100 100 | 26, 54, 123, 169      | 0     |
| 1   | M     | 163/183 (89%) | -1.70  | 0 100 100 | 23, 38, 71, 137       | 0     |
| 1   | N     | 163/183 (89%) | -1.72  | 0 100 100 | 23, 37, 74, 128       | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|-----------|-----------------------|-------|
| 1   | O     | 163/183 (89%) | -1.69  | 0 100 100 | 28, 46, 84, 129       | 0     |
| 1   | P     | 163/183 (89%) | -1.63  | 0 100 100 | 25, 47, 100, 159      | 0     |
| 1   | Q     | 163/183 (89%) | -1.65  | 0 100 100 | 26, 45, 113, 151      | 0     |
| 1   | R     | 163/183 (89%) | -1.59  | 0 100 100 | 29, 54, 124, 176      | 0     |
| 1   | S     | 163/183 (89%) | -1.71  | 0 100 100 | 29, 45, 81, 123       | 0     |
| 1   | T     | 163/183 (89%) | -1.66  | 0 100 100 | 26, 44, 81, 120       | 0     |
| 1   | U     | 163/183 (89%) | -1.58  | 0 100 100 | 36, 52, 96, 140       | 0     |
| 1   | V     | 163/183 (89%) | -1.61  | 0 100 100 | 28, 53, 116, 150      | 0     |
| 1   | W     | 163/183 (89%) | -1.60  | 0 100 100 | 27, 47, 104, 156      | 0     |
| 1   | X     | 163/183 (89%) | -1.61  | 0 100 100 | 28, 47, 116, 193      | 0     |
| 1   | Y     | 163/183 (89%) | -1.68  | 0 100 100 | 25, 42, 79, 121       | 0     |
| 1   | Z     | 163/183 (89%) | -1.68  | 0 100 100 | 31, 48, 81, 143       | 0     |
| 1   | a     | 163/183 (89%) | -1.60  | 0 100 100 | 36, 62, 110, 149      | 0     |
| 1   | b     | 163/183 (89%) | -1.66  | 0 100 100 | 31, 53, 104, 147      | 0     |
| 1   | c     | 163/183 (89%) | -1.52  | 0 100 100 | 36, 66, 120, 135      | 0     |
| 1   | d     | 163/183 (89%) | -1.67  | 0 100 100 | 25, 43, 103, 156      | 0     |
| 1   | e     | 163/183 (89%) | -1.62  | 0 100 100 | 28, 49, 106, 153      | 0     |
| 1   | f     | 163/183 (89%) | -1.57  | 0 100 100 | 37, 59, 114, 159      | 0     |
| 1   | g     | 163/183 (89%) | -1.68  | 0 100 100 | 29, 48, 81, 120       | 0     |
| 1   | h     | 163/183 (89%) | -1.70  | 0 100 100 | 26, 43, 79, 121       | 0     |
| 1   | i     | 163/183 (89%) | -1.67  | 0 100 100 | 26, 45, 87, 114       | 0     |
| 1   | j     | 163/183 (89%) | -1.61  | 0 100 100 | 26, 49, 102, 165      | 0     |
| 1   | k     | 163/183 (89%) | -1.61  | 0 100 100 | 34, 47, 102, 151      | 0     |
| 1   | l     | 163/183 (89%) | -1.61  | 0 100 100 | 31, 52, 115, 265      | 0     |
| 1   | m     | 163/183 (89%) | -1.74  | 0 100 100 | 25, 36, 71, 115       | 0     |
| 1   | n     | 163/183 (89%) | -1.70  | 0 100 100 | 28, 44, 78, 137       | 0     |
| 1   | o     | 163/183 (89%) | -1.65  | 0 100 100 | 26, 39, 79, 124       | 0     |
| 1   | p     | 163/183 (89%) | -1.68  | 0 100 100 | 28, 43, 90, 120       | 0     |
| 1   | q     | 163/183 (89%) | -1.65  | 0 100 100 | 26, 47, 95, 118       | 0     |
| 1   | r     | 163/183 (89%) | -1.60  | 0 100 100 | 38, 57, 99, 128       | 0     |
| 1   | s     | 163/183 (89%) | -1.58  | 0 100 100 | 39, 61, 103, 139      | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2 | OWAB(Å²) | Q<0.9            |   |
|-----|-------|------------------|--------|---------|----------|------------------|---|
| 1   | t     | 163/183 (89%)    | -1.65  | 0       | 100 100  | 33, 52, 103, 141 | 0 |
| 1   | u     | 163/183 (89%)    | -1.53  | 0       | 100 100  | 41, 65, 114, 144 | 0 |
| 1   | v     | 163/183 (89%)    | -1.62  | 0       | 100 100  | 35, 55, 93, 129  | 0 |
| 1   | w     | 163/183 (89%)    | -1.66  | 0       | 100 100  | 29, 44, 93, 117  | 0 |
| 1   | x     | 163/183 (89%)    | -1.65  | 0       | 100 100  | 26, 49, 97, 122  | 0 |
| All | All   | 9780/10980 (89%) | -1.64  | 0       | 100 100  | 23, 48, 102, 265 | 0 |

There are no RSRZ outliers to report.

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.