



Full wwPDB X-ray Structure Validation Report

Jun 16, 2014 – 06:41 PM BST

PDB ID : 4V7G
Title : Crystal Structure of Lumazine Synthase from Bacillus Anthracis
Authors : Morgunova, E.; Illarionov, B.; Saller, S.; Popov, A.; Sambaiah, T.; Bacher, A.;
Cushman, M.; Fischer, M.; Ladenstein, R.
Deposited on : 2009-09-16
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

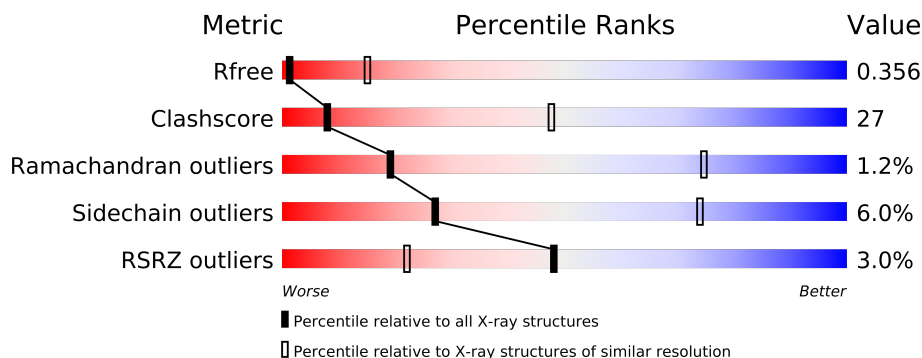
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1243 (3.70-3.30) |
| Clashscore | 79885 | 1039 (3.66-3.34) |
| Ramachandran outliers | 78287 | 1000 (3.66-3.34) |
| Sidechain outliers | 78261 | 1000 (3.66-3.34) |
| RSRZ outliers | 66119 | 1243 (3.70-3.30) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A1 | 153 | |
| 1 | A2 | 153 | |
| 1 | A3 | 153 | |
| 1 | A4 | 153 | |
| 1 | AA | 153 | |
| 1 | AB | 153 | |
| 1 | AC | 153 | |
| 1 | AD | 153 | |
| 1 | AE | 153 | |
| 1 | AF | 153 | |
| 1 | AG | 153 | |
| 1 | AH | 153 | |
| 1 | AI | 153 | |
| 1 | AJ | 153 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AK | 153 | |
| 1 | AL | 153 | |
| 1 | AM | 153 | |
| 1 | AN | 153 | |
| 1 | AO | 153 | |
| 1 | AP | 153 | |
| 1 | AQ | 153 | |
| 1 | AR | 153 | |
| 1 | AS | 153 | |
| 1 | AT | 153 | |
| 1 | AU | 153 | |
| 1 | AV | 153 | |
| 1 | AW | 153 | |
| 1 | AX | 153 | |
| 1 | AY | 153 | |
| 1 | AZ | 153 | |
| 1 | B1 | 153 | |
| 1 | B2 | 153 | |
| 1 | B3 | 153 | |
| 1 | B4 | 153 | |
| 1 | BA | 153 | |
| 1 | BB | 153 | |
| 1 | BC | 153 | |
| 1 | BD | 153 | |
| 1 | BE | 153 | |
| 1 | BF | 153 | |
| 1 | BG | 153 | |
| 1 | BH | 153 | |
| 1 | BI | 153 | |
| 1 | BJ | 153 | |
| 1 | BK | 153 | |
| 1 | BL | 153 | |
| 1 | BM | 153 | |
| 1 | BN | 153 | |
| 1 | BO | 153 | |
| 1 | BP | 153 | |
| 1 | BQ | 153 | |
| 1 | BR | 153 | |
| 1 | BS | 153 | |
| 1 | BT | 153 | |
| 1 | BU | 153 | |
| 1 | BV | 153 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | BW | 153 | |
| 1 | BX | 153 | |
| 1 | BY | 153 | |
| 1 | BZ | 153 | |
| 1 | C1 | 153 | |
| 1 | C2 | 153 | |
| 1 | C3 | 153 | |
| 1 | C4 | 153 | |
| 1 | CA | 153 | |
| 1 | CB | 153 | |
| 1 | CC | 153 | |
| 1 | CD | 153 | |
| 1 | CE | 153 | |
| 1 | CF | 153 | |
| 1 | CG | 153 | |
| 1 | CH | 153 | |
| 1 | CI | 153 | |
| 1 | CJ | 153 | |
| 1 | CK | 153 | |
| 1 | CL | 153 | |
| 1 | CM | 153 | |
| 1 | CN | 153 | |
| 1 | CO | 153 | |
| 1 | CP | 153 | |
| 1 | CQ | 153 | |
| 1 | CR | 153 | |
| 1 | CS | 153 | |
| 1 | CT | 153 | |
| 1 | CU | 153 | |
| 1 | CV | 153 | |
| 1 | CW | 153 | |
| 1 | CX | 153 | |
| 1 | CY | 153 | |
| 1 | CZ | 153 | |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 2 | PO4 | AI | 1001 | - | X |
| 2 | PO4 | AX | 1001 | - | X |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 102534 atoms, of which 0 are hydrogen and 0 are deuterium.

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 6,7-dimethyl-8-ribityllumazinesynthase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | AA | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AB | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AC | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AD | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AE | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AF | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AG | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AH | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AI | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AJ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AK | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AL | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AM | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AN | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AO | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AP | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | AQ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AR | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AS | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AT | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AU | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AV | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | AW | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AX | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AY | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | AZ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | A1 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 723 | 193 | 210 | 3 | | | |
| 1 | A2 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | A3 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | A4 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 724 | 193 | 212 | 3 | | | |
| 1 | BA | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BB | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BC | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BD | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BE | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BF | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BG | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | BH | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BI | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BJ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BK | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BL | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BM | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BN | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BO | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BP | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BQ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BR | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BS | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BT | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BU | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BV | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BW | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BX | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BY | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | BZ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | B1 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | B2 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |

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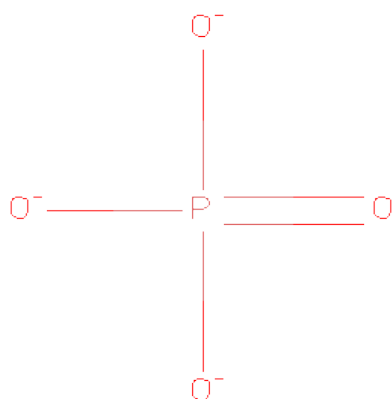
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | B3 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | B4 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CA | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CB | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CC | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CD | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CE | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CF | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CG | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CH | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CI | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CJ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CK | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CL | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CM | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CN | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CO | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CP | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CQ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CR | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CS | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | CT | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CU | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CV | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CW | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CX | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CY | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | CZ | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | C1 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | C2 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | C3 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |
| 1 | C4 | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 193 | 214 | 3 | | | |

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | AA | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AB | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AC | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AD | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AE | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AF | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AG | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AH | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AI | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AJ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AK | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AL | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AM | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AN | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AO | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AP | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AQ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AR | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AS | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AT | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AU | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AV | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | AW | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AX | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AY | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | AZ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A1 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A2 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A3 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A4 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BA | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BB | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BC | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BD | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BE | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BF | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BG | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BH | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BI | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BJ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BK | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BL | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BM | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | BN | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BO | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BP | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BQ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BR | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BS | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BT | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BU | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BV | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BW | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BX | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BY | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | BZ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B1 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B2 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B3 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B4 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CA | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CB | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CC | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CD | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | CE | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CF | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CG | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CH | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CI | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CJ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CK | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CL | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CM | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CN | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CO | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CP | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CQ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CR | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CS | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CT | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CU | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CV | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CW | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CX | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | CY | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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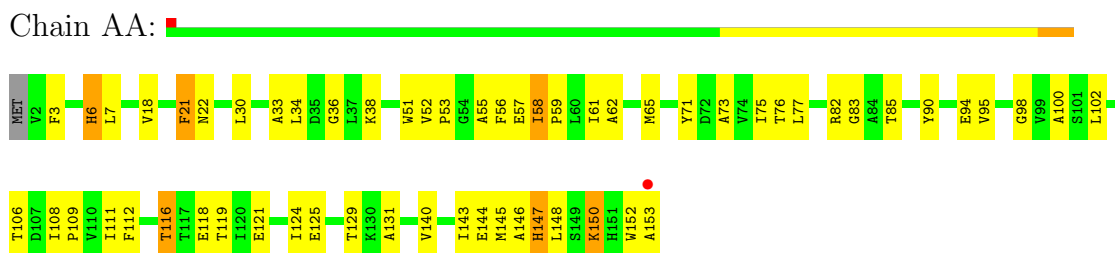
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | CZ | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C1 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C2 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C3 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C4 | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

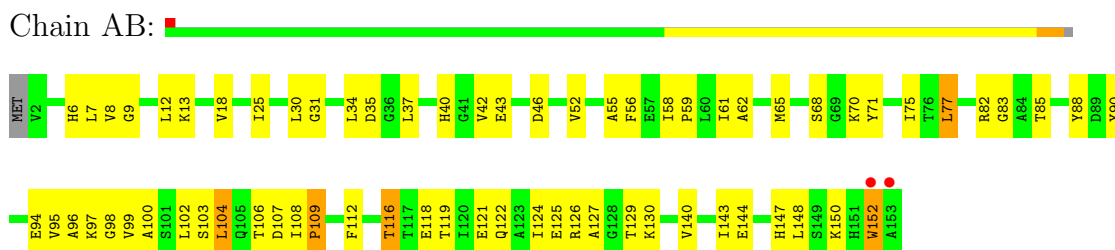
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

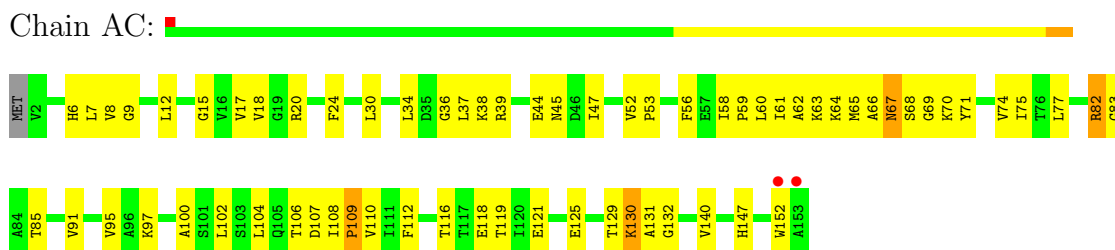
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase



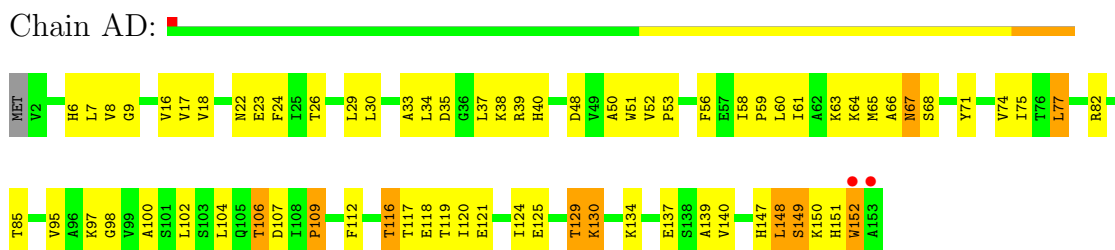
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

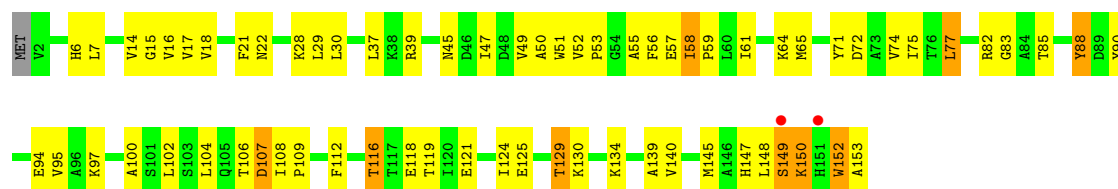


- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase



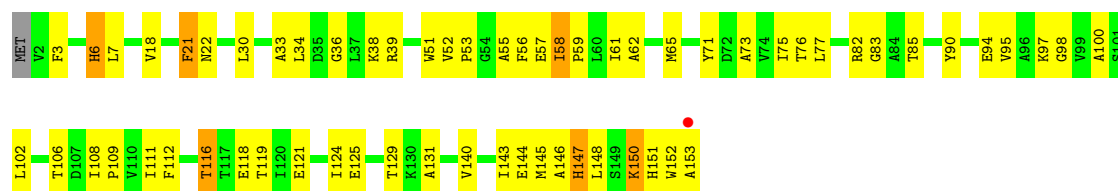
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AE:



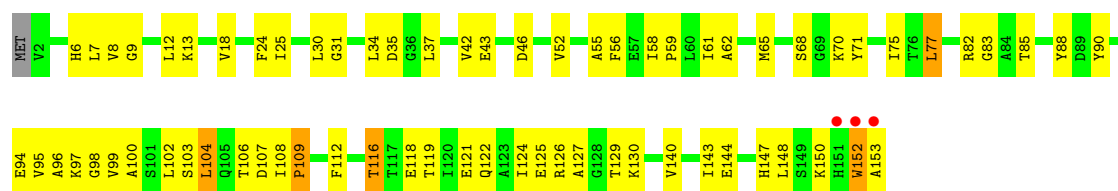
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AF:



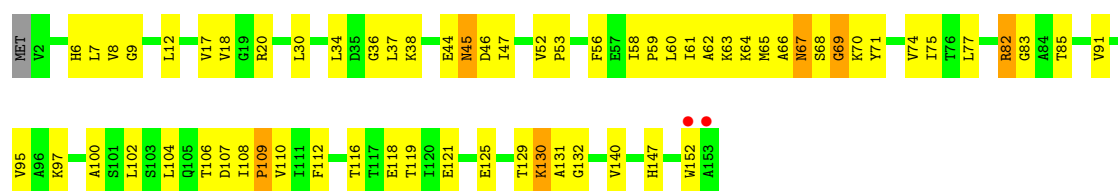
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AG:



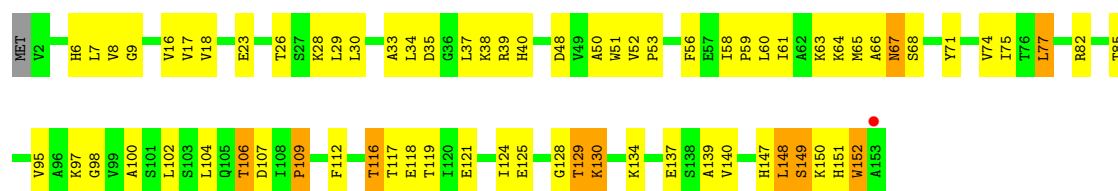
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AH:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

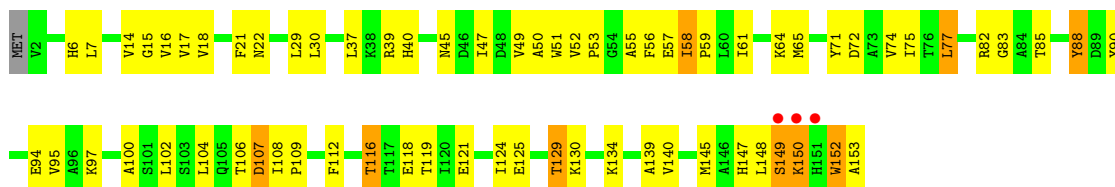
Chain AI:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

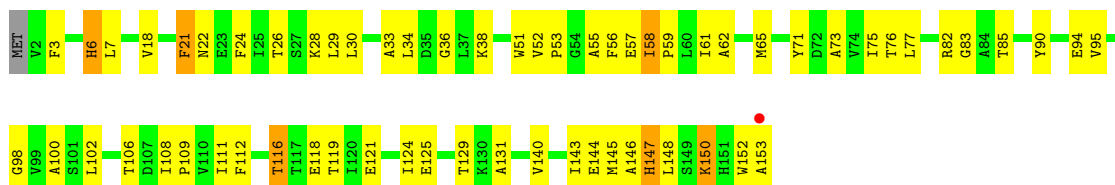
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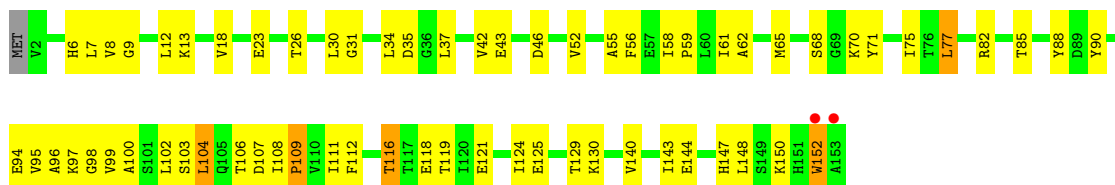
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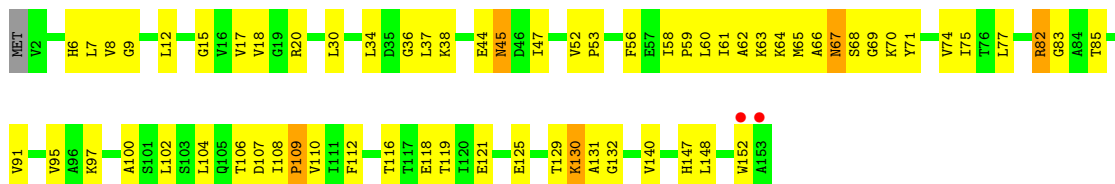
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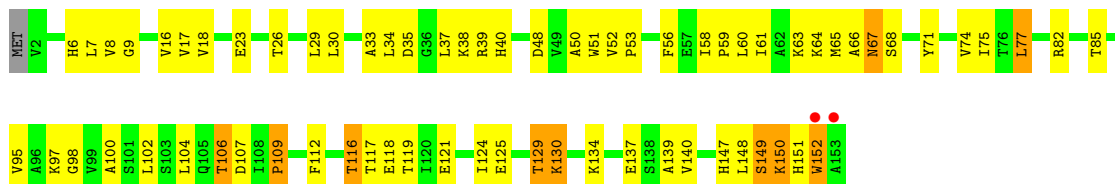
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AM:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AN:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AO:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AP:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AQ:

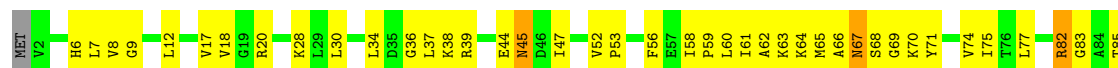
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AR:



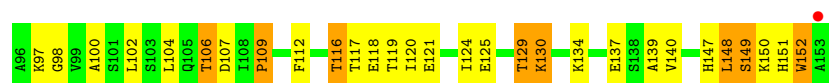
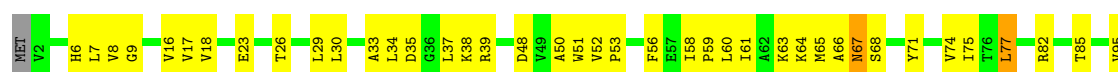
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AS:



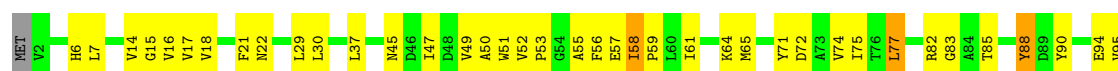
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AS:



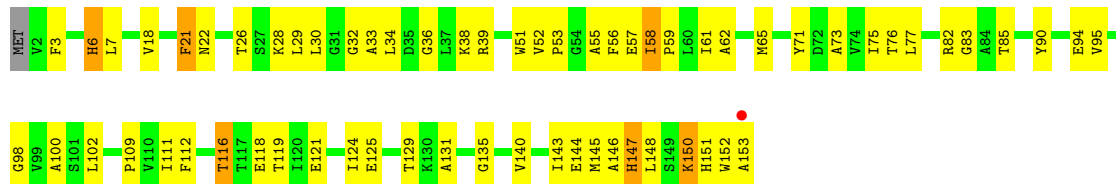
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AT:



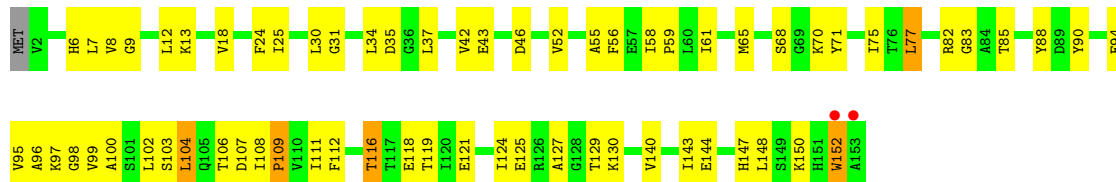
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AU:



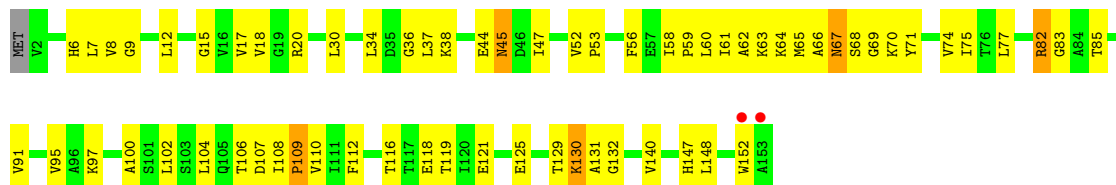
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AV:



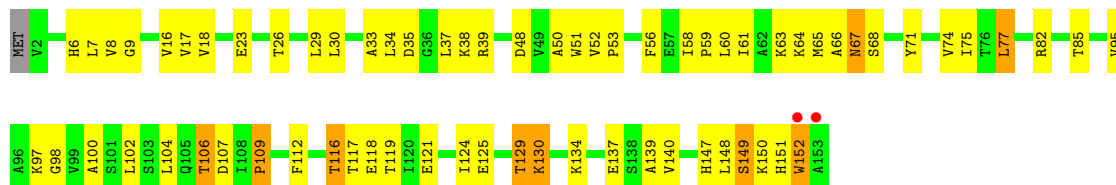
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AW:



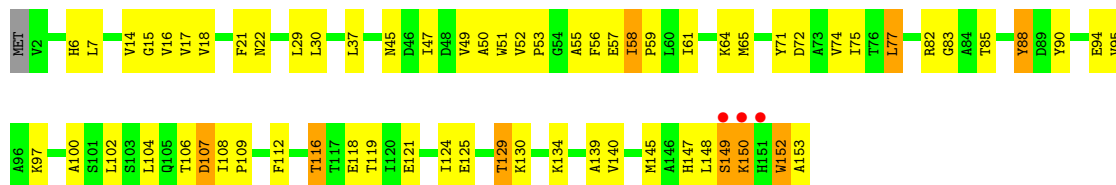
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain AX:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

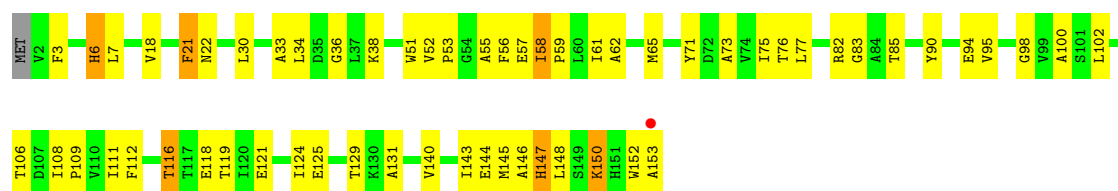
Chain AY:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

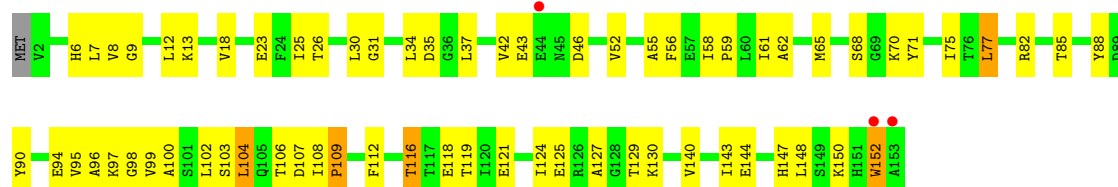
Chain AZ:





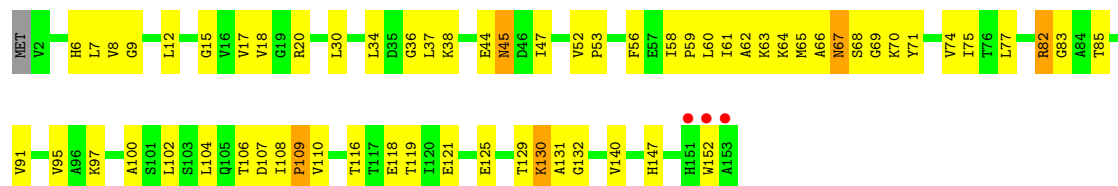
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain A1:



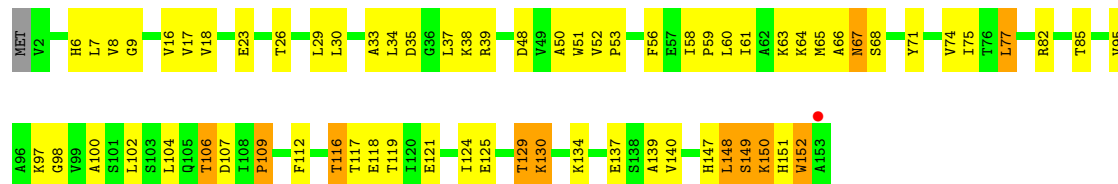
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain A2:



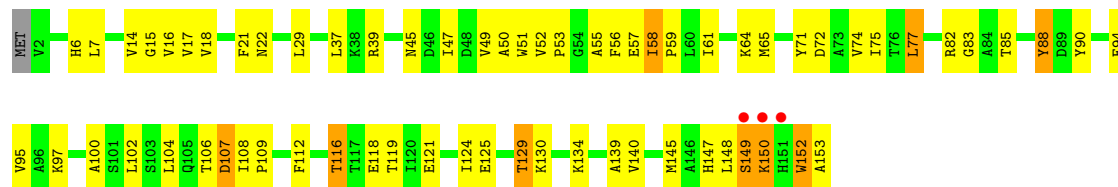
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain A3:



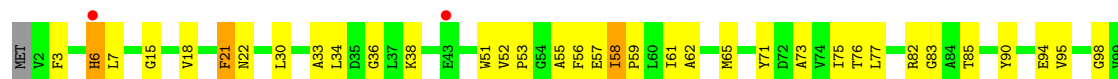
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

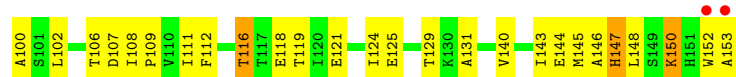
Chain A4:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BA:





- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BB:



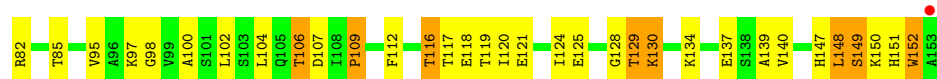
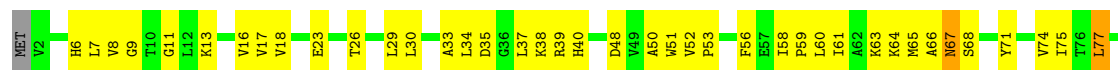
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BC:



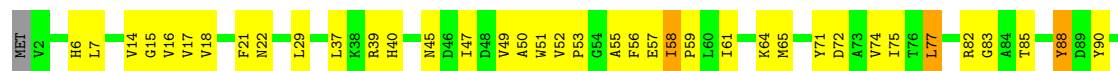
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BD:



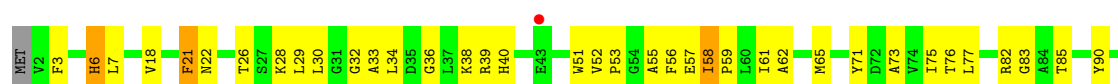
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BE:



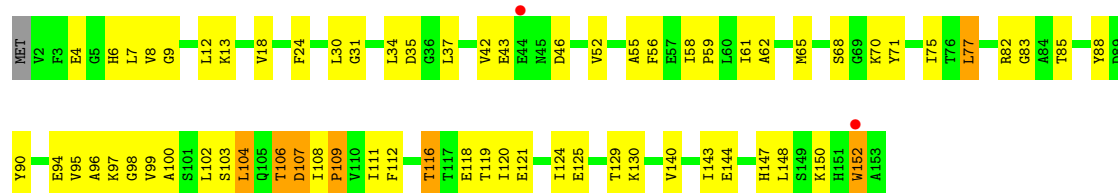
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BF:



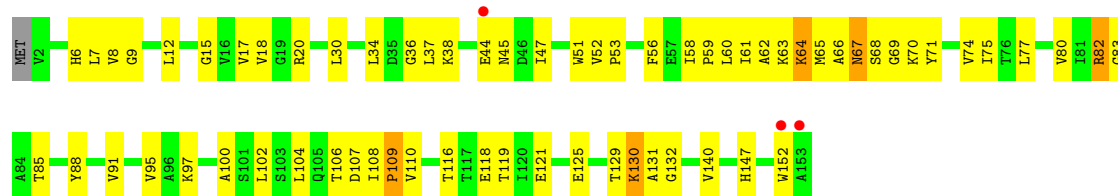
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BG:



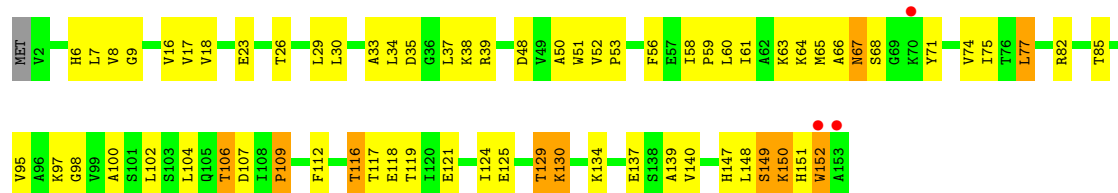
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BH:



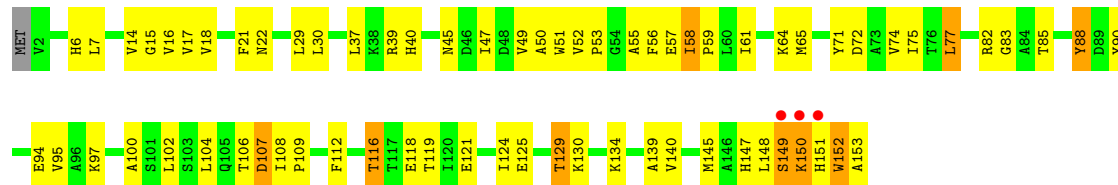
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BI:



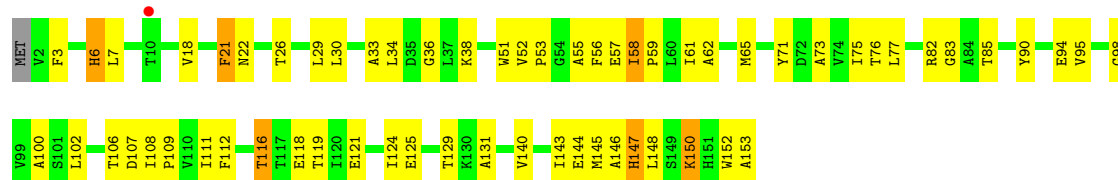
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BJ:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

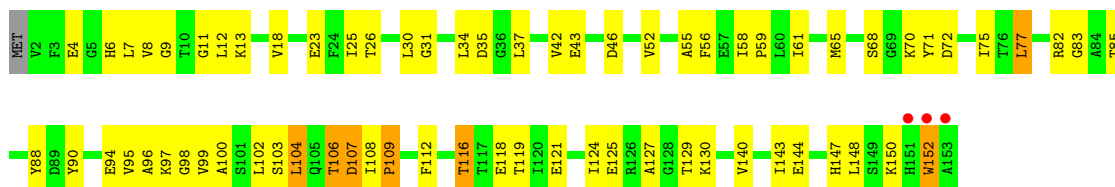
Chain BK:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

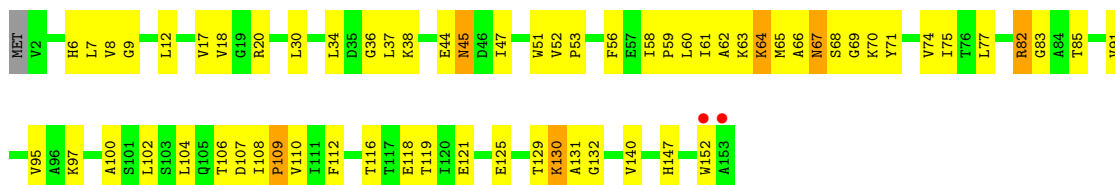
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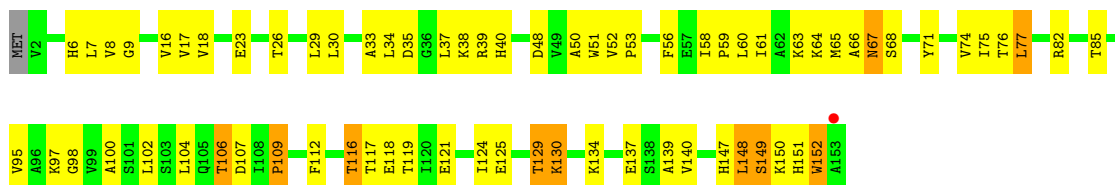
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BM:



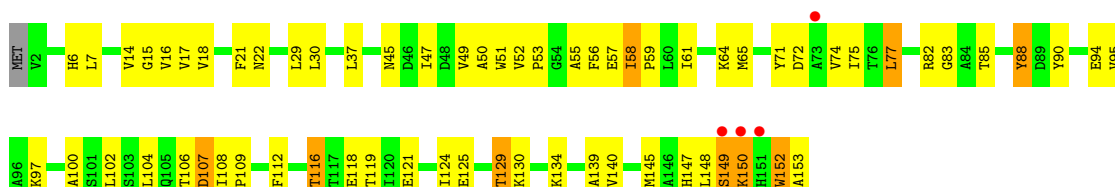
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

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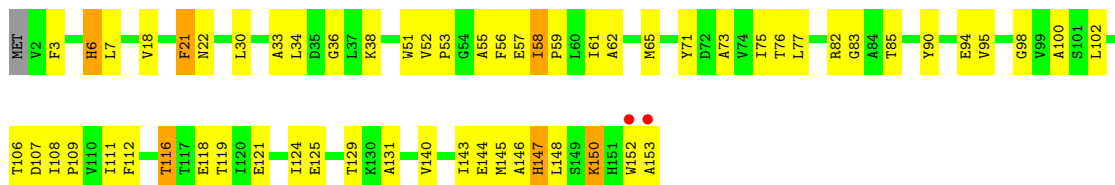
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BO:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BP:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

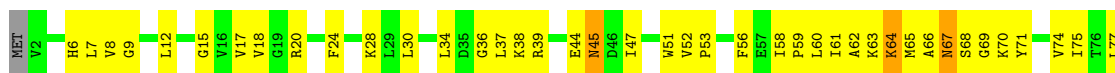
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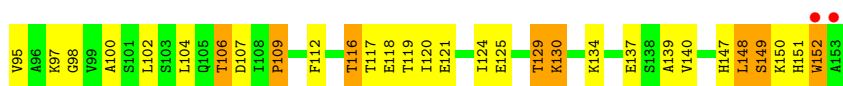
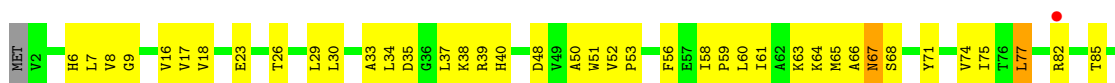
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BR:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BS:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BT:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BU:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BV:





- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BW:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BX:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BY:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain BZ:



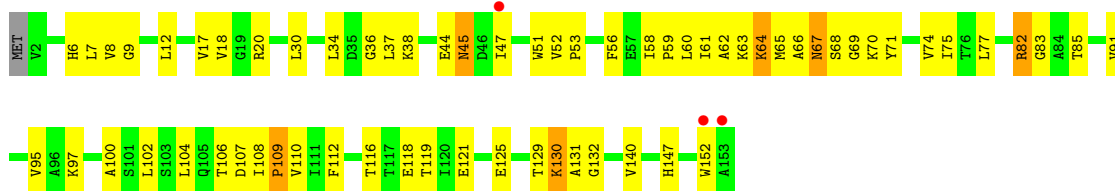
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Chain B1:



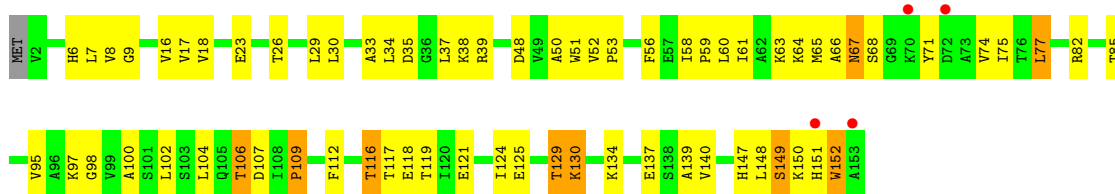
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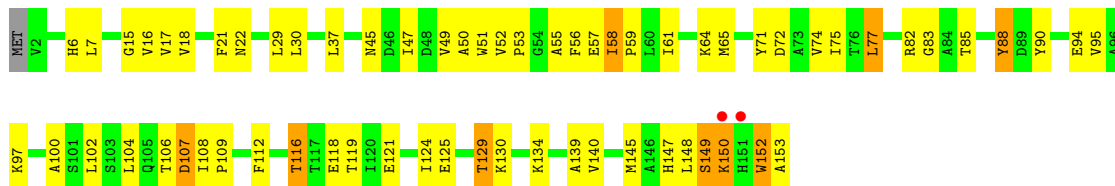
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

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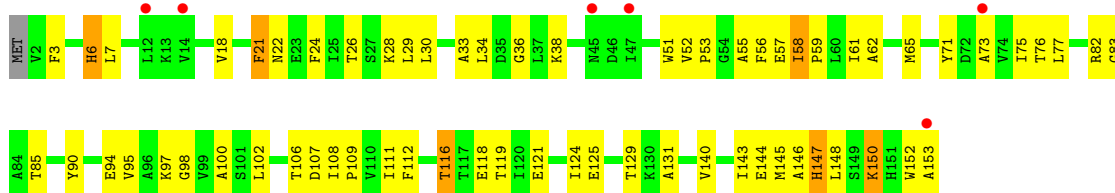
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Chain B4:



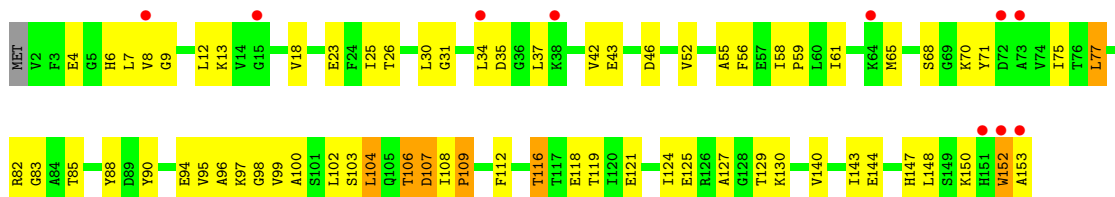
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CA:

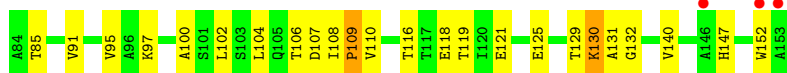
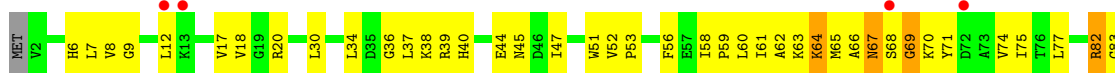


- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

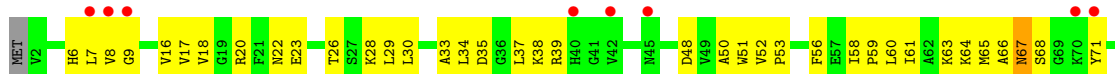
Chain CB:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CC: 

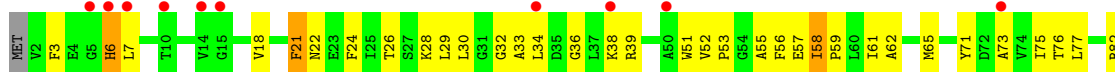
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CD: 

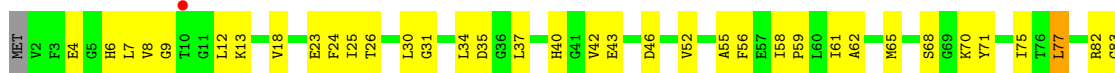
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CE: 

- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

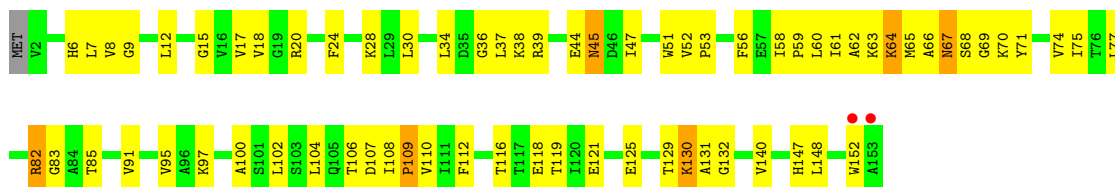
Chain CF: 

- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CG: 

- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CH: 



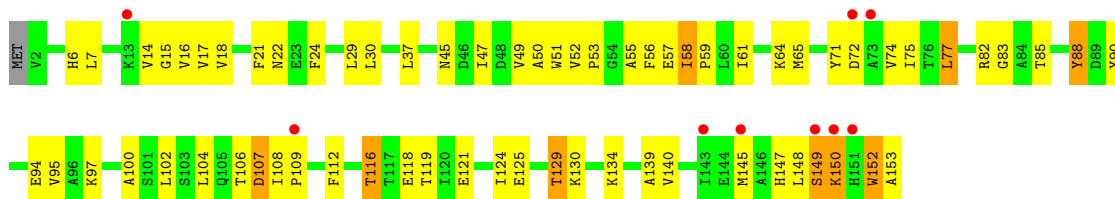
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CI:



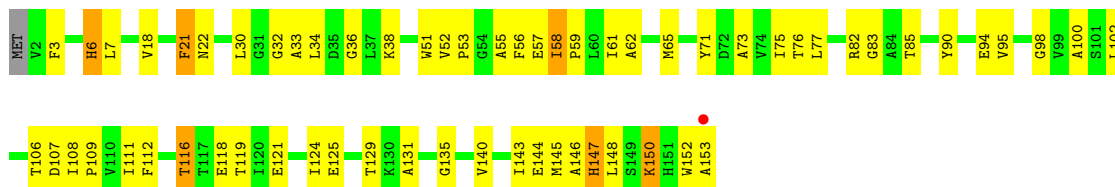
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CJ:



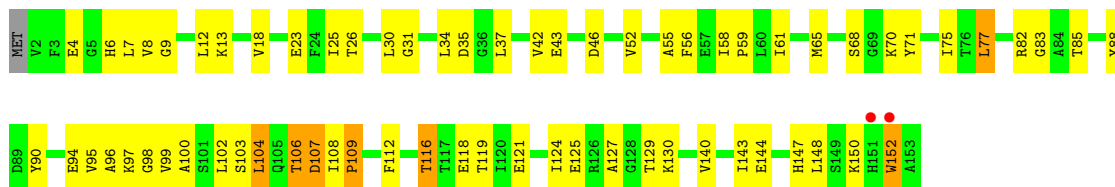
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CK:



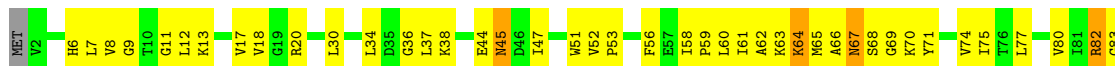
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CL:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CM:





- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CN:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

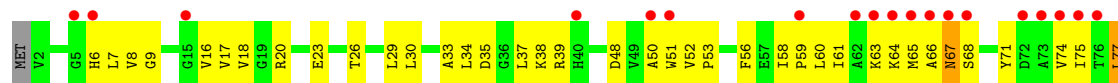
Chain CO:





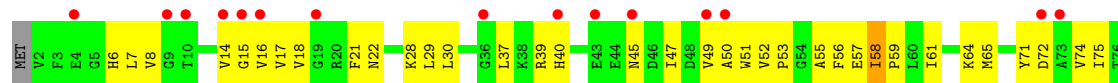
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CS:



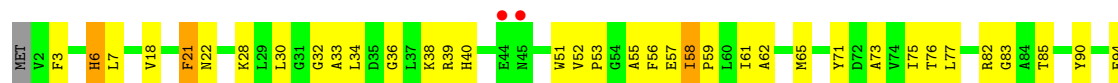
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CT:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CU:



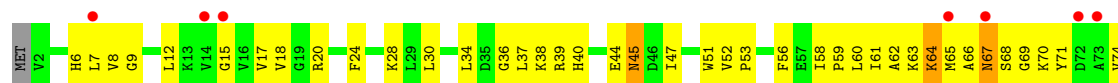
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CV:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

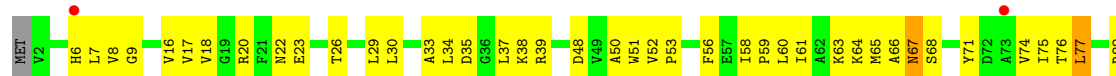
Chain CW:





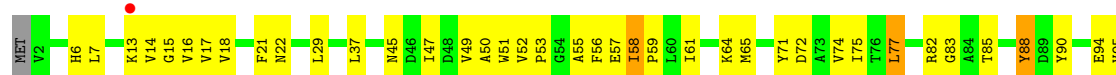
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CX:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CY:



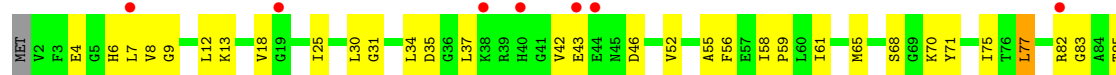
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain CZ:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain C1:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

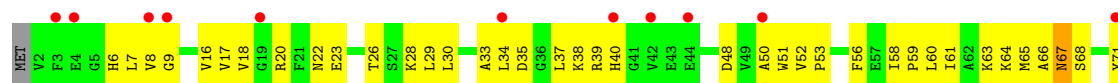
Chain C2:





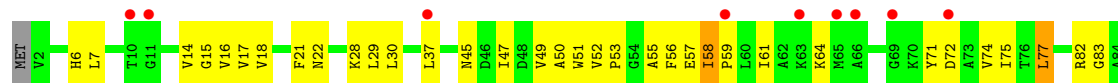
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain C3:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase

Chain C4:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 157.20Å 222.24Å 473.49Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 3.50 39.90 – 3.50 | Depositor EDS |
| % Data completeness (in resolution range) | 89.8 (15.00-3.50) 93.0 (39.90-3.50) | Depositor EDS |
| R_{merge} | 0.29 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.93 (at 3.48Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine) | Depositor |
| R, R_{free} | 0.235 , 0.286 0.353 , 0.356 | Depositor DCC |
| R_{free} test set | 3896 reflections (2.05%) | DCC |
| Wilson B-factor (Å ²) | 67.0 | Xtriage |
| Anisotropy | 0.104 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 44.4 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$ | Xtriage |
| Outliers | 1 of 194062 reflections (0.001%) | Xtriage |
| F_o, F_c correlation | 0.72 | EDS |
| Total number of atoms | 102534 | wwPDB-VP |
| Average B, all atoms (Å ²) | 104.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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 | A1 | 0.44 | 0/1149 | 0.71 | 2/1558 (0.1%) |
| 1 | A2 | 0.32 | 0/1152 | 0.62 | 1/1562 (0.1%) |
| 1 | A3 | 0.31 | 0/1152 | 0.85 | 5/1562 (0.3%) |
| 1 | A4 | 0.34 | 0/1152 | 0.58 | 1/1562 (0.1%) |
| 1 | AA | 0.33 | 0/1149 | 0.49 | 1/1558 (0.1%) |
| 1 | AB | 0.44 | 0/1149 | 0.71 | 2/1558 (0.1%) |
| 1 | AC | 0.32 | 0/1152 | 0.62 | 1/1562 (0.1%) |
| 1 | AD | 0.31 | 0/1152 | 0.85 | 5/1562 (0.3%) |
| 1 | AE | 0.34 | 0/1152 | 0.58 | 1/1562 (0.1%) |
| 1 | AF | 0.33 | 0/1149 | 0.49 | 1/1558 (0.1%) |
| 1 | AG | 0.44 | 0/1149 | 0.71 | 2/1558 (0.1%) |
| 1 | AH | 0.32 | 0/1152 | 0.63 | 1/1562 (0.1%) |
| 1 | AI | 0.31 | 0/1152 | 0.85 | 5/1562 (0.3%) |
| 1 | AJ | 0.34 | 0/1152 | 0.58 | 1/1562 (0.1%) |
| 1 | AK | 0.33 | 0/1149 | 0.49 | 1/1558 (0.1%) |
| 1 | AL | 0.44 | 0/1149 | 0.71 | 2/1558 (0.1%) |
| 1 | AM | 0.32 | 0/1152 | 0.63 | 1/1562 (0.1%) |
| 1 | AN | 0.31 | 0/1152 | 0.85 | 5/1562 (0.3%) |
| 1 | AO | 0.34 | 0/1152 | 0.58 | 1/1562 (0.1%) |
| 1 | AP | 0.33 | 0/1149 | 0.49 | 1/1558 (0.1%) |
| 1 | AQ | 0.44 | 0/1149 | 0.71 | 2/1558 (0.1%) |
| 1 | AR | 0.32 | 0/1152 | 0.62 | 1/1562 (0.1%) |
| 1 | AS | 0.31 | 0/1152 | 0.85 | 5/1562 (0.3%) |
| 1 | AT | 0.34 | 0/1152 | 0.58 | 1/1562 (0.1%) |
| 1 | AU | 0.33 | 0/1149 | 0.49 | 1/1558 (0.1%) |
| 1 | AV | 0.44 | 0/1149 | 0.71 | 2/1558 (0.1%) |
| 1 | AW | 0.32 | 0/1152 | 0.63 | 1/1562 (0.1%) |
| 1 | AX | 0.31 | 0/1152 | 0.85 | 5/1562 (0.3%) |
| 1 | AY | 0.34 | 0/1152 | 0.58 | 1/1562 (0.1%) |
| 1 | AZ | 0.33 | 0/1149 | 0.49 | 1/1558 (0.1%) |
| 1 | B1 | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | B2 | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | B3 | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | B4 | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | BA | 0.32 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | BB | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | BC | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | BD | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | BE | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | BF | 0.32 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | BG | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | BH | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | BI | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | BJ | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | BK | 0.32 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | BL | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | BM | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | BN | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | BO | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | BP | 0.33 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | BQ | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | BR | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | BS | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | BT | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | BU | 0.33 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | BV | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | BW | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | BX | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | BY | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | BZ | 0.33 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | C1 | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | C2 | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | C3 | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | C4 | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | CA | 0.33 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | CB | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | CC | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | CD | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | CE | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | CF | 0.33 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | CG | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | CH | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | CI | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | CJ | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | CK | 0.33 | 0/1156 | 0.51 | 2/1567 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | CL | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | CM | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | CN | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | CO | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | CP | 0.32 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | CQ | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | CR | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | CS | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | CT | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | CU | 0.33 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| 1 | CV | 0.44 | 0/1156 | 0.72 | 3/1567 (0.2%) |
| 1 | CW | 0.32 | 0/1156 | 0.62 | 1/1567 (0.1%) |
| 1 | CX | 0.31 | 0/1156 | 0.85 | 5/1567 (0.3%) |
| 1 | CY | 0.34 | 0/1156 | 0.58 | 1/1567 (0.1%) |
| 1 | CZ | 0.33 | 0/1156 | 0.51 | 2/1567 (0.1%) |
| All | All | 0.35 | 0/103884 | 0.67 | 204/140832 (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 | A1 | 0 | 1 |
| 1 | AB | 0 | 1 |
| 1 | AG | 0 | 1 |
| 1 | AL | 0 | 1 |
| 1 | AQ | 0 | 1 |
| 1 | AV | 0 | 1 |
| 1 | B1 | 0 | 1 |
| 1 | BB | 0 | 1 |
| 1 | BG | 0 | 1 |
| 1 | BL | 0 | 1 |
| 1 | BQ | 0 | 1 |
| 1 | BV | 0 | 1 |
| 1 | C1 | 0 | 1 |
| 1 | CB | 0 | 1 |
| 1 | CG | 0 | 1 |
| 1 | CL | 0 | 1 |
| 1 | CQ | 0 | 1 |
| 1 | CV | 0 | 1 |
| All | All | 0 | 18 |

There are no bond length outliers.

All (204) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | BD | 149 | SER | CB-CA-C | -14.91 | 81.78 | 110.10 |
| 1 | CD | 149 | SER | CB-CA-C | -14.90 | 81.79 | 110.10 |
| 1 | C3 | 149 | SER | CB-CA-C | -14.89 | 81.80 | 110.10 |
| 1 | BI | 149 | SER | CB-CA-C | -14.89 | 81.81 | 110.10 |
| 1 | CX | 149 | SER | CB-CA-C | -14.89 | 81.81 | 110.10 |
| 1 | AS | 149 | SER | CB-CA-C | -14.88 | 81.82 | 110.10 |
| 1 | AX | 149 | SER | CB-CA-C | -14.88 | 81.83 | 110.10 |
| 1 | CS | 149 | SER | CB-CA-C | -14.88 | 81.83 | 110.10 |
| 1 | AD | 149 | SER | CB-CA-C | -14.88 | 81.83 | 110.10 |
| 1 | B3 | 149 | SER | CB-CA-C | -14.88 | 81.83 | 110.10 |
| 1 | AI | 149 | SER | CB-CA-C | -14.88 | 81.83 | 110.10 |
| 1 | BX | 149 | SER | CB-CA-C | -14.88 | 81.84 | 110.10 |
| 1 | CI | 149 | SER | CB-CA-C | -14.87 | 81.84 | 110.10 |
| 1 | BN | 149 | SER | CB-CA-C | -14.87 | 81.85 | 110.10 |
| 1 | BS | 149 | SER | CB-CA-C | -14.87 | 81.85 | 110.10 |
| 1 | AN | 149 | SER | CB-CA-C | -14.86 | 81.86 | 110.10 |
| 1 | A3 | 149 | SER | CB-CA-C | -14.86 | 81.88 | 110.10 |
| 1 | CN | 149 | SER | CB-CA-C | -14.86 | 81.88 | 110.10 |
| 1 | CX | 150 | LYS | N-CA-CB | -13.59 | 86.14 | 110.60 |
| 1 | BN | 150 | LYS | N-CA-CB | -13.59 | 86.14 | 110.60 |
| 1 | C3 | 150 | LYS | N-CA-CB | -13.59 | 86.14 | 110.60 |
| 1 | BD | 150 | LYS | N-CA-CB | -13.58 | 86.15 | 110.60 |
| 1 | AN | 150 | LYS | N-CA-CB | -13.58 | 86.16 | 110.60 |
| 1 | CS | 150 | LYS | N-CA-CB | -13.58 | 86.16 | 110.60 |
| 1 | BI | 150 | LYS | N-CA-CB | -13.57 | 86.16 | 110.60 |
| 1 | CD | 150 | LYS | N-CA-CB | -13.57 | 86.17 | 110.60 |
| 1 | AI | 150 | LYS | N-CA-CB | -13.57 | 86.18 | 110.60 |
| 1 | AD | 150 | LYS | N-CA-CB | -13.56 | 86.19 | 110.60 |
| 1 | AS | 150 | LYS | N-CA-CB | -13.56 | 86.19 | 110.60 |
| 1 | A3 | 150 | LYS | N-CA-CB | -13.56 | 86.20 | 110.60 |
| 1 | BS | 150 | LYS | N-CA-CB | -13.55 | 86.20 | 110.60 |
| 1 | B3 | 150 | LYS | N-CA-CB | -13.55 | 86.21 | 110.60 |
| 1 | CN | 150 | LYS | N-CA-CB | -13.55 | 86.21 | 110.60 |
| 1 | AX | 150 | LYS | N-CA-CB | -13.54 | 86.22 | 110.60 |
| 1 | CI | 150 | LYS | N-CA-CB | -13.54 | 86.22 | 110.60 |
| 1 | BX | 150 | LYS | N-CA-CB | -13.53 | 86.24 | 110.60 |
| 1 | CI | 109 | PRO | CA-N-CD | -12.47 | 94.04 | 111.50 |
| 1 | B3 | 109 | PRO | CA-N-CD | -12.46 | 94.05 | 111.50 |
| 1 | BX | 109 | PRO | CA-N-CD | -12.46 | 94.06 | 111.50 |
| 1 | A3 | 109 | PRO | CA-N-CD | -12.45 | 94.07 | 111.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | BD | 109 | PRO | CA-N-CD | -12.45 | 94.07 | 111.50 |
| 1 | CS | 109 | PRO | CA-N-CD | -12.45 | 94.07 | 111.50 |
| 1 | AD | 109 | PRO | CA-N-CD | -12.45 | 94.07 | 111.50 |
| 1 | BS | 109 | PRO | CA-N-CD | -12.45 | 94.08 | 111.50 |
| 1 | CD | 109 | PRO | CA-N-CD | -12.44 | 94.08 | 111.50 |
| 1 | AN | 109 | PRO | CA-N-CD | -12.44 | 94.08 | 111.50 |
| 1 | BN | 109 | PRO | CA-N-CD | -12.44 | 94.08 | 111.50 |
| 1 | BI | 109 | PRO | CA-N-CD | -12.44 | 94.08 | 111.50 |
| 1 | AI | 109 | PRO | CA-N-CD | -12.44 | 94.09 | 111.50 |
| 1 | C3 | 109 | PRO | CA-N-CD | -12.43 | 94.10 | 111.50 |
| 1 | AX | 109 | PRO | CA-N-CD | -12.43 | 94.10 | 111.50 |
| 1 | CX | 109 | PRO | CA-N-CD | -12.42 | 94.11 | 111.50 |
| 1 | AS | 109 | PRO | CA-N-CD | -12.42 | 94.11 | 111.50 |
| 1 | CN | 109 | PRO | CA-N-CD | -12.42 | 94.12 | 111.50 |
| 1 | CG | 109 | PRO | CA-N-CD | -11.82 | 94.94 | 111.50 |
| 1 | CV | 109 | PRO | CA-N-CD | -11.81 | 94.96 | 111.50 |
| 1 | AG | 109 | PRO | CA-N-CD | -11.81 | 94.97 | 111.50 |
| 1 | BL | 109 | PRO | CA-N-CD | -11.81 | 94.97 | 111.50 |
| 1 | B1 | 109 | PRO | CA-N-CD | -11.81 | 94.97 | 111.50 |
| 1 | BG | 109 | PRO | CA-N-CD | -11.80 | 94.97 | 111.50 |
| 1 | BB | 109 | PRO | CA-N-CD | -11.80 | 94.98 | 111.50 |
| 1 | BQ | 109 | PRO | CA-N-CD | -11.80 | 94.98 | 111.50 |
| 1 | AB | 109 | PRO | CA-N-CD | -11.79 | 94.99 | 111.50 |
| 1 | AQ | 109 | PRO | CA-N-CD | -11.79 | 95.00 | 111.50 |
| 1 | A1 | 109 | PRO | CA-N-CD | -11.79 | 95.00 | 111.50 |
| 1 | BV | 109 | PRO | CA-N-CD | -11.79 | 95.00 | 111.50 |
| 1 | CQ | 109 | PRO | CA-N-CD | -11.79 | 95.00 | 111.50 |
| 1 | CB | 109 | PRO | CA-N-CD | -11.79 | 95.00 | 111.50 |
| 1 | AV | 109 | PRO | CA-N-CD | -11.77 | 95.02 | 111.50 |
| 1 | CL | 109 | PRO | CA-N-CD | -11.77 | 95.02 | 111.50 |
| 1 | AL | 109 | PRO | CA-N-CD | -11.77 | 95.03 | 111.50 |
| 1 | C1 | 109 | PRO | CA-N-CD | -11.77 | 95.03 | 111.50 |
| 1 | AN | 149 | SER | N-CA-C | 9.93 | 137.81 | 111.00 |
| 1 | A3 | 149 | SER | N-CA-C | 9.91 | 137.76 | 111.00 |
| 1 | AS | 149 | SER | N-CA-C | 9.91 | 137.76 | 111.00 |
| 1 | BS | 149 | SER | N-CA-C | 9.91 | 137.76 | 111.00 |
| 1 | CS | 149 | SER | N-CA-C | 9.91 | 137.76 | 111.00 |
| 1 | BN | 149 | SER | N-CA-C | 9.91 | 137.75 | 111.00 |
| 1 | AD | 149 | SER | N-CA-C | 9.91 | 137.75 | 111.00 |
| 1 | CI | 149 | SER | N-CA-C | 9.91 | 137.75 | 111.00 |
| 1 | B3 | 149 | SER | N-CA-C | 9.91 | 137.75 | 111.00 |
| 1 | AI | 149 | SER | N-CA-C | 9.90 | 137.74 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | BD | 149 | SER | N-CA-C | 9.90 | 137.75 | 111.00 |
| 1 | AX | 149 | SER | N-CA-C | 9.90 | 137.72 | 111.00 |
| 1 | BI | 149 | SER | N-CA-C | 9.90 | 137.72 | 111.00 |
| 1 | CD | 149 | SER | N-CA-C | 9.90 | 137.72 | 111.00 |
| 1 | C3 | 149 | SER | N-CA-C | 9.90 | 137.72 | 111.00 |
| 1 | BX | 149 | SER | N-CA-C | 9.89 | 137.71 | 111.00 |
| 1 | CN | 149 | SER | N-CA-C | 9.89 | 137.71 | 111.00 |
| 1 | CX | 149 | SER | N-CA-C | 9.88 | 137.69 | 111.00 |
| 1 | B2 | 109 | PRO | CA-N-CD | -8.02 | 100.28 | 111.50 |
| 1 | BR | 109 | PRO | CA-N-CD | -8.01 | 100.28 | 111.50 |
| 1 | BM | 109 | PRO | CA-N-CD | -8.00 | 100.30 | 111.50 |
| 1 | BW | 109 | PRO | CA-N-CD | -8.00 | 100.30 | 111.50 |
| 1 | CR | 109 | PRO | CA-N-CD | -8.00 | 100.30 | 111.50 |
| 1 | AH | 109 | PRO | CA-N-CD | -7.99 | 100.31 | 111.50 |
| 1 | BH | 109 | PRO | CA-N-CD | -7.99 | 100.32 | 111.50 |
| 1 | AC | 109 | PRO | CA-N-CD | -7.98 | 100.33 | 111.50 |
| 1 | CW | 109 | PRO | CA-N-CD | -7.98 | 100.33 | 111.50 |
| 1 | C2 | 109 | PRO | CA-N-CD | -7.98 | 100.33 | 111.50 |
| 1 | AM | 109 | PRO | CA-N-CD | -7.97 | 100.34 | 111.50 |
| 1 | AW | 109 | PRO | CA-N-CD | -7.97 | 100.34 | 111.50 |
| 1 | A2 | 109 | PRO | CA-N-CD | -7.97 | 100.35 | 111.50 |
| 1 | BC | 109 | PRO | CA-N-CD | -7.97 | 100.35 | 111.50 |
| 1 | AR | 109 | PRO | CA-N-CD | -7.96 | 100.35 | 111.50 |
| 1 | CH | 109 | PRO | CA-N-CD | -7.96 | 100.36 | 111.50 |
| 1 | CM | 109 | PRO | CA-N-CD | -7.95 | 100.37 | 111.50 |
| 1 | CC | 109 | PRO | CA-N-CD | -7.94 | 100.38 | 111.50 |
| 1 | BS | 148 | LEU | N-CA-C | -5.84 | 95.23 | 111.00 |
| 1 | AX | 148 | LEU | N-CA-C | -5.84 | 95.23 | 111.00 |
| 1 | CS | 148 | LEU | N-CA-C | -5.84 | 95.24 | 111.00 |
| 1 | B3 | 148 | LEU | N-CA-C | -5.83 | 95.25 | 111.00 |
| 1 | CI | 148 | LEU | N-CA-C | -5.83 | 95.25 | 111.00 |
| 1 | A3 | 148 | LEU | N-CA-C | -5.83 | 95.25 | 111.00 |
| 1 | BD | 148 | LEU | N-CA-C | -5.83 | 95.25 | 111.00 |
| 1 | AD | 148 | LEU | N-CA-C | -5.83 | 95.26 | 111.00 |
| 1 | BX | 148 | LEU | N-CA-C | -5.83 | 95.27 | 111.00 |
| 1 | AN | 148 | LEU | N-CA-C | -5.83 | 95.27 | 111.00 |
| 1 | CN | 148 | LEU | N-CA-C | -5.83 | 95.27 | 111.00 |
| 1 | CX | 148 | LEU | N-CA-C | -5.83 | 95.27 | 111.00 |
| 1 | AI | 148 | LEU | N-CA-C | -5.82 | 95.28 | 111.00 |
| 1 | BI | 148 | LEU | N-CA-C | -5.82 | 95.28 | 111.00 |
| 1 | CD | 148 | LEU | N-CA-C | -5.82 | 95.28 | 111.00 |
| 1 | AS | 148 | LEU | N-CA-C | -5.82 | 95.29 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C3 | 148 | LEU | N-CA-C | -5.82 | 95.29 | 111.00 |
| 1 | BN | 148 | LEU | N-CA-C | -5.82 | 95.30 | 111.00 |
| 1 | B1 | 150 | LYS | N-CA-C | -5.70 | 95.61 | 111.00 |
| 1 | CB | 150 | LYS | N-CA-C | -5.70 | 95.61 | 111.00 |
| 1 | CQ | 150 | LYS | N-CA-C | -5.69 | 95.63 | 111.00 |
| 1 | CV | 150 | LYS | N-CA-C | -5.69 | 95.63 | 111.00 |
| 1 | BQ | 150 | LYS | N-CA-C | -5.69 | 95.63 | 111.00 |
| 1 | BV | 150 | LYS | N-CA-C | -5.69 | 95.64 | 111.00 |
| 1 | CG | 150 | LYS | N-CA-C | -5.69 | 95.64 | 111.00 |
| 1 | AQ | 150 | LYS | N-CA-C | -5.69 | 95.64 | 111.00 |
| 1 | AB | 150 | LYS | N-CA-C | -5.69 | 95.64 | 111.00 |
| 1 | AV | 150 | LYS | N-CA-C | -5.69 | 95.65 | 111.00 |
| 1 | BL | 150 | LYS | N-CA-C | -5.69 | 95.65 | 111.00 |
| 1 | CL | 150 | LYS | N-CA-C | -5.69 | 95.65 | 111.00 |
| 1 | A1 | 150 | LYS | N-CA-C | -5.68 | 95.66 | 111.00 |
| 1 | BB | 150 | LYS | N-CA-C | -5.68 | 95.66 | 111.00 |
| 1 | BG | 150 | LYS | N-CA-C | -5.68 | 95.66 | 111.00 |
| 1 | AG | 150 | LYS | N-CA-C | -5.68 | 95.67 | 111.00 |
| 1 | AL | 150 | LYS | N-CA-C | -5.68 | 95.67 | 111.00 |
| 1 | C1 | 150 | LYS | N-CA-C | -5.68 | 95.67 | 111.00 |
| 1 | C4 | 58 | ILE | CB-CA-C | -5.29 | 101.02 | 111.60 |
| 1 | BE | 58 | ILE | CB-CA-C | -5.29 | 101.03 | 111.60 |
| 1 | BY | 58 | ILE | CB-CA-C | -5.28 | 101.03 | 111.60 |
| 1 | BJ | 58 | ILE | CB-CA-C | -5.28 | 101.04 | 111.60 |
| 1 | CO | 58 | ILE | CB-CA-C | -5.28 | 101.04 | 111.60 |
| 1 | AO | 58 | ILE | CB-CA-C | -5.28 | 101.05 | 111.60 |
| 1 | B4 | 58 | ILE | CB-CA-C | -5.27 | 101.06 | 111.60 |
| 1 | CJ | 58 | ILE | CB-CA-C | -5.27 | 101.06 | 111.60 |
| 1 | CY | 58 | ILE | CB-CA-C | -5.27 | 101.06 | 111.60 |
| 1 | AY | 58 | ILE | CB-CA-C | -5.27 | 101.06 | 111.60 |
| 1 | AE | 58 | ILE | CB-CA-C | -5.27 | 101.07 | 111.60 |
| 1 | AT | 58 | ILE | CB-CA-C | -5.27 | 101.06 | 111.60 |
| 1 | A4 | 58 | ILE | CB-CA-C | -5.27 | 101.06 | 111.60 |
| 1 | CT | 58 | ILE | CB-CA-C | -5.27 | 101.07 | 111.60 |
| 1 | AJ | 58 | ILE | CB-CA-C | -5.26 | 101.07 | 111.60 |
| 1 | BT | 58 | ILE | CB-CA-C | -5.26 | 101.08 | 111.60 |
| 1 | CE | 58 | ILE | CB-CA-C | -5.26 | 101.09 | 111.60 |
| 1 | BO | 58 | ILE | CB-CA-C | -5.24 | 101.12 | 111.60 |
| 1 | BL | 107 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 1 | CZ | 107 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 1 | BA | 107 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 1 | BU | 107 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | BZ | 107 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 1 | CA | 107 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 1 | CP | 107 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 1 | BF | 107 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 1 | CU | 107 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 1 | CV | 107 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 1 | BQ | 107 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 1 | B1 | 107 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 1 | CB | 107 | ASP | CB-CG-OD2 | 5.18 | 122.97 | 118.30 |
| 1 | CL | 107 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | BB | 107 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | BP | 107 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 1 | CQ | 107 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 1 | CG | 107 | ASP | CB-CG-OD2 | 5.16 | 122.95 | 118.30 |
| 1 | BK | 107 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 1 | CK | 107 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 1 | BV | 107 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 1 | BK | 58 | ILE | CB-CA-C | -5.15 | 101.29 | 111.60 |
| 1 | C1 | 107 | ASP | CB-CG-OD2 | 5.15 | 122.94 | 118.30 |
| 1 | AP | 58 | ILE | CB-CA-C | -5.15 | 101.31 | 111.60 |
| 1 | CA | 58 | ILE | CB-CA-C | -5.15 | 101.31 | 111.60 |
| 1 | CU | 58 | ILE | CB-CA-C | -5.15 | 101.31 | 111.60 |
| 1 | BA | 58 | ILE | CB-CA-C | -5.15 | 101.31 | 111.60 |
| 1 | AK | 58 | ILE | CB-CA-C | -5.14 | 101.31 | 111.60 |
| 1 | BZ | 58 | ILE | CB-CA-C | -5.14 | 101.31 | 111.60 |
| 1 | CP | 58 | ILE | CB-CA-C | -5.14 | 101.31 | 111.60 |
| 1 | BF | 58 | ILE | CB-CA-C | -5.14 | 101.32 | 111.60 |
| 1 | AA | 58 | ILE | CB-CA-C | -5.14 | 101.32 | 111.60 |
| 1 | BU | 58 | ILE | CB-CA-C | -5.14 | 101.32 | 111.60 |
| 1 | CF | 107 | ASP | CB-CG-OD2 | 5.14 | 122.92 | 118.30 |
| 1 | AF | 58 | ILE | CB-CA-C | -5.14 | 101.32 | 111.60 |
| 1 | AU | 58 | ILE | CB-CA-C | -5.14 | 101.33 | 111.60 |
| 1 | CZ | 58 | ILE | CB-CA-C | -5.14 | 101.33 | 111.60 |
| 1 | CK | 58 | ILE | CB-CA-C | -5.13 | 101.33 | 111.60 |
| 1 | BG | 107 | ASP | CB-CG-OD2 | 5.13 | 122.92 | 118.30 |
| 1 | AZ | 58 | ILE | CB-CA-C | -5.12 | 101.36 | 111.60 |
| 1 | BP | 58 | ILE | CB-CA-C | -5.12 | 101.36 | 111.60 |
| 1 | CF | 58 | ILE | CB-CA-C | -5.11 | 101.38 | 111.60 |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A1 | 99 | VAL | Peptide |
| 1 | AB | 99 | VAL | Peptide |
| 1 | AG | 99 | VAL | Peptide |
| 1 | AL | 99 | VAL | Peptide |
| 1 | AQ | 99 | VAL | Peptide |
| 1 | AV | 99 | VAL | Peptide |
| 1 | B1 | 99 | VAL | Peptide |
| 1 | BB | 99 | VAL | Peptide |
| 1 | BG | 99 | VAL | Peptide |
| 1 | BL | 99 | VAL | Peptide |
| 1 | BQ | 99 | VAL | Peptide |
| 1 | BV | 99 | VAL | Peptide |
| 1 | C1 | 99 | VAL | Peptide |
| 1 | CB | 99 | VAL | Peptide |
| 1 | CG | 99 | VAL | Peptide |
| 1 | CL | 99 | VAL | Peptide |
| 1 | CQ | 99 | VAL | Peptide |
| 1 | CV | 99 | VAL | Peptide |

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A1 | 1129 | 0 | 1143 | 68 | 0 |
| 1 | A2 | 1132 | 0 | 1145 | 77 | 0 |
| 1 | A3 | 1132 | 0 | 1145 | 64 | 0 |
| 1 | A4 | 1132 | 0 | 1145 | 75 | 0 |
| 1 | AA | 1129 | 0 | 1143 | 52 | 0 |
| 1 | AB | 1129 | 0 | 1143 | 73 | 0 |
| 1 | AC | 1132 | 0 | 1145 | 81 | 0 |
| 1 | AD | 1132 | 0 | 1145 | 71 | 0 |
| 1 | AE | 1132 | 0 | 1145 | 82 | 0 |
| 1 | AF | 1129 | 0 | 1143 | 57 | 0 |
| 1 | AG | 1129 | 0 | 1143 | 68 | 2 |
| 1 | AH | 1132 | 0 | 1145 | 76 | 3 |
| 1 | AI | 1132 | 0 | 1145 | 70 | 0 |
| 1 | AJ | 1132 | 0 | 1145 | 81 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AK | 1129 | 0 | 1143 | 55 | 0 |
| 1 | AL | 1129 | 0 | 1143 | 68 | 0 |
| 1 | AM | 1132 | 0 | 1145 | 78 | 0 |
| 1 | AN | 1132 | 0 | 1145 | 64 | 0 |
| 1 | AO | 1132 | 0 | 1145 | 80 | 0 |
| 1 | AP | 1129 | 0 | 1143 | 53 | 0 |
| 1 | AQ | 1129 | 0 | 1143 | 90 | 0 |
| 1 | AR | 1132 | 0 | 1145 | 85 | 0 |
| 1 | AS | 1132 | 0 | 1145 | 65 | 0 |
| 1 | AT | 1132 | 0 | 1145 | 75 | 0 |
| 1 | AU | 1129 | 0 | 1143 | 58 | 0 |
| 1 | AV | 1129 | 0 | 1143 | 67 | 0 |
| 1 | AW | 1132 | 0 | 1145 | 78 | 0 |
| 1 | AX | 1132 | 0 | 1145 | 62 | 0 |
| 1 | AY | 1132 | 0 | 1145 | 75 | 0 |
| 1 | AZ | 1129 | 0 | 1143 | 50 | 0 |
| 1 | B1 | 1136 | 0 | 1149 | 73 | 0 |
| 1 | B2 | 1136 | 0 | 1149 | 78 | 0 |
| 1 | B3 | 1136 | 0 | 1149 | 60 | 0 |
| 1 | B4 | 1136 | 0 | 1149 | 73 | 0 |
| 1 | BA | 1136 | 0 | 1149 | 49 | 0 |
| 1 | BB | 1136 | 0 | 1149 | 81 | 0 |
| 1 | BC | 1136 | 0 | 1149 | 88 | 0 |
| 1 | BD | 1136 | 0 | 1149 | 75 | 0 |
| 1 | BE | 1136 | 0 | 1149 | 74 | 0 |
| 1 | BF | 1136 | 0 | 1149 | 64 | 0 |
| 1 | BG | 1136 | 0 | 1149 | 76 | 0 |
| 1 | BH | 1136 | 0 | 1149 | 80 | 0 |
| 1 | BI | 1136 | 0 | 1149 | 63 | 0 |
| 1 | BJ | 1136 | 0 | 1149 | 78 | 1 |
| 1 | BK | 1136 | 0 | 1149 | 51 | 0 |
| 1 | BL | 1136 | 0 | 1149 | 74 | 3 |
| 1 | BM | 1136 | 0 | 1149 | 78 | 0 |
| 1 | BN | 1136 | 0 | 1149 | 65 | 0 |
| 1 | BO | 1136 | 0 | 1149 | 75 | 0 |
| 1 | BP | 1136 | 0 | 1149 | 49 | 0 |
| 1 | BQ | 1136 | 0 | 1149 | 81 | 0 |
| 1 | BR | 1136 | 0 | 1149 | 90 | 0 |
| 1 | BS | 1136 | 0 | 1149 | 67 | 0 |
| 1 | BT | 1136 | 0 | 1149 | 74 | 0 |
| 1 | BU | 1136 | 0 | 1149 | 77 | 0 |
| 1 | BV | 1136 | 0 | 1149 | 75 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | BW | 1136 | 0 | 1149 | 80 | 0 |
| 1 | BX | 1136 | 0 | 1149 | 63 | 0 |
| 1 | BY | 1136 | 0 | 1149 | 77 | 0 |
| 1 | BZ | 1136 | 0 | 1149 | 49 | 0 |
| 1 | C1 | 1136 | 0 | 1149 | 74 | 0 |
| 1 | C2 | 1136 | 0 | 1149 | 91 | 0 |
| 1 | C3 | 1136 | 0 | 1149 | 76 | 0 |
| 1 | C4 | 1136 | 0 | 1149 | 74 | 1 |
| 1 | CA | 1136 | 0 | 1149 | 55 | 0 |
| 1 | CB | 1136 | 0 | 1149 | 75 | 2 |
| 1 | CC | 1136 | 0 | 1149 | 96 | 2 |
| 1 | CD | 1136 | 0 | 1149 | 75 | 0 |
| 1 | CE | 1136 | 0 | 1149 | 76 | 0 |
| 1 | CF | 1136 | 0 | 1149 | 64 | 0 |
| 1 | CG | 1136 | 0 | 1149 | 84 | 3 |
| 1 | CH | 1136 | 0 | 1149 | 86 | 3 |
| 1 | CI | 1136 | 0 | 1149 | 68 | 0 |
| 1 | CJ | 1136 | 0 | 1149 | 77 | 0 |
| 1 | CK | 1136 | 0 | 1149 | 52 | 0 |
| 1 | CL | 1136 | 0 | 1149 | 74 | 0 |
| 1 | CM | 1136 | 0 | 1149 | 86 | 3 |
| 1 | CN | 1136 | 0 | 1149 | 68 | 0 |
| 1 | CO | 1136 | 0 | 1149 | 80 | 0 |
| 1 | CP | 1136 | 0 | 1149 | 59 | 0 |
| 1 | CQ | 1136 | 0 | 1149 | 81 | 0 |
| 1 | CR | 1136 | 0 | 1149 | 96 | 0 |
| 1 | CS | 1136 | 0 | 1149 | 71 | 0 |
| 1 | CT | 1136 | 0 | 1149 | 83 | 0 |
| 1 | CU | 1136 | 0 | 1149 | 61 | 0 |
| 1 | CV | 1136 | 0 | 1149 | 77 | 0 |
| 1 | CW | 1136 | 0 | 1149 | 92 | 0 |
| 1 | CX | 1136 | 0 | 1149 | 69 | 0 |
| 1 | CY | 1136 | 0 | 1149 | 73 | 1 |
| 1 | CZ | 1136 | 0 | 1149 | 52 | 1 |
| 2 | A1 | 5 | 0 | 0 | 0 | 0 |
| 2 | A2 | 5 | 0 | 0 | 3 | 0 |
| 2 | A3 | 5 | 0 | 0 | 0 | 0 |
| 2 | A4 | 5 | 0 | 0 | 2 | 0 |
| 2 | AA | 5 | 0 | 0 | 1 | 0 |
| 2 | AB | 5 | 0 | 0 | 1 | 0 |
| 2 | AC | 5 | 0 | 0 | 3 | 0 |
| 2 | AD | 5 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | AE | 5 | 0 | 0 | 2 | 0 |
| 2 | AF | 5 | 0 | 0 | 1 | 0 |
| 2 | AG | 5 | 0 | 0 | 1 | 0 |
| 2 | AH | 5 | 0 | 0 | 3 | 0 |
| 2 | AI | 5 | 0 | 0 | 0 | 0 |
| 2 | AJ | 5 | 0 | 0 | 2 | 0 |
| 2 | AK | 5 | 0 | 0 | 1 | 0 |
| 2 | AL | 5 | 0 | 0 | 0 | 0 |
| 2 | AM | 5 | 0 | 0 | 3 | 0 |
| 2 | AN | 5 | 0 | 0 | 0 | 0 |
| 2 | AO | 5 | 0 | 0 | 2 | 0 |
| 2 | AP | 5 | 0 | 0 | 1 | 0 |
| 2 | AQ | 5 | 0 | 0 | 1 | 0 |
| 2 | AR | 5 | 0 | 0 | 3 | 0 |
| 2 | AS | 5 | 0 | 0 | 0 | 0 |
| 2 | AT | 5 | 0 | 0 | 2 | 0 |
| 2 | AU | 5 | 0 | 0 | 1 | 0 |
| 2 | AV | 5 | 0 | 0 | 1 | 0 |
| 2 | AW | 5 | 0 | 0 | 3 | 0 |
| 2 | AX | 5 | 0 | 0 | 0 | 0 |
| 2 | AY | 5 | 0 | 0 | 2 | 0 |
| 2 | AZ | 5 | 0 | 0 | 1 | 0 |
| 2 | B1 | 5 | 0 | 0 | 1 | 0 |
| 2 | B2 | 5 | 0 | 0 | 3 | 0 |
| 2 | B3 | 5 | 0 | 0 | 0 | 0 |
| 2 | B4 | 5 | 0 | 0 | 2 | 0 |
| 2 | BA | 5 | 0 | 0 | 1 | 0 |
| 2 | BB | 5 | 0 | 0 | 1 | 0 |
| 2 | BC | 5 | 0 | 0 | 3 | 0 |
| 2 | BD | 5 | 0 | 0 | 0 | 0 |
| 2 | BE | 5 | 0 | 0 | 2 | 0 |
| 2 | BF | 5 | 0 | 0 | 1 | 0 |
| 2 | BG | 5 | 0 | 0 | 1 | 0 |
| 2 | BH | 5 | 0 | 0 | 3 | 0 |
| 2 | BI | 5 | 0 | 0 | 0 | 0 |
| 2 | BJ | 5 | 0 | 0 | 2 | 0 |
| 2 | BK | 5 | 0 | 0 | 1 | 0 |
| 2 | BL | 5 | 0 | 0 | 1 | 0 |
| 2 | BM | 5 | 0 | 0 | 3 | 0 |
| 2 | BN | 5 | 0 | 0 | 0 | 0 |
| 2 | BO | 5 | 0 | 0 | 2 | 0 |
| 2 | BP | 5 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2 | BQ | 5 | 0 | 0 | 1 | 0 |
| 2 | BR | 5 | 0 | 0 | 3 | 0 |
| 2 | BS | 5 | 0 | 0 | 0 | 0 |
| 2 | BT | 5 | 0 | 0 | 2 | 0 |
| 2 | BU | 5 | 0 | 0 | 1 | 0 |
| 2 | BV | 5 | 0 | 0 | 0 | 0 |
| 2 | BW | 5 | 0 | 0 | 3 | 0 |
| 2 | BX | 5 | 0 | 0 | 0 | 0 |
| 2 | BY | 5 | 0 | 0 | 2 | 0 |
| 2 | BZ | 5 | 0 | 0 | 1 | 0 |
| 2 | C1 | 5 | 0 | 0 | 1 | 0 |
| 2 | C2 | 5 | 0 | 0 | 3 | 0 |
| 2 | C3 | 5 | 0 | 0 | 0 | 0 |
| 2 | C4 | 5 | 0 | 0 | 2 | 0 |
| 2 | CA | 5 | 0 | 0 | 1 | 0 |
| 2 | CB | 5 | 0 | 0 | 1 | 0 |
| 2 | CC | 5 | 0 | 0 | 3 | 0 |
| 2 | CD | 5 | 0 | 0 | 0 | 0 |
| 2 | CE | 5 | 0 | 0 | 2 | 0 |
| 2 | CF | 5 | 0 | 0 | 1 | 0 |
| 2 | CG | 5 | 0 | 0 | 1 | 0 |
| 2 | CH | 5 | 0 | 0 | 3 | 0 |
| 2 | CI | 5 | 0 | 0 | 0 | 0 |
| 2 | CJ | 5 | 0 | 0 | 2 | 0 |
| 2 | CK | 5 | 0 | 0 | 1 | 0 |
| 2 | CL | 5 | 0 | 0 | 1 | 0 |
| 2 | CM | 5 | 0 | 0 | 3 | 0 |
| 2 | CN | 5 | 0 | 0 | 0 | 0 |
| 2 | CO | 5 | 0 | 0 | 2 | 0 |
| 2 | CP | 5 | 0 | 0 | 1 | 0 |
| 2 | CQ | 5 | 0 | 0 | 0 | 0 |
| 2 | CR | 5 | 0 | 0 | 3 | 0 |
| 2 | CS | 5 | 0 | 0 | 0 | 0 |
| 2 | CT | 5 | 0 | 0 | 2 | 0 |
| 2 | CU | 5 | 0 | 0 | 1 | 0 |
| 2 | CV | 5 | 0 | 0 | 0 | 0 |
| 2 | CW | 5 | 0 | 0 | 3 | 0 |
| 2 | CX | 5 | 0 | 0 | 0 | 0 |
| 2 | CY | 5 | 0 | 0 | 2 | 0 |
| 2 | CZ | 5 | 0 | 0 | 1 | 0 |
| All | All | 102534 | 0 | 103266 | 5521 | 13 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 27.

All (5521) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CT:53:PRO:CG | 1:CT:57:GLU:HG3 | 1.49 | 1.43 |
| 1:CJ:53:PRO:CG | 1:CJ:57:GLU:HG3 | 1.49 | 1.42 |
| 1:AE:53:PRO:CG | 1:AE:57:GLU:HG3 | 1.49 | 1.42 |
| 1:B4:53:PRO:CG | 1:B4:57:GLU:HG3 | 1.49 | 1.42 |
| 1:C4:53:PRO:CG | 1:C4:57:GLU:HG3 | 1.49 | 1.42 |
| 1:CY:53:PRO:CG | 1:CY:57:GLU:HG3 | 1.49 | 1.42 |
| 1:A4:53:PRO:CG | 1:A4:57:GLU:HG3 | 1.49 | 1.42 |
| 1:AJ:53:PRO:CG | 1:AJ:57:GLU:HG3 | 1.49 | 1.41 |
| 1:BJ:53:PRO:CG | 1:BJ:57:GLU:HG3 | 1.49 | 1.41 |
| 1:AO:53:PRO:CG | 1:AO:57:GLU:HG3 | 1.49 | 1.41 |
| 1:BO:53:PRO:CG | 1:BO:57:GLU:HG3 | 1.49 | 1.41 |
| 1:AT:53:PRO:CG | 1:AT:57:GLU:HG3 | 1.49 | 1.41 |
| 1:CE:53:PRO:CG | 1:CE:57:GLU:HG3 | 1.49 | 1.40 |
| 1:BY:53:PRO:CG | 1:BY:57:GLU:HG3 | 1.49 | 1.40 |
| 1:CO:53:PRO:CG | 1:CO:57:GLU:HG3 | 1.49 | 1.40 |
| 1:AY:53:PRO:CG | 1:AY:57:GLU:HG3 | 1.49 | 1.39 |
| 1:BT:53:PRO:CG | 1:BT:57:GLU:HG3 | 1.49 | 1.39 |
| 1:BE:53:PRO:CG | 1:BE:57:GLU:HG3 | 1.49 | 1.39 |
| 1:AQ:69:GLY:O | 1:BU:10:THR:HG23 | 1.27 | 1.33 |
| 1:CE:53:PRO:HG2 | 1:CE:57:GLU:CG | 1.59 | 1.32 |
| 1:CO:53:PRO:HG2 | 1:CO:57:GLU:CG | 1.59 | 1.32 |
| 1:CT:53:PRO:HG2 | 1:CT:57:GLU:CG | 1.59 | 1.32 |
| 1:AJ:53:PRO:HG2 | 1:AJ:57:GLU:CG | 1.59 | 1.32 |
| 1:CY:53:PRO:HG2 | 1:CY:57:GLU:CG | 1.59 | 1.32 |
| 1:AO:53:PRO:HG2 | 1:AO:57:GLU:CG | 1.59 | 1.31 |
| 1:AE:53:PRO:HG2 | 1:AE:57:GLU:CG | 1.59 | 1.31 |
| 1:CJ:53:PRO:HG2 | 1:CJ:57:GLU:CG | 1.59 | 1.31 |
| 1:AT:53:PRO:HG2 | 1:AT:57:GLU:CG | 1.59 | 1.31 |
| 1:BO:53:PRO:HG2 | 1:BO:57:GLU:CG | 1.59 | 1.30 |
| 1:C4:53:PRO:HG2 | 1:C4:57:GLU:CG | 1.59 | 1.30 |
| 1:B4:53:PRO:HG2 | 1:B4:57:GLU:CG | 1.59 | 1.30 |
| 1:A4:53:PRO:HG2 | 1:A4:57:GLU:CG | 1.59 | 1.30 |
| 1:BJ:53:PRO:HG2 | 1:BJ:57:GLU:CG | 1.59 | 1.30 |
| 1:BY:53:PRO:HG2 | 1:BY:57:GLU:CG | 1.59 | 1.30 |
| 1:BT:53:PRO:HG2 | 1:BT:57:GLU:CG | 1.59 | 1.29 |
| 1:BE:53:PRO:HG2 | 1:BE:57:GLU:CG | 1.59 | 1.29 |
| 1:AY:53:PRO:HG2 | 1:AY:57:GLU:CG | 1.59 | 1.29 |
| 1:AR:129:THR:HG22 | 1:AR:130:LYS:H | 1.05 | 1.20 |
| 1:BH:129:THR:HG22 | 1:BH:130:LYS:H | 1.05 | 1.20 |
| 1:C2:129:THR:HG22 | 1:C2:130:LYS:H | 1.05 | 1.19 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:AC:129:THR:HG22 | 1:AC:130:LYS:H | 1.05 | 1.17 |
| 1:CR:129:THR:HG22 | 1:CR:130:LYS:H | 1.05 | 1.17 |
| 1:B2:129:THR:HG22 | 1:B2:130:LYS:H | 1.05 | 1.16 |
| 1:BB:107:ASP:OD2 | 1:BC:64:LYS:NZ | 1.76 | 1.15 |
| 1:BM:129:THR:HG22 | 1:BM:130:LYS:H | 1.05 | 1.15 |
| 1:CM:129:THR:HG22 | 1:CM:130:LYS:H | 1.05 | 1.15 |
| 1:CW:129:THR:HG22 | 1:CW:130:LYS:H | 1.05 | 1.15 |
| 1:AM:129:THR:HG22 | 1:AM:130:LYS:H | 1.05 | 1.15 |
| 1:C1:107:ASP:OD2 | 1:C2:64:LYS:NZ | 1.76 | 1.14 |
| 1:AG:104:LEU:HD21 | 1:AH:60:LEU:HA | 1.30 | 1.14 |
| 1:A2:129:THR:HG22 | 1:A2:130:LYS:H | 1.05 | 1.14 |
| 1:BL:104:LEU:HD21 | 1:BM:60:LEU:HA | 1.30 | 1.14 |
| 1:BG:104:LEU:HD21 | 1:BH:60:LEU:HA | 1.30 | 1.13 |
| 1:A1:104:LEU:HD21 | 1:A2:60:LEU:HA | 1.30 | 1.12 |
| 1:CL:104:LEU:HD21 | 1:CM:60:LEU:HA | 1.30 | 1.12 |
| 1:CC:129:THR:HG22 | 1:CC:130:LYS:H | 1.05 | 1.12 |
| 1:AL:104:LEU:HD21 | 1:AM:60:LEU:HA | 1.30 | 1.12 |
| 1:BV:104:LEU:HD21 | 1:BW:60:LEU:HA | 1.30 | 1.12 |
| 1:CV:107:ASP:OD2 | 1:CW:64:LYS:NZ | 1.76 | 1.11 |
| 1:BW:129:THR:HG22 | 1:BW:130:LYS:H | 1.05 | 1.11 |
| 1:BR:129:THR:HG22 | 1:BR:130:LYS:H | 1.05 | 1.11 |
| 1:AW:129:THR:HG22 | 1:AW:130:LYS:H | 1.05 | 1.11 |
| 1:AQ:13:LYS:NZ | 1:BU:43:GLU:HG2 | 1.65 | 1.11 |
| 1:AH:129:THR:HG22 | 1:AH:130:LYS:H | 1.05 | 1.11 |
| 1:CG:104:LEU:HD21 | 1:CH:60:LEU:HA | 1.30 | 1.10 |
| 1:B1:107:ASP:OD2 | 1:B2:64:LYS:NZ | 1.76 | 1.10 |
| 1:CV:104:LEU:HD21 | 1:CW:60:LEU:HA | 1.30 | 1.10 |
| 1:CB:107:ASP:OD2 | 1:CC:64:LYS:NZ | 1.76 | 1.09 |
| 1:AV:104:LEU:HD21 | 1:AW:60:LEU:HA | 1.30 | 1.09 |
| 1:CB:104:LEU:HD21 | 1:CC:60:LEU:HA | 1.30 | 1.09 |
| 1:CH:129:THR:HG22 | 1:CH:130:LYS:H | 1.05 | 1.08 |
| 1:AQ:104:LEU:HD21 | 1:AR:60:LEU:HA | 1.30 | 1.08 |
| 1:B1:104:LEU:HD21 | 1:B2:60:LEU:HA | 1.30 | 1.07 |
| 1:BV:107:ASP:OD2 | 1:BW:64:LYS:NZ | 1.76 | 1.07 |
| 1:CQ:107:ASP:OD2 | 1:CR:64:LYS:NZ | 1.76 | 1.07 |
| 1:BC:129:THR:HG22 | 1:BC:130:LYS:H | 1.05 | 1.07 |
| 1:BG:107:ASP:OD2 | 1:BH:64:LYS:NZ | 1.76 | 1.07 |
| 1:AB:104:LEU:HD21 | 1:AC:60:LEU:HA | 1.30 | 1.07 |
| 1:C1:104:LEU:HD21 | 1:C2:60:LEU:HA | 1.30 | 1.06 |
| 1:BQ:104:LEU:HD21 | 1:BR:60:LEU:HA | 1.30 | 1.06 |
| 1:AE:72:ASP:O | 1:AE:150:LYS:HD3 | 1.56 | 1.06 |
| 1:AO:72:ASP:O | 1:AO:150:LYS:HD3 | 1.56 | 1.05 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BB:104:LEU:HD21 | 1:BC:60:LEU:HA | 1.30 | 1.05 |
| 1:BY:72:ASP:O | 1:BY:150:LYS:HD3 | 1.56 | 1.05 |
| 1:CO:72:ASP:O | 1:CO:150:LYS:HD3 | 1.56 | 1.05 |
| 1:CJ:72:ASP:O | 1:CJ:150:LYS:HD3 | 1.56 | 1.05 |
| 1:CE:72:ASP:O | 1:CE:150:LYS:HD3 | 1.56 | 1.05 |
| 1:BD:11:GLY:HA3 | 1:CM:11:GLY:HA3 | 1.38 | 1.05 |
| 1:CL:107:ASP:OD2 | 1:CM:64:LYS:NZ | 1.76 | 1.05 |
| 1:AJ:72:ASP:O | 1:AJ:150:LYS:HD3 | 1.56 | 1.04 |
| 1:BE:72:ASP:O | 1:BE:150:LYS:HD3 | 1.56 | 1.04 |
| 1:CQ:104:LEU:HD21 | 1:CR:60:LEU:HA | 1.30 | 1.04 |
| 1:BL:107:ASP:OD2 | 1:BM:64:LYS:NZ | 1.76 | 1.04 |
| 1:A4:72:ASP:O | 1:A4:150:LYS:HD3 | 1.56 | 1.04 |
| 1:BO:72:ASP:O | 1:BO:150:LYS:HD3 | 1.56 | 1.04 |
| 1:AT:72:ASP:O | 1:AT:150:LYS:HD3 | 1.56 | 1.04 |
| 1:AY:72:ASP:O | 1:AY:150:LYS:HD3 | 1.56 | 1.03 |
| 1:CY:72:ASP:O | 1:CY:150:LYS:HD3 | 1.56 | 1.03 |
| 1:B4:72:ASP:O | 1:B4:150:LYS:HD3 | 1.56 | 1.03 |
| 1:BJ:72:ASP:O | 1:BJ:150:LYS:HD3 | 1.56 | 1.03 |
| 1:BT:72:ASP:O | 1:BT:150:LYS:HD3 | 1.56 | 1.03 |
| 1:C3:107:ASP:O | 1:C3:107:ASP:OD1 | 1.77 | 1.02 |
| 1:BI:107:ASP:OD1 | 1:BI:107:ASP:O | 1.77 | 1.02 |
| 1:CT:72:ASP:O | 1:CT:150:LYS:HD3 | 1.56 | 1.02 |
| 1:AI:107:ASP:OD1 | 1:AI:107:ASP:O | 1.77 | 1.02 |
| 1:CG:107:ASP:OD2 | 1:CH:64:LYS:NZ | 1.76 | 1.02 |
| 1:BN:107:ASP:O | 1:BN:107:ASP:OD1 | 1.77 | 1.02 |
| 1:C4:72:ASP:O | 1:C4:150:LYS:HD3 | 1.56 | 1.02 |
| 1:AN:107:ASP:OD1 | 1:AN:107:ASP:O | 1.77 | 1.01 |
| 1:CN:107:ASP:O | 1:CN:107:ASP:OD1 | 1.77 | 1.01 |
| 1:CI:107:ASP:O | 1:CI:107:ASP:OD1 | 1.77 | 1.01 |
| 1:A3:107:ASP:OD1 | 1:A3:107:ASP:O | 1.77 | 1.01 |
| 1:AD:107:ASP:OD1 | 1:AD:107:ASP:O | 1.77 | 1.01 |
| 1:BB:107:ASP:HB2 | 1:BB:152:TRP:CZ3 | 1.96 | 1.01 |
| 1:BL:107:ASP:HB2 | 1:BL:152:TRP:CZ3 | 1.96 | 1.01 |
| 1:B1:52:VAL:HG12 | 1:B1:61:ILE:HD12 | 1.43 | 1.01 |
| 1:AX:107:ASP:O | 1:AX:107:ASP:OD1 | 1.77 | 1.01 |
| 1:CQ:107:ASP:HB2 | 1:CQ:152:TRP:CZ3 | 1.96 | 1.01 |
| 1:CX:107:ASP:OD1 | 1:CX:107:ASP:O | 1.77 | 1.01 |
| 1:CV:107:ASP:HB2 | 1:CV:152:TRP:CZ3 | 1.96 | 1.00 |
| 1:CL:107:ASP:HB2 | 1:CL:152:TRP:CZ3 | 1.96 | 1.00 |
| 1:BV:52:VAL:HG12 | 1:BV:61:ILE:HD12 | 1.43 | 1.00 |
| 1:CD:107:ASP:O | 1:CD:107:ASP:OD1 | 1.77 | 1.00 |
| 1:AQ:52:VAL:HG12 | 1:AQ:61:ILE:HD12 | 1.43 | 1.00 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:CD1 | 1.91 | 1.00 |
| 1:CB:107:ASP:HB2 | 1:CB:152:TRP:CZ3 | 1.96 | 1.00 |
| 1:BV:107:ASP:HB2 | 1:BV:152:TRP:CZ3 | 1.96 | 1.00 |
| 1:CS:107:ASP:OD1 | 1:CS:107:ASP:O | 1.77 | 1.00 |
| 1:B1:107:ASP:HB2 | 1:B1:152:TRP:CZ3 | 1.96 | 1.00 |
| 1:BD:107:ASP:OD1 | 1:BD:107:ASP:O | 1.77 | 1.00 |
| 1:CB:52:VAL:HG12 | 1:CB:61:ILE:HD12 | 1.43 | 1.00 |
| 1:AS:107:ASP:O | 1:AS:107:ASP:OD1 | 1.77 | 1.00 |
| 1:AG:52:VAL:HG12 | 1:AG:61:ILE:HD12 | 1.43 | 1.00 |
| 1:BX:107:ASP:O | 1:BX:107:ASP:OD1 | 1.77 | 1.00 |
| 1:BL:52:VAL:HG12 | 1:BL:61:ILE:HD12 | 1.43 | 1.00 |
| 1:BQ:107:ASP:OD2 | 1:BR:64:LYS:NZ | 1.76 | 1.00 |
| 1:BG:107:ASP:HB2 | 1:BG:152:TRP:CZ3 | 1.96 | 0.99 |
| 1:B3:107:ASP:OD1 | 1:B3:107:ASP:O | 1.77 | 0.99 |
| 1:AQ:69:GLY:O | 1:BU:10:THR:CG2 | 2.08 | 0.99 |
| 1:BB:52:VAL:HG12 | 1:BB:61:ILE:HD12 | 1.43 | 0.99 |
| 1:BQ:107:ASP:HB2 | 1:BQ:152:TRP:CZ3 | 1.96 | 0.99 |
| 1:BS:107:ASP:O | 1:BS:107:ASP:OD1 | 1.77 | 0.99 |
| 1:AL:52:VAL:HG12 | 1:AL:61:ILE:HD12 | 1.43 | 0.99 |
| 1:C1:107:ASP:HB2 | 1:C1:152:TRP:CZ3 | 1.96 | 0.99 |
| 1:CG:107:ASP:HB2 | 1:CG:152:TRP:CZ3 | 1.96 | 0.99 |
| 1:CQ:52:VAL:HG12 | 1:CQ:61:ILE:HD12 | 1.43 | 0.99 |
| 1:A1:52:VAL:HG12 | 1:A1:61:ILE:HD12 | 1.43 | 0.98 |
| 1:CL:52:VAL:HG12 | 1:CL:61:ILE:HD12 | 1.43 | 0.98 |
| 1:C1:52:VAL:HG12 | 1:C1:61:ILE:HD12 | 1.43 | 0.98 |
| 1:CV:52:VAL:HG12 | 1:CV:61:ILE:HD12 | 1.43 | 0.98 |
| 1:CG:52:VAL:HG12 | 1:CG:61:ILE:HD12 | 1.43 | 0.97 |
| 1:BG:52:VAL:HG12 | 1:BG:61:ILE:HD12 | 1.43 | 0.97 |
| 1:AB:52:VAL:HG12 | 1:AB:61:ILE:HD12 | 1.43 | 0.97 |
| 1:BQ:52:VAL:HG12 | 1:BQ:61:ILE:HD12 | 1.43 | 0.97 |
| 1:AV:52:VAL:HG12 | 1:AV:61:ILE:HD12 | 1.43 | 0.97 |
| 1:BB:96:ALA:C | 1:BB:100:ALA:HB2 | 1.86 | 0.97 |
| 1:AV:96:ALA:C | 1:AV:100:ALA:HB2 | 1.86 | 0.96 |
| 1:CB:96:ALA:C | 1:CB:100:ALA:HB2 | 1.86 | 0.96 |
| 1:AG:96:ALA:C | 1:AG:100:ALA:HB2 | 1.86 | 0.96 |
| 1:BL:96:ALA:C | 1:BL:100:ALA:HB2 | 1.86 | 0.96 |
| 1:AL:96:ALA:C | 1:AL:100:ALA:HB2 | 1.86 | 0.96 |
| 1:C1:96:ALA:C | 1:C1:100:ALA:HB2 | 1.86 | 0.96 |
| 1:AQ:96:ALA:C | 1:AQ:100:ALA:HB2 | 1.86 | 0.96 |
| 1:AB:96:ALA:C | 1:AB:100:ALA:HB2 | 1.86 | 0.96 |
| 1:B1:96:ALA:C | 1:B1:100:ALA:HB2 | 1.86 | 0.96 |
| 1:CL:96:ALA:C | 1:CL:100:ALA:HB2 | 1.86 | 0.95 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:CQ:96:ALA:C | 1:CQ:100:ALA:HB2 | 1.86 | 0.95 |
| 1:BV:96:ALA:C | 1:BV:100:ALA:HB2 | 1.86 | 0.95 |
| 1:BQ:96:ALA:C | 1:BQ:100:ALA:HB2 | 1.86 | 0.95 |
| 1:BG:96:ALA:C | 1:BG:100:ALA:HB2 | 1.86 | 0.95 |
| 1:CG:96:ALA:C | 1:CG:100:ALA:HB2 | 1.86 | 0.95 |
| 1:CV:96:ALA:C | 1:CV:100:ALA:HB2 | 1.86 | 0.95 |
| 1:AX:52:VAL:HG12 | 1:AX:61:ILE:HD12 | 1.49 | 0.94 |
| 1:A1:96:ALA:C | 1:A1:100:ALA:HB2 | 1.86 | 0.94 |
| 1:AD:52:VAL:HG12 | 1:AD:61:ILE:HD12 | 1.49 | 0.94 |
| 1:AN:52:VAL:HG12 | 1:AN:61:ILE:HD12 | 1.49 | 0.94 |
| 1:B3:52:VAL:HG12 | 1:B3:61:ILE:HD12 | 1.49 | 0.94 |
| 1:CI:52:VAL:HG12 | 1:CI:61:ILE:HD12 | 1.49 | 0.94 |
| 1:BS:52:VAL:HG12 | 1:BS:61:ILE:HD12 | 1.49 | 0.94 |
| 1:BJ:52:VAL:HG12 | 1:BJ:61:ILE:HD12 | 1.50 | 0.94 |
| 1:BD:52:VAL:HG12 | 1:BD:61:ILE:HD12 | 1.49 | 0.94 |
| 1:BX:52:VAL:HG12 | 1:BX:61:ILE:HD12 | 1.49 | 0.93 |
| 1:BO:52:VAL:HG12 | 1:BO:61:ILE:HD12 | 1.50 | 0.93 |
| 1:C3:52:VAL:HG12 | 1:C3:61:ILE:HD12 | 1.49 | 0.93 |
| 1:AE:52:VAL:HG12 | 1:AE:61:ILE:HD12 | 1.51 | 0.93 |
| 1:AJ:52:VAL:HG12 | 1:AJ:61:ILE:HD12 | 1.51 | 0.93 |
| 1:AY:52:VAL:HG12 | 1:AY:61:ILE:HD12 | 1.50 | 0.93 |
| 1:BY:52:VAL:HG12 | 1:BY:61:ILE:HD12 | 1.51 | 0.93 |
| 1:C4:52:VAL:HG12 | 1:C4:61:ILE:HD12 | 1.51 | 0.93 |
| 1:B4:52:VAL:HG12 | 1:B4:61:ILE:HD12 | 1.51 | 0.93 |
| 1:AQ:13:LYS:HZ3 | 1:BU:43:GLU:HG2 | 1.19 | 0.93 |
| 1:AS:52:VAL:HG12 | 1:AS:61:ILE:HD12 | 1.49 | 0.93 |
| 1:A4:52:VAL:HG12 | 1:A4:61:ILE:HD12 | 1.51 | 0.93 |
| 1:AI:52:VAL:HG12 | 1:AI:61:ILE:HD12 | 1.49 | 0.93 |
| 1:AC:52:VAL:HG12 | 1:AC:61:ILE:HD12 | 1.51 | 0.93 |
| 1:CM:52:VAL:HG12 | 1:CM:61:ILE:HD12 | 1.51 | 0.93 |
| 1:A3:52:VAL:HG12 | 1:A3:61:ILE:HD12 | 1.50 | 0.93 |
| 1:CE:52:VAL:HG12 | 1:CE:61:ILE:HD12 | 1.51 | 0.93 |
| 1:BT:52:VAL:HG12 | 1:BT:61:ILE:HD12 | 1.50 | 0.93 |
| 1:BH:52:VAL:HG12 | 1:BH:61:ILE:HD12 | 1.51 | 0.93 |
| 1:BC:52:VAL:HG12 | 1:BC:61:ILE:HD12 | 1.51 | 0.92 |
| 1:AT:52:VAL:HG12 | 1:AT:61:ILE:HD12 | 1.51 | 0.92 |
| 1:BN:52:VAL:HG12 | 1:BN:61:ILE:HD12 | 1.49 | 0.92 |
| 1:CN:52:VAL:HG12 | 1:CN:61:ILE:HD12 | 1.49 | 0.92 |
| 1:AO:52:VAL:HG12 | 1:AO:61:ILE:HD12 | 1.51 | 0.92 |
| 1:AH:52:VAL:HG12 | 1:AH:61:ILE:HD12 | 1.51 | 0.92 |
| 1:CR:52:VAL:HG12 | 1:CR:61:ILE:HD12 | 1.51 | 0.92 |
| 1:A2:52:VAL:HG12 | 1:A2:61:ILE:HD12 | 1.51 | 0.92 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:AM:52:VAL:HG12 | 1:AM:61:ILE:HD12 | 1.51 | 0.92 |
| 1:BE:52:VAL:HG12 | 1:BE:61:ILE:HD12 | 1.50 | 0.92 |
| 1:BR:52:VAL:HG12 | 1:BR:61:ILE:HD12 | 1.51 | 0.92 |
| 1:CC:52:VAL:HG12 | 1:CC:61:ILE:HD12 | 1.51 | 0.92 |
| 1:AW:52:VAL:HG12 | 1:AW:61:ILE:HD12 | 1.52 | 0.92 |
| 1:CS:52:VAL:HG12 | 1:CS:61:ILE:HD12 | 1.49 | 0.92 |
| 1:CJ:52:VAL:HG12 | 1:CJ:61:ILE:HD12 | 1.51 | 0.91 |
| 1:BI:52:VAL:HG12 | 1:BI:61:ILE:HD12 | 1.49 | 0.91 |
| 1:CH:52:VAL:HG12 | 1:CH:61:ILE:HD12 | 1.51 | 0.91 |
| 1:CX:52:VAL:HG12 | 1:CX:61:ILE:HD12 | 1.49 | 0.91 |
| 1:B2:52:VAL:HG12 | 1:B2:61:ILE:HD12 | 1.51 | 0.91 |
| 1:BM:52:VAL:HG12 | 1:BM:61:ILE:HD12 | 1.51 | 0.91 |
| 1:CD:52:VAL:HG12 | 1:CD:61:ILE:HD12 | 1.49 | 0.91 |
| 1:BW:52:VAL:HG12 | 1:BW:61:ILE:HD12 | 1.51 | 0.90 |
| 1:CO:52:VAL:HG12 | 1:CO:61:ILE:HD12 | 1.50 | 0.90 |
| 1:AR:52:VAL:HG12 | 1:AR:61:ILE:HD12 | 1.51 | 0.90 |
| 1:C2:52:VAL:HG12 | 1:C2:61:ILE:HD12 | 1.52 | 0.90 |
| 1:CY:52:VAL:HG12 | 1:CY:61:ILE:HD12 | 1.51 | 0.90 |
| 1:CW:52:VAL:HG12 | 1:CW:61:ILE:HD12 | 1.51 | 0.90 |
| 1:BP:52:VAL:HG12 | 1:BP:61:ILE:HD12 | 1.54 | 0.90 |
| 1:AP:52:VAL:HG12 | 1:AP:61:ILE:HD12 | 1.54 | 0.90 |
| 1:CK:52:VAL:HG12 | 1:CK:61:ILE:HD12 | 1.54 | 0.89 |
| 1:CT:52:VAL:HG12 | 1:CT:61:ILE:HD12 | 1.51 | 0.89 |
| 1:AU:52:VAL:HG12 | 1:AU:61:ILE:HD12 | 1.54 | 0.89 |
| 1:AF:52:VAL:HG12 | 1:AF:61:ILE:HD12 | 1.54 | 0.89 |
| 1:CU:52:VAL:HG12 | 1:CU:61:ILE:HD12 | 1.54 | 0.89 |
| 1:BO:52:VAL:HB | 1:BO:53:PRO:HD2 | 1.55 | 0.89 |
| 1:CT:52:VAL:HB | 1:CT:53:PRO:HD2 | 1.55 | 0.89 |
| 1:B4:52:VAL:HB | 1:B4:53:PRO:HD2 | 1.55 | 0.89 |
| 1:CJ:52:VAL:HB | 1:CJ:53:PRO:HD2 | 1.55 | 0.88 |
| 1:CR:129:THR:HG22 | 1:CR:130:LYS:N | 1.88 | 0.88 |
| 1:AK:52:VAL:HG12 | 1:AK:61:ILE:HD12 | 1.54 | 0.88 |
| 1:BY:52:VAL:HB | 1:BY:53:PRO:HD2 | 1.55 | 0.88 |
| 1:BT:52:VAL:HB | 1:BT:53:PRO:HD2 | 1.55 | 0.88 |
| 1:CH:129:THR:HG22 | 1:CH:130:LYS:N | 1.88 | 0.88 |
| 1:BK:52:VAL:HG12 | 1:BK:61:ILE:HD12 | 1.54 | 0.88 |
| 1:BF:52:VAL:HG12 | 1:BF:61:ILE:HD12 | 1.54 | 0.88 |
| 1:AJ:52:VAL:HB | 1:AJ:53:PRO:HD2 | 1.55 | 0.88 |
| 1:AY:52:VAL:HB | 1:AY:53:PRO:HD2 | 1.55 | 0.88 |
| 1:BW:129:THR:HG22 | 1:BW:130:LYS:N | 1.89 | 0.88 |
| 1:BA:52:VAL:HG12 | 1:BA:61:ILE:HD12 | 1.54 | 0.88 |
| 1:A4:52:VAL:HB | 1:A4:53:PRO:HD2 | 1.55 | 0.88 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:AO:52:VAL:HB | 1:AO:53:PRO:HD2 | 1.55 | 0.88 |
| 1:BE:52:VAL:HB | 1:BE:53:PRO:HD2 | 1.55 | 0.88 |
| 1:AR:129:THR:HG22 | 1:AR:130:LYS:N | 1.88 | 0.88 |
| 1:CF:52:VAL:HG12 | 1:CF:61:ILE:HD12 | 1.54 | 0.88 |
| 1:CC:129:THR:HG22 | 1:CC:130:LYS:N | 1.88 | 0.88 |
| 1:CA:52:VAL:HG12 | 1:CA:61:ILE:HD12 | 1.54 | 0.88 |
| 1:AT:52:VAL:HB | 1:AT:53:PRO:HD2 | 1.55 | 0.87 |
| 1:C4:52:VAL:HB | 1:C4:53:PRO:HD2 | 1.55 | 0.87 |
| 1:BH:129:THR:HG22 | 1:BH:130:LYS:N | 1.89 | 0.87 |
| 1:CM:129:THR:HG22 | 1:CM:130:LYS:N | 1.88 | 0.87 |
| 1:BR:129:THR:HG22 | 1:BR:130:LYS:N | 1.89 | 0.87 |
| 1:CP:52:VAL:HG12 | 1:CP:61:ILE:HD12 | 1.54 | 0.87 |
| 1:BZ:52:VAL:HG12 | 1:BZ:61:ILE:HD12 | 1.54 | 0.87 |
| 1:B2:129:THR:HG22 | 1:B2:130:LYS:N | 1.88 | 0.87 |
| 1:AH:129:THR:HG22 | 1:AH:130:LYS:N | 1.89 | 0.87 |
| 1:CO:52:VAL:HB | 1:CO:53:PRO:HD2 | 1.55 | 0.87 |
| 1:AW:129:THR:HG22 | 1:AW:130:LYS:N | 1.88 | 0.87 |
| 1:CE:52:VAL:HB | 1:CE:53:PRO:HD2 | 1.55 | 0.87 |
| 1:C2:129:THR:HG22 | 1:C2:130:LYS:N | 1.88 | 0.87 |
| 1:AC:129:THR:HG22 | 1:AC:130:LYS:N | 1.88 | 0.86 |
| 1:BC:129:THR:HG21 | 1:BS:120:ILE:CD1 | 2.05 | 0.86 |
| 1:A2:129:THR:HG22 | 1:A2:130:LYS:N | 1.88 | 0.86 |
| 1:AW:129:THR:CG2 | 1:AW:130:LYS:H | 1.89 | 0.86 |
| 1:BU:52:VAL:HG12 | 1:BU:61:ILE:HD12 | 1.54 | 0.86 |
| 1:AE:52:VAL:HB | 1:AE:53:PRO:HD2 | 1.55 | 0.86 |
| 1:CY:52:VAL:HB | 1:CY:53:PRO:HD2 | 1.55 | 0.86 |
| 1:BJ:52:VAL:HB | 1:BJ:53:PRO:HD2 | 1.55 | 0.86 |
| 1:AA:52:VAL:HG12 | 1:AA:61:ILE:HD12 | 1.54 | 0.86 |
| 1:BM:129:THR:HG22 | 1:BM:130:LYS:N | 1.88 | 0.86 |
| 1:AM:129:THR:HG22 | 1:AM:130:LYS:N | 1.88 | 0.85 |
| 1:CZ:52:VAL:HG12 | 1:CZ:61:ILE:HD12 | 1.54 | 0.85 |
| 1:AZ:52:VAL:HG12 | 1:AZ:61:ILE:HD12 | 1.54 | 0.85 |
| 1:AQ:13:LYS:NZ | 1:BU:43:GLU:CG | 2.39 | 0.85 |
| 1:C1:55:ALA:HB1 | 1:C1:95:VAL:HG21 | 1.59 | 0.85 |
| 1:CQ:55:ALA:HB1 | 1:CQ:95:VAL:HG21 | 1.59 | 0.85 |
| 1:CV:55:ALA:HB1 | 1:CV:95:VAL:HG21 | 1.59 | 0.85 |
| 1:BC:129:THR:CG2 | 1:BC:130:LYS:H | 1.89 | 0.85 |
| 1:C2:129:THR:CG2 | 1:C2:130:LYS:H | 1.89 | 0.85 |
| 1:AM:129:THR:CG2 | 1:AM:130:LYS:H | 1.89 | 0.85 |
| 1:BG:55:ALA:HB1 | 1:BG:95:VAL:HG21 | 1.59 | 0.85 |
| 1:A1:55:ALA:HB1 | 1:A1:95:VAL:HG21 | 1.59 | 0.85 |
| 1:AB:55:ALA:HB1 | 1:AB:95:VAL:HG21 | 1.59 | 0.85 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:B1:55:ALA:HB1 | 1:B1:95:VAL:HG21 | 1.59 | 0.84 |
| 1:BC:129:THR:HG22 | 1:BC:130:LYS:N | 1.88 | 0.84 |
| 1:BB:55:ALA:HB1 | 1:BB:95:VAL:HG21 | 1.59 | 0.84 |
| 1:CB:55:ALA:HB1 | 1:CB:95:VAL:HG21 | 1.59 | 0.84 |
| 1:AG:55:ALA:HB1 | 1:AG:95:VAL:HG21 | 1.59 | 0.84 |
| 1:CM:129:THR:CG2 | 1:CM:130:LYS:H | 1.89 | 0.84 |
| 1:CH:129:THR:CG2 | 1:CH:130:LYS:H | 1.89 | 0.84 |
| 1:BT:124:ILE:O | 1:BT:129:THR:OG1 | 1.96 | 0.84 |
| 1:BV:55:ALA:HB1 | 1:BV:95:VAL:HG21 | 1.59 | 0.84 |
| 1:AO:124:ILE:O | 1:AO:129:THR:OG1 | 1.96 | 0.84 |
| 1:BO:124:ILE:O | 1:BO:129:THR:OG1 | 1.96 | 0.84 |
| 1:CT:124:ILE:O | 1:CT:129:THR:OG1 | 1.96 | 0.83 |
| 1:AY:124:ILE:O | 1:AY:129:THR:OG1 | 1.96 | 0.83 |
| 1:BY:124:ILE:O | 1:BY:129:THR:OG1 | 1.96 | 0.83 |
| 1:A4:124:ILE:O | 1:A4:129:THR:OG1 | 1.96 | 0.83 |
| 1:AV:55:ALA:HB1 | 1:AV:95:VAL:HG21 | 1.59 | 0.83 |
| 1:AJ:108:ILE:HG12 | 1:AJ:150:LYS:HE3 | 1.61 | 0.83 |
| 1:CO:124:ILE:O | 1:CO:129:THR:OG1 | 1.96 | 0.83 |
| 1:CO:108:ILE:HG12 | 1:CO:150:LYS:HE3 | 1.61 | 0.83 |
| 1:BT:108:ILE:HG12 | 1:BT:150:LYS:HE3 | 1.61 | 0.83 |
| 1:CY:124:ILE:O | 1:CY:129:THR:OG1 | 1.96 | 0.83 |
| 1:B2:129:THR:CG2 | 1:B2:130:LYS:H | 1.89 | 0.83 |
| 1:BL:55:ALA:HB1 | 1:BL:95:VAL:HG21 | 1.59 | 0.83 |
| 1:AJ:124:ILE:O | 1:AJ:129:THR:OG1 | 1.96 | 0.83 |
| 1:BE:124:ILE:O | 1:BE:129:THR:OG1 | 1.96 | 0.83 |
| 1:BO:108:ILE:HG12 | 1:BO:150:LYS:HE3 | 1.61 | 0.83 |
| 1:BQ:55:ALA:HB1 | 1:BQ:95:VAL:HG21 | 1.59 | 0.83 |
| 1:BD:11:GLY:HA3 | 1:CM:11:GLY:CA | 2.09 | 0.83 |
| 1:AT:108:ILE:HG12 | 1:AT:150:LYS:HE3 | 1.61 | 0.83 |
| 1:AQ:55:ALA:HB1 | 1:AQ:95:VAL:HG21 | 1.59 | 0.83 |
| 1:CL:55:ALA:HB1 | 1:CL:95:VAL:HG21 | 1.59 | 0.83 |
| 1:CG:55:ALA:HB1 | 1:CG:95:VAL:HG21 | 1.59 | 0.83 |
| 1:BJ:124:ILE:O | 1:BJ:129:THR:OG1 | 1.96 | 0.83 |
| 1:CR:129:THR:CG2 | 1:CR:130:LYS:H | 1.89 | 0.82 |
| 1:AE:108:ILE:HG12 | 1:AE:150:LYS:HE3 | 1.61 | 0.82 |
| 1:BE:108:ILE:HG12 | 1:BE:150:LYS:HE3 | 1.61 | 0.82 |
| 1:AO:108:ILE:HG12 | 1:AO:150:LYS:HE3 | 1.61 | 0.82 |
| 1:CY:108:ILE:HG12 | 1:CY:150:LYS:HE3 | 1.61 | 0.82 |
| 1:CE:124:ILE:O | 1:CE:129:THR:OG1 | 1.96 | 0.82 |
| 1:BJ:108:ILE:HG12 | 1:BJ:150:LYS:HE3 | 1.61 | 0.82 |
| 1:AL:55:ALA:HB1 | 1:AL:95:VAL:HG21 | 1.59 | 0.82 |
| 1:AE:124:ILE:O | 1:AE:129:THR:OG1 | 1.96 | 0.82 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AY:108:ILE:HG12 | 1:AY:150:LYS:HE3 | 1.61 | 0.82 |
| 1:B4:108:ILE:HG12 | 1:B4:150:LYS:HE3 | 1.61 | 0.82 |
| 1:CJ:124:ILE:O | 1:CJ:129:THR:OG1 | 1.96 | 0.82 |
| 1:CW:129:THR:HG22 | 1:CW:130:LYS:N | 1.88 | 0.82 |
| 1:B4:124:ILE:O | 1:B4:129:THR:OG1 | 1.96 | 0.82 |
| 1:CJ:108:ILE:HG12 | 1:CJ:150:LYS:HE3 | 1.61 | 0.82 |
| 1:C4:124:ILE:O | 1:C4:129:THR:OG1 | 1.96 | 0.82 |
| 1:AT:124:ILE:O | 1:AT:129:THR:OG1 | 1.96 | 0.82 |
| 1:C4:108:ILE:HG12 | 1:C4:150:LYS:HE3 | 1.61 | 0.81 |
| 1:CE:108:ILE:HG12 | 1:CE:150:LYS:HE3 | 1.61 | 0.81 |
| 1:A4:108:ILE:HG12 | 1:A4:150:LYS:HE3 | 1.61 | 0.81 |
| 1:AR:129:THR:CG2 | 1:AR:130:LYS:H | 1.89 | 0.81 |
| 1:AM:38:LYS:HZ2 | 1:AM:44:GLU:HG3 | 1.45 | 0.81 |
| 1:BY:108:ILE:HG12 | 1:BY:150:LYS:HE3 | 1.61 | 0.81 |
| 1:B2:7:LEU:HD11 | 1:B2:140:VAL:HG13 | 1.63 | 0.81 |
| 1:AQ:13:LYS:HZ3 | 1:BU:43:GLU:CG | 1.94 | 0.81 |
| 1:AR:7:LEU:HD11 | 1:AR:140:VAL:HG13 | 1.63 | 0.81 |
| 1:CT:108:ILE:HG12 | 1:CT:150:LYS:HE3 | 1.61 | 0.81 |
| 1:BR:7:LEU:HD11 | 1:BR:140:VAL:HG13 | 1.63 | 0.81 |
| 1:BM:7:LEU:HD11 | 1:BM:140:VAL:HG13 | 1.63 | 0.81 |
| 1:CW:7:LEU:HD11 | 1:CW:140:VAL:HG13 | 1.63 | 0.80 |
| 1:BM:129:THR:CG2 | 1:BM:130:LYS:H | 1.89 | 0.80 |
| 1:AQ:13:LYS:HZ1 | 1:BU:43:GLU:CB | 1.94 | 0.80 |
| 1:BD:11:GLY:CA | 1:CM:11:GLY:HA3 | 2.11 | 0.80 |
| 1:B3:18:VAL:HG12 | 1:B3:77:LEU:HB2 | 1.64 | 0.80 |
| 1:BN:18:VAL:HG12 | 1:BN:77:LEU:HB2 | 1.63 | 0.80 |
| 1:AD:18:VAL:HG12 | 1:AD:77:LEU:HB2 | 1.64 | 0.80 |
| 1:CD:28:LYS:NZ | 1:CF:28:LYS:HZ2 | 1.79 | 0.80 |
| 1:CC:7:LEU:HD11 | 1:CC:140:VAL:HG13 | 1.63 | 0.80 |
| 1:AH:7:LEU:HD11 | 1:AH:140:VAL:HG13 | 1.63 | 0.80 |
| 1:AS:18:VAL:HG12 | 1:AS:77:LEU:HB2 | 1.64 | 0.80 |
| 1:AX:18:VAL:HG12 | 1:AX:77:LEU:HB2 | 1.63 | 0.80 |
| 1:BD:18:VAL:HG12 | 1:BD:77:LEU:HB2 | 1.64 | 0.80 |
| 1:AL:7:LEU:HD11 | 1:AL:140:VAL:HG13 | 1.64 | 0.80 |
| 1:AB:7:LEU:HD11 | 1:AB:140:VAL:HG13 | 1.64 | 0.80 |
| 1:AC:7:LEU:HD11 | 1:AC:140:VAL:HG13 | 1.63 | 0.80 |
| 1:CM:7:LEU:HD11 | 1:CM:140:VAL:HG13 | 1.63 | 0.80 |
| 1:CR:7:LEU:HD11 | 1:CR:140:VAL:HG13 | 1.63 | 0.80 |
| 1:A2:7:LEU:HD11 | 1:A2:140:VAL:HG13 | 1.63 | 0.80 |
| 1:CB:7:LEU:HD11 | 1:CB:140:VAL:HG13 | 1.64 | 0.80 |
| 1:CW:129:THR:CG2 | 1:CW:130:LYS:H | 1.89 | 0.80 |
| 1:CG:7:LEU:HD11 | 1:CG:140:VAL:HG13 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CW:38:LYS:HZ2 | 1:CW:44:GLU:HG3 | 1.47 | 0.79 |
| 1:AO:72:ASP:C | 1:AO:150:LYS:HD3 | 2.03 | 0.79 |
| 1:CQ:7:LEU:HD11 | 1:CQ:140:VAL:HG13 | 1.64 | 0.79 |
| 1:BX:18:VAL:HG12 | 1:BX:77:LEU:HB2 | 1.64 | 0.79 |
| 1:AW:7:LEU:HD11 | 1:AW:140:VAL:HG13 | 1.63 | 0.79 |
| 1:AT:72:ASP:C | 1:AT:150:LYS:HD3 | 2.03 | 0.79 |
| 1:AY:72:ASP:C | 1:AY:150:LYS:HD3 | 2.03 | 0.79 |
| 1:BB:7:LEU:HD11 | 1:BB:140:VAL:HG13 | 1.64 | 0.79 |
| 1:CL:7:LEU:HD11 | 1:CL:140:VAL:HG13 | 1.64 | 0.79 |
| 1:BI:18:VAL:HG12 | 1:BI:77:LEU:HB2 | 1.64 | 0.79 |
| 1:CE:72:ASP:C | 1:CE:150:LYS:HD3 | 2.03 | 0.79 |
| 1:BH:7:LEU:HD11 | 1:BH:140:VAL:HG13 | 1.63 | 0.79 |
| 1:BW:7:LEU:HD11 | 1:BW:140:VAL:HG13 | 1.63 | 0.79 |
| 1:CI:18:VAL:HG12 | 1:CI:77:LEU:HB2 | 1.63 | 0.79 |
| 1:BO:72:ASP:C | 1:BO:150:LYS:HD3 | 2.03 | 0.79 |
| 1:CJ:72:ASP:C | 1:CJ:150:LYS:HD3 | 2.03 | 0.79 |
| 1:CX:18:VAL:HG12 | 1:CX:77:LEU:HB2 | 1.64 | 0.79 |
| 1:BH:129:THR:CG2 | 1:BH:130:LYS:H | 1.89 | 0.79 |
| 1:AC:129:THR:CG2 | 1:AC:130:LYS:H | 1.89 | 0.79 |
| 1:BD:120:ILE:CD1 | 1:BR:129:THR:HG21 | 2.12 | 0.79 |
| 1:CW:34:LEU:HD22 | 1:CW:38:LYS:HE2 | 1.65 | 0.79 |
| 1:CS:18:VAL:HG12 | 1:CS:77:LEU:HB2 | 1.63 | 0.79 |
| 1:C2:7:LEU:HD11 | 1:C2:140:VAL:HG13 | 1.63 | 0.79 |
| 1:CN:18:VAL:HG12 | 1:CN:77:LEU:HB2 | 1.64 | 0.79 |
| 1:BH:34:LEU:HD22 | 1:BH:38:LYS:HE2 | 1.65 | 0.79 |
| 1:BS:18:VAL:HG12 | 1:BS:77:LEU:HB2 | 1.63 | 0.79 |
| 1:CV:7:LEU:HD11 | 1:CV:140:VAL:HG13 | 1.64 | 0.79 |
| 1:C2:82:ARG:HH11 | 1:C2:82:ARG:HG3 | 1.49 | 0.79 |
| 1:AH:82:ARG:HG3 | 1:AH:82:ARG:HH11 | 1.48 | 0.78 |
| 1:BR:82:ARG:HH11 | 1:BR:82:ARG:HG3 | 1.48 | 0.78 |
| 1:B1:7:LEU:HD11 | 1:B1:140:VAL:HG13 | 1.64 | 0.78 |
| 1:B2:34:LEU:HD22 | 1:B2:38:LYS:HE2 | 1.65 | 0.78 |
| 1:AV:7:LEU:HD11 | 1:AV:140:VAL:HG13 | 1.64 | 0.78 |
| 1:CR:82:ARG:HH11 | 1:CR:82:ARG:HG3 | 1.49 | 0.78 |
| 1:BW:119:THR:HG22 | 1:BW:121:GLU:H | 1.49 | 0.78 |
| 1:BW:129:THR:CG2 | 1:BW:130:LYS:H | 1.89 | 0.78 |
| 1:CT:72:ASP:C | 1:CT:150:LYS:HD3 | 2.03 | 0.78 |
| 1:A3:18:VAL:HG12 | 1:A3:77:LEU:HB2 | 1.64 | 0.78 |
| 1:BH:82:ARG:HH11 | 1:BH:82:ARG:HG3 | 1.49 | 0.78 |
| 1:BC:7:LEU:HD11 | 1:BC:140:VAL:HG13 | 1.63 | 0.78 |
| 1:CD:18:VAL:HG12 | 1:CD:77:LEU:HB2 | 1.64 | 0.78 |
| 1:BC:82:ARG:HG3 | 1:BC:82:ARG:HH11 | 1.49 | 0.78 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AR:34:LEU:HD22 | 1:AR:38:LYS:HE2 | 1.65 | 0.78 |
| 1:AN:18:VAL:HG12 | 1:AN:77:LEU:HB2 | 1.64 | 0.78 |
| 1:AW:82:ARG:HH11 | 1:AW:82:ARG:HG3 | 1.49 | 0.78 |
| 1:BW:82:ARG:HH11 | 1:BW:82:ARG:HG3 | 1.49 | 0.78 |
| 1:AD:120:ILE:CD1 | 1:AR:129:THR:HG21 | 2.14 | 0.78 |
| 1:BT:72:ASP:C | 1:BT:150:LYS:HD3 | 2.03 | 0.78 |
| 1:BR:119:THR:HG22 | 1:BR:121:GLU:H | 1.49 | 0.78 |
| 1:BE:72:ASP:C | 1:BE:150:LYS:HD3 | 2.03 | 0.78 |
| 1:AC:34:LEU:HD22 | 1:AC:38:LYS:HE2 | 1.65 | 0.78 |
| 1:BM:119:THR:HG22 | 1:BM:121:GLU:H | 1.49 | 0.78 |
| 1:AM:7:LEU:HD11 | 1:AM:140:VAL:HG13 | 1.63 | 0.78 |
| 1:BL:7:LEU:HD11 | 1:BL:140:VAL:HG13 | 1.64 | 0.78 |
| 1:A2:34:LEU:HD22 | 1:A2:38:LYS:HE2 | 1.65 | 0.78 |
| 1:B2:119:THR:HG22 | 1:B2:121:GLU:H | 1.49 | 0.78 |
| 1:CM:119:THR:HG22 | 1:CM:121:GLU:H | 1.49 | 0.78 |
| 1:BG:7:LEU:HD11 | 1:BG:140:VAL:HG13 | 1.64 | 0.78 |
| 1:C3:18:VAL:HG12 | 1:C3:77:LEU:HB2 | 1.64 | 0.78 |
| 1:CO:72:ASP:C | 1:CO:150:LYS:HD3 | 2.03 | 0.78 |
| 1:BI:16:VAL:HG12 | 1:BI:75:ILE:HB | 1.66 | 0.78 |
| 1:CW:82:ARG:HG3 | 1:CW:82:ARG:HH11 | 1.49 | 0.78 |
| 1:AI:18:VAL:HG12 | 1:AI:77:LEU:HB2 | 1.64 | 0.78 |
| 1:BC:119:THR:HG22 | 1:BC:121:GLU:H | 1.49 | 0.78 |
| 1:CW:119:THR:HG22 | 1:CW:121:GLU:H | 1.49 | 0.78 |
| 1:AR:119:THR:HG22 | 1:AR:121:GLU:H | 1.49 | 0.78 |
| 1:BM:34:LEU:HD22 | 1:BM:38:LYS:HE2 | 1.65 | 0.78 |
| 1:A2:82:ARG:HG3 | 1:A2:82:ARG:HH11 | 1.48 | 0.78 |
| 1:C2:119:THR:HG22 | 1:C2:121:GLU:H | 1.49 | 0.78 |
| 1:B4:72:ASP:C | 1:B4:150:LYS:HD3 | 2.03 | 0.78 |
| 1:BR:34:LEU:HD22 | 1:BR:38:LYS:HE2 | 1.65 | 0.78 |
| 1:BC:34:LEU:HD22 | 1:BC:38:LYS:HE2 | 1.65 | 0.78 |
| 1:BM:82:ARG:HG3 | 1:BM:82:ARG:HH11 | 1.49 | 0.78 |
| 1:AW:119:THR:HG22 | 1:AW:121:GLU:H | 1.49 | 0.78 |
| 1:CH:34:LEU:HD22 | 1:CH:38:LYS:HE2 | 1.65 | 0.78 |
| 1:C4:72:ASP:C | 1:C4:150:LYS:HD3 | 2.03 | 0.78 |
| 1:AX:16:VAL:HG12 | 1:AX:75:ILE:HB | 1.66 | 0.78 |
| 1:BD:16:VAL:HG12 | 1:BD:75:ILE:HB | 1.66 | 0.78 |
| 1:CX:16:VAL:HG12 | 1:CX:75:ILE:HB | 1.66 | 0.78 |
| 1:C3:16:VAL:HG12 | 1:C3:75:ILE:HB | 1.66 | 0.78 |
| 1:C1:7:LEU:HD11 | 1:C1:140:VAL:HG13 | 1.64 | 0.78 |
| 1:CR:38:LYS:HZ2 | 1:CR:44:GLU:HG3 | 1.48 | 0.78 |
| 1:AH:34:LEU:HD22 | 1:AH:38:LYS:HE2 | 1.65 | 0.78 |
| 1:AJ:72:ASP:C | 1:AJ:150:LYS:HD3 | 2.03 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CS:16:VAL:HG12 | 1:CS:75:ILE:HB | 1.66 | 0.77 |
| 1:CH:7:LEU:HD11 | 1:CH:140:VAL:HG13 | 1.63 | 0.77 |
| 1:AM:119:THR:HG22 | 1:AM:121:GLU:H | 1.49 | 0.77 |
| 1:CC:34:LEU:HD22 | 1:CC:38:LYS:HE2 | 1.65 | 0.77 |
| 1:CC:82:ARG:HH11 | 1:CC:82:ARG:HG3 | 1.48 | 0.77 |
| 1:CC:119:THR:HG22 | 1:CC:121:GLU:H | 1.49 | 0.77 |
| 1:AE:72:ASP:C | 1:AE:150:LYS:HD3 | 2.03 | 0.77 |
| 1:BJ:72:ASP:C | 1:BJ:150:LYS:HD3 | 2.03 | 0.77 |
| 1:BQ:7:LEU:HD11 | 1:BQ:140:VAL:HG13 | 1.64 | 0.77 |
| 1:AN:16:VAL:HG12 | 1:AN:75:ILE:HB | 1.66 | 0.77 |
| 1:CM:38:LYS:HZ2 | 1:CM:44:GLU:HG3 | 1.49 | 0.77 |
| 1:CR:34:LEU:HD22 | 1:CR:38:LYS:HE2 | 1.65 | 0.77 |
| 1:BY:18:VAL:HG12 | 1:BY:77:LEU:HB2 | 1.67 | 0.77 |
| 1:AY:18:VAL:HG12 | 1:AY:77:LEU:HB2 | 1.67 | 0.77 |
| 1:CY:18:VAL:HG12 | 1:CY:77:LEU:HB2 | 1.67 | 0.77 |
| 1:BO:18:VAL:HG12 | 1:BO:77:LEU:HB2 | 1.67 | 0.77 |
| 1:CY:72:ASP:C | 1:CY:150:LYS:HD3 | 2.03 | 0.77 |
| 1:A3:16:VAL:HG12 | 1:A3:75:ILE:HB | 1.66 | 0.77 |
| 1:AM:82:ARG:HG3 | 1:AM:82:ARG:HH11 | 1.49 | 0.77 |
| 1:BY:72:ASP:C | 1:BY:150:LYS:HD3 | 2.03 | 0.77 |
| 1:A4:72:ASP:C | 1:A4:150:LYS:HD3 | 2.03 | 0.77 |
| 1:AQ:7:LEU:HD11 | 1:AQ:140:VAL:HG13 | 1.64 | 0.77 |
| 1:BT:18:VAL:HG12 | 1:BT:77:LEU:HB2 | 1.67 | 0.77 |
| 1:AW:34:LEU:HD22 | 1:AW:38:LYS:HE2 | 1.65 | 0.77 |
| 1:BG:104:LEU:HD13 | 1:BH:102:LEU:HD22 | 1.67 | 0.77 |
| 1:AC:82:ARG:HG3 | 1:AC:82:ARG:HH11 | 1.49 | 0.77 |
| 1:AO:18:VAL:HG12 | 1:AO:77:LEU:HB2 | 1.67 | 0.77 |
| 1:CN:16:VAL:HG12 | 1:CN:75:ILE:HB | 1.66 | 0.77 |
| 1:BW:34:LEU:HD22 | 1:BW:38:LYS:HE2 | 1.65 | 0.77 |
| 1:BV:104:LEU:HD13 | 1:BW:102:LEU:HD22 | 1.67 | 0.77 |
| 1:CB:104:LEU:HD13 | 1:CC:102:LEU:HD22 | 1.67 | 0.77 |
| 1:BX:16:VAL:HG12 | 1:BX:75:ILE:HB | 1.66 | 0.77 |
| 1:AC:119:THR:HG22 | 1:AC:121:GLU:H | 1.49 | 0.77 |
| 1:BV:7:LEU:HD11 | 1:BV:140:VAL:HG13 | 1.64 | 0.77 |
| 1:CM:82:ARG:HH11 | 1:CM:82:ARG:HG3 | 1.49 | 0.77 |
| 1:C1:104:LEU:HD13 | 1:C2:102:LEU:HD22 | 1.67 | 0.77 |
| 1:BS:16:VAL:HG12 | 1:BS:75:ILE:HB | 1.66 | 0.77 |
| 1:AE:18:VAL:HG12 | 1:AE:77:LEU:HB2 | 1.67 | 0.77 |
| 1:CV:104:LEU:HD13 | 1:CW:102:LEU:HD22 | 1.67 | 0.77 |
| 1:B1:104:LEU:HD13 | 1:B2:102:LEU:HD22 | 1.67 | 0.77 |
| 1:AD:16:VAL:HG12 | 1:AD:75:ILE:HB | 1.66 | 0.77 |
| 1:AS:16:VAL:HG12 | 1:AS:75:ILE:HB | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AJ:18:VAL:HG12 | 1:AJ:77:LEU:HB2 | 1.67 | 0.77 |
| 1:C2:34:LEU:HD22 | 1:C2:38:LYS:HE2 | 1.65 | 0.77 |
| 1:AH:129:THR:CG2 | 1:AH:130:LYS:H | 1.89 | 0.76 |
| 1:CJ:109:PRO:HD2 | 1:CJ:150:LYS:HD2 | 1.67 | 0.76 |
| 1:CQ:104:LEU:HD13 | 1:CR:102:LEU:HD22 | 1.67 | 0.76 |
| 1:BO:109:PRO:HD2 | 1:BO:150:LYS:HD2 | 1.67 | 0.76 |
| 1:AM:34:LEU:HD22 | 1:AM:38:LYS:HE2 | 1.65 | 0.76 |
| 1:CC:7:LEU:HD23 | 1:CR:40:HIS:CE1 | 2.20 | 0.76 |
| 1:AH:119:THR:HG22 | 1:AH:121:GLU:H | 1.49 | 0.76 |
| 1:A1:104:LEU:HD13 | 1:A2:102:LEU:HD22 | 1.67 | 0.76 |
| 1:AI:16:VAL:HG12 | 1:AI:75:ILE:HB | 1.66 | 0.76 |
| 1:CM:34:LEU:HD22 | 1:CM:38:LYS:HE2 | 1.65 | 0.76 |
| 1:CO:18:VAL:HG12 | 1:CO:77:LEU:HB2 | 1.67 | 0.76 |
| 1:A2:119:THR:HG22 | 1:A2:121:GLU:H | 1.49 | 0.76 |
| 1:AG:7:LEU:HD11 | 1:AG:140:VAL:HG13 | 1.64 | 0.76 |
| 1:B4:109:PRO:HD2 | 1:B4:150:LYS:HD2 | 1.68 | 0.76 |
| 1:A1:7:LEU:HD11 | 1:A1:140:VAL:HG13 | 1.64 | 0.76 |
| 1:AQ:104:LEU:HD13 | 1:AR:102:LEU:HD22 | 1.67 | 0.76 |
| 1:CY:109:PRO:HD2 | 1:CY:150:LYS:HD2 | 1.68 | 0.76 |
| 1:B3:16:VAL:HG12 | 1:B3:75:ILE:HB | 1.66 | 0.76 |
| 1:CE:18:VAL:HG12 | 1:CE:77:LEU:HB2 | 1.67 | 0.76 |
| 1:CH:119:THR:HG22 | 1:CH:121:GLU:H | 1.49 | 0.76 |
| 1:BB:104:LEU:HD13 | 1:BC:102:LEU:HD22 | 1.67 | 0.76 |
| 1:AJ:109:PRO:HD2 | 1:AJ:150:LYS:HD2 | 1.67 | 0.76 |
| 1:A4:109:PRO:HD2 | 1:A4:150:LYS:HD2 | 1.67 | 0.76 |
| 1:AR:68:SER:O | 1:AR:70:LYS:HG2 | 1.86 | 0.76 |
| 1:AW:68:SER:O | 1:AW:70:LYS:HG2 | 1.86 | 0.76 |
| 1:BE:18:VAL:HG12 | 1:BE:77:LEU:HB2 | 1.67 | 0.76 |
| 1:AO:109:PRO:HD2 | 1:AO:150:LYS:HD2 | 1.68 | 0.76 |
| 1:AH:68:SER:O | 1:AH:70:LYS:HG2 | 1.86 | 0.76 |
| 1:AL:104:LEU:HD13 | 1:AM:102:LEU:HD22 | 1.67 | 0.76 |
| 1:CC:129:THR:CG2 | 1:CC:130:LYS:H | 1.89 | 0.76 |
| 1:BY:109:PRO:HD2 | 1:BY:150:LYS:HD2 | 1.67 | 0.76 |
| 1:CE:109:PRO:HD2 | 1:CE:150:LYS:HD2 | 1.68 | 0.76 |
| 1:BE:109:PRO:HD2 | 1:BE:150:LYS:HD2 | 1.67 | 0.76 |
| 1:CJ:18:VAL:HG12 | 1:CJ:77:LEU:HB2 | 1.67 | 0.76 |
| 1:BJ:18:VAL:HG12 | 1:BJ:77:LEU:HB2 | 1.67 | 0.76 |
| 1:BH:68:SER:O | 1:BH:70:LYS:HG2 | 1.86 | 0.76 |
| 1:CC:68:SER:O | 1:CC:70:LYS:HG2 | 1.86 | 0.76 |
| 1:A2:129:THR:CG2 | 1:A2:130:LYS:H | 1.89 | 0.76 |
| 1:BJ:109:PRO:HD2 | 1:BJ:150:LYS:HD2 | 1.68 | 0.76 |
| 1:CH:38:LYS:HZ2 | 1:CH:44:GLU:HG3 | 1.50 | 0.76 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AR:82:ARG:HH11 | 1:AR:82:ARG:HG3 | 1.48 | 0.76 |
| 1:AT:18:VAL:HG12 | 1:AT:77:LEU:HB2 | 1.67 | 0.76 |
| 1:CR:68:SER:O | 1:CR:70:LYS:HG2 | 1.86 | 0.76 |
| 1:CK:55:ALA:HB1 | 1:CK:95:VAL:HG21 | 1.68 | 0.76 |
| 1:C4:18:VAL:HG12 | 1:C4:77:LEU:HB2 | 1.67 | 0.76 |
| 1:CF:125:GLU:HA | 1:CF:129:THR:OG1 | 1.87 | 0.76 |
| 1:BH:119:THR:HG22 | 1:BH:121:GLU:H | 1.49 | 0.76 |
| 1:CR:119:THR:HG22 | 1:CR:121:GLU:H | 1.49 | 0.76 |
| 1:AB:104:LEU:HD13 | 1:AC:102:LEU:HD22 | 1.67 | 0.75 |
| 1:CO:109:PRO:HD2 | 1:CO:150:LYS:HD2 | 1.67 | 0.75 |
| 1:BN:16:VAL:HG12 | 1:BN:75:ILE:HB | 1.66 | 0.75 |
| 1:B2:38:LYS:HZ2 | 1:B2:44:GLU:HG3 | 1.51 | 0.75 |
| 1:BP:125:GLU:HA | 1:BP:129:THR:OG1 | 1.87 | 0.75 |
| 1:AA:55:ALA:HB1 | 1:AA:95:VAL:HG21 | 1.68 | 0.75 |
| 1:B2:68:SER:O | 1:B2:70:LYS:HG2 | 1.86 | 0.75 |
| 1:BK:125:GLU:HA | 1:BK:129:THR:OG1 | 1.87 | 0.75 |
| 1:CG:104:LEU:HD13 | 1:CH:102:LEU:HD22 | 1.67 | 0.75 |
| 1:CD:16:VAL:HG12 | 1:CD:75:ILE:HB | 1.66 | 0.75 |
| 1:AU:55:ALA:HB1 | 1:AU:95:VAL:HG21 | 1.68 | 0.75 |
| 1:AU:125:GLU:HA | 1:AU:129:THR:OG1 | 1.87 | 0.75 |
| 1:BM:68:SER:O | 1:BM:70:LYS:HG2 | 1.86 | 0.75 |
| 1:B4:18:VAL:HG12 | 1:B4:77:LEU:HB2 | 1.67 | 0.75 |
| 1:BW:68:SER:O | 1:BW:70:LYS:HG2 | 1.86 | 0.75 |
| 1:AE:109:PRO:HD2 | 1:AE:150:LYS:HD2 | 1.68 | 0.75 |
| 1:CI:16:VAL:HG12 | 1:CI:75:ILE:HB | 1.66 | 0.75 |
| 1:CP:125:GLU:HA | 1:CP:129:THR:OG1 | 1.87 | 0.75 |
| 1:B2:82:ARG:HG3 | 1:B2:82:ARG:HH11 | 1.49 | 0.75 |
| 1:CL:104:LEU:HD13 | 1:CM:102:LEU:HD22 | 1.67 | 0.75 |
| 1:BA:55:ALA:HB1 | 1:BA:95:VAL:HG21 | 1.68 | 0.75 |
| 1:BA:125:GLU:HA | 1:BA:129:THR:OG1 | 1.87 | 0.75 |
| 1:A4:18:VAL:HG12 | 1:A4:77:LEU:HB2 | 1.67 | 0.75 |
| 1:AV:104:LEU:HD13 | 1:AW:102:LEU:HD22 | 1.67 | 0.75 |
| 1:BA:119:THR:HG22 | 1:BA:121:GLU:H | 1.52 | 0.75 |
| 1:BZ:125:GLU:HA | 1:BZ:129:THR:OG1 | 1.87 | 0.75 |
| 1:CH:82:ARG:HG3 | 1:CH:82:ARG:HH11 | 1.48 | 0.75 |
| 1:CZ:55:ALA:HB1 | 1:CZ:95:VAL:HG21 | 1.68 | 0.75 |
| 1:A2:68:SER:O | 1:A2:70:LYS:HG2 | 1.86 | 0.75 |
| 1:CT:119:THR:HG22 | 1:CT:121:GLU:H | 1.52 | 0.75 |
| 1:BZ:55:ALA:HB1 | 1:BZ:95:VAL:HG21 | 1.68 | 0.75 |
| 1:AG:104:LEU:HD13 | 1:AH:102:LEU:HD22 | 1.67 | 0.75 |
| 1:AU:119:THR:HG22 | 1:AU:121:GLU:H | 1.52 | 0.75 |
| 1:BC:68:SER:O | 1:BC:70:LYS:HG2 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BU:119:THR:HG22 | 1:BU:121:GLU:H | 1.52 | 0.75 |
| 1:CM:68:SER:O | 1:CM:70:LYS:HG2 | 1.86 | 0.75 |
| 1:CU:125:GLU:HA | 1:CU:129:THR:OG1 | 1.86 | 0.75 |
| 1:BO:119:THR:HG22 | 1:BO:121:GLU:H | 1.52 | 0.75 |
| 1:AM:68:SER:O | 1:AM:70:LYS:HG2 | 1.86 | 0.75 |
| 1:BL:104:LEU:HD13 | 1:BM:102:LEU:HD22 | 1.67 | 0.75 |
| 1:CF:119:THR:HG22 | 1:CF:121:GLU:H | 1.52 | 0.75 |
| 1:AZ:55:ALA:HB1 | 1:AZ:95:VAL:HG21 | 1.68 | 0.75 |
| 1:CO:119:THR:HG22 | 1:CO:121:GLU:H | 1.52 | 0.75 |
| 1:BR:68:SER:O | 1:BR:70:LYS:HG2 | 1.86 | 0.75 |
| 1:CH:68:SER:O | 1:CH:70:LYS:HG2 | 1.86 | 0.75 |
| 1:CY:119:THR:HG22 | 1:CY:121:GLU:H | 1.52 | 0.75 |
| 1:CA:125:GLU:HA | 1:CA:129:THR:OG1 | 1.87 | 0.75 |
| 1:CZ:125:GLU:HA | 1:CZ:129:THR:OG1 | 1.87 | 0.75 |
| 1:CT:18:VAL:HG12 | 1:CT:77:LEU:HB2 | 1.67 | 0.75 |
| 1:CK:119:THR:HG22 | 1:CK:121:GLU:H | 1.52 | 0.75 |
| 1:CT:109:PRO:HD2 | 1:CT:150:LYS:HD2 | 1.68 | 0.74 |
| 1:BH:38:LYS:HZ2 | 1:BH:44:GLU:HG3 | 1.51 | 0.74 |
| 1:BZ:119:THR:HG22 | 1:BZ:121:GLU:H | 1.52 | 0.74 |
| 1:AC:68:SER:O | 1:AC:70:LYS:HG2 | 1.86 | 0.74 |
| 1:BU:55:ALA:HB1 | 1:BU:95:VAL:HG21 | 1.68 | 0.74 |
| 1:AF:125:GLU:HA | 1:AF:129:THR:OG1 | 1.87 | 0.74 |
| 1:BP:119:THR:HG22 | 1:BP:121:GLU:H | 1.52 | 0.74 |
| 1:CU:119:THR:HG22 | 1:CU:121:GLU:H | 1.52 | 0.74 |
| 1:AA:119:THR:HG22 | 1:AA:121:GLU:H | 1.52 | 0.74 |
| 1:CU:55:ALA:HB1 | 1:CU:95:VAL:HG21 | 1.68 | 0.74 |
| 1:BT:119:THR:HG22 | 1:BT:121:GLU:H | 1.52 | 0.74 |
| 1:CW:68:SER:O | 1:CW:70:LYS:HG2 | 1.86 | 0.74 |
| 1:BF:125:GLU:HA | 1:BF:129:THR:OG1 | 1.87 | 0.74 |
| 1:BA:76:THR:HG22 | 1:BA:111:ILE:O | 1.88 | 0.74 |
| 1:AT:109:PRO:HD2 | 1:AT:150:LYS:HD2 | 1.67 | 0.74 |
| 1:AR:38:LYS:HZ2 | 1:AR:44:GLU:HG3 | 1.51 | 0.74 |
| 1:CZ:119:THR:HG22 | 1:CZ:121:GLU:H | 1.52 | 0.74 |
| 1:AK:76:THR:HG22 | 1:AK:111:ILE:O | 1.88 | 0.74 |
| 1:C2:68:SER:O | 1:C2:70:LYS:HG2 | 1.86 | 0.74 |
| 1:CF:39:ARG:O | 1:CQ:7:LEU:HB3 | 1.87 | 0.74 |
| 1:CZ:76:THR:HG22 | 1:CZ:111:ILE:O | 1.88 | 0.74 |
| 1:BU:125:GLU:HA | 1:BU:129:THR:OG1 | 1.87 | 0.74 |
| 1:CA:119:THR:HG22 | 1:CA:121:GLU:H | 1.52 | 0.74 |
| 1:BJ:119:THR:HG22 | 1:BJ:121:GLU:H | 1.52 | 0.74 |
| 1:AA:125:GLU:HA | 1:AA:129:THR:OG1 | 1.87 | 0.74 |
| 1:AZ:125:GLU:HA | 1:AZ:129:THR:OG1 | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:C4:119:THR:HG22 | 1:C4:121:GLU:H | 1.52 | 0.74 |
| 1:BF:76:THR:HG22 | 1:BF:111:ILE:O | 1.88 | 0.74 |
| 1:BF:55:ALA:HB1 | 1:BF:95:VAL:HG21 | 1.68 | 0.74 |
| 1:BZ:76:THR:HG22 | 1:BZ:111:ILE:O | 1.88 | 0.74 |
| 1:CU:76:THR:HG22 | 1:CU:111:ILE:O | 1.88 | 0.74 |
| 1:AZ:119:THR:HG22 | 1:AZ:121:GLU:H | 1.52 | 0.74 |
| 1:CE:119:THR:HG22 | 1:CE:121:GLU:H | 1.52 | 0.74 |
| 1:BP:76:THR:HG22 | 1:BP:111:ILE:O | 1.88 | 0.74 |
| 1:CA:76:THR:HG22 | 1:CA:111:ILE:O | 1.88 | 0.74 |
| 1:AK:55:ALA:HB1 | 1:AK:95:VAL:HG21 | 1.68 | 0.74 |
| 1:CF:76:THR:HG22 | 1:CF:111:ILE:O | 1.88 | 0.74 |
| 1:BK:76:THR:HG22 | 1:BK:111:ILE:O | 1.88 | 0.74 |
| 1:BK:55:ALA:HB1 | 1:BK:95:VAL:HG21 | 1.68 | 0.74 |
| 1:AP:55:ALA:HB1 | 1:AP:95:VAL:HG21 | 1.68 | 0.74 |
| 1:AP:125:GLU:HA | 1:AP:129:THR:OG1 | 1.87 | 0.74 |
| 1:BQ:104:LEU:HD13 | 1:BR:102:LEU:HD22 | 1.67 | 0.74 |
| 1:BT:109:PRO:HD2 | 1:BT:150:LYS:HD2 | 1.67 | 0.74 |
| 1:AT:119:THR:HG22 | 1:AT:121:GLU:H | 1.52 | 0.74 |
| 1:AE:119:THR:HG22 | 1:AE:121:GLU:H | 1.52 | 0.74 |
| 1:AY:119:THR:HG22 | 1:AY:121:GLU:H | 1.52 | 0.74 |
| 1:AY:109:PRO:HD2 | 1:AY:150:LYS:HD2 | 1.68 | 0.74 |
| 1:AZ:76:THR:HG22 | 1:AZ:111:ILE:O | 1.88 | 0.74 |
| 1:BU:76:THR:HG22 | 1:BU:111:ILE:O | 1.88 | 0.74 |
| 1:CA:55:ALA:HB1 | 1:CA:95:VAL:HG21 | 1.68 | 0.74 |
| 1:CP:76:THR:HG22 | 1:CP:111:ILE:O | 1.88 | 0.74 |
| 1:AF:76:THR:HG22 | 1:AF:111:ILE:O | 1.88 | 0.74 |
| 1:CT:40:HIS:CE1 | 1:C3:7:LEU:HD23 | 2.23 | 0.73 |
| 1:AK:125:GLU:HA | 1:AK:129:THR:OG1 | 1.87 | 0.73 |
| 1:B4:119:THR:HG22 | 1:B4:121:GLU:H | 1.52 | 0.73 |
| 1:C4:109:PRO:HD2 | 1:C4:150:LYS:HD2 | 1.68 | 0.73 |
| 1:A4:119:THR:HG22 | 1:A4:121:GLU:H | 1.52 | 0.73 |
| 1:CK:76:THR:HG22 | 1:CK:111:ILE:O | 1.88 | 0.73 |
| 1:CP:119:THR:HG22 | 1:CP:121:GLU:H | 1.52 | 0.73 |
| 1:CK:125:GLU:HA | 1:CK:129:THR:OG1 | 1.87 | 0.73 |
| 1:BF:119:THR:HG22 | 1:BF:121:GLU:H | 1.52 | 0.73 |
| 1:CF:55:ALA:HB1 | 1:CF:95:VAL:HG21 | 1.68 | 0.73 |
| 1:CP:55:ALA:HB1 | 1:CP:95:VAL:HG21 | 1.68 | 0.73 |
| 1:AA:76:THR:HG22 | 1:AA:111:ILE:O | 1.88 | 0.73 |
| 1:AJ:119:THR:HG22 | 1:AJ:121:GLU:H | 1.52 | 0.73 |
| 1:AF:119:THR:HG22 | 1:AF:121:GLU:H | 1.52 | 0.73 |
| 1:AK:119:THR:HG22 | 1:AK:121:GLU:H | 1.52 | 0.73 |
| 1:BP:55:ALA:HB1 | 1:BP:95:VAL:HG21 | 1.68 | 0.73 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BE:119:THR:HG22 | 1:BE:121:GLU:H | 1.52 | 0.73 |
| 1:CG:40:HIS:CE1 | 1:CU:7:LEU:HD23 | 2.23 | 0.73 |
| 1:BB:7:LEU:HB3 | 1:BU:39:ARG:O | 1.89 | 0.72 |
| 1:BW:38:LYS:HZ2 | 1:BW:44:GLU:HG3 | 1.53 | 0.72 |
| 1:AF:55:ALA:HB1 | 1:AF:95:VAL:HG21 | 1.68 | 0.72 |
| 1:CJ:119:THR:HG22 | 1:CJ:121:GLU:H | 1.52 | 0.72 |
| 1:BK:119:THR:HG22 | 1:BK:121:GLU:H | 1.52 | 0.72 |
| 1:AU:76:THR:HG22 | 1:AU:111:ILE:O | 1.88 | 0.72 |
| 1:BB:40:HIS:CE1 | 1:BU:7:LEU:HD23 | 2.23 | 0.72 |
| 1:BY:119:THR:HG22 | 1:BY:121:GLU:H | 1.52 | 0.72 |
| 1:AP:76:THR:HG22 | 1:AP:111:ILE:O | 1.88 | 0.72 |
| 1:AP:119:THR:HG22 | 1:AP:121:GLU:H | 1.52 | 0.72 |
| 1:AO:119:THR:HG22 | 1:AO:121:GLU:H | 1.52 | 0.72 |
| 1:AB:104:LEU:CD2 | 1:AC:60:LEU:HA | 2.17 | 0.72 |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:HD13 | 1.72 | 0.71 |
| 1:B1:104:LEU:CD2 | 1:B2:60:LEU:HA | 2.17 | 0.71 |
| 1:AX:149:SER:O | 1:AX:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:BN:149:SER:O | 1:BN:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:AI:149:SER:O | 1:AI:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:A1:119:THR:HG22 | 1:A1:121:GLU:H | 1.55 | 0.71 |
| 1:BG:119:THR:HG22 | 1:BG:121:GLU:H | 1.55 | 0.71 |
| 1:BQ:119:THR:HG22 | 1:BQ:121:GLU:H | 1.55 | 0.71 |
| 1:BX:149:SER:O | 1:BX:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:CN:149:SER:O | 1:CN:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:AV:119:THR:HG22 | 1:AV:121:GLU:H | 1.55 | 0.71 |
| 1:A3:149:SER:O | 1:A3:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:AQ:104:LEU:CD2 | 1:AR:60:LEU:HA | 2.17 | 0.71 |
| 1:BM:38:LYS:HZ2 | 1:BM:44:GLU:HG3 | 1.54 | 0.71 |
| 1:CC:38:LYS:HZ2 | 1:CC:44:GLU:HG3 | 1.55 | 0.71 |
| 1:AS:149:SER:O | 1:AS:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:BD:149:SER:O | 1:BD:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:C3:149:SER:O | 1:C3:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:CQ:119:THR:HG22 | 1:CQ:121:GLU:H | 1.55 | 0.71 |
| 1:CL:119:THR:HG22 | 1:CL:121:GLU:H | 1.55 | 0.71 |
| 1:BS:149:SER:O | 1:BS:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:BB:119:THR:HG22 | 1:BB:121:GLU:H | 1.55 | 0.71 |
| 1:CD:107:ASP:CG | 1:CD:107:ASP:O | 2.29 | 0.71 |
| 1:B3:149:SER:O | 1:B3:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:BI:149:SER:O | 1:BI:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:CB:119:THR:HG22 | 1:CB:121:GLU:H | 1.55 | 0.71 |
| 1:BV:119:THR:HG22 | 1:BV:121:GLU:H | 1.55 | 0.71 |
| 1:AN:149:SER:O | 1:AN:152:TRP:CZ2 | 2.43 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CV:119:THR:HG22 | 1:CV:121:GLU:H | 1.55 | 0.71 |
| 1:BC:129:THR:HG21 | 1:BS:120:ILE:HD11 | 1.73 | 0.71 |
| 1:C3:107:ASP:O | 1:C3:107:ASP:CG | 2.29 | 0.71 |
| 1:AN:107:ASP:CG | 1:AN:107:ASP:O | 2.29 | 0.71 |
| 1:CI:149:SER:O | 1:CI:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:AD:149:SER:O | 1:AD:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:CS:149:SER:O | 1:CS:152:TRP:CZ2 | 2.43 | 0.71 |
| 1:AX:107:ASP:CG | 1:AX:107:ASP:O | 2.29 | 0.71 |
| 1:AL:119:THR:HG22 | 1:AL:121:GLU:H | 1.55 | 0.71 |
| 1:BF:7:LEU:HD23 | 1:BQ:40:HIS:CE1 | 2.26 | 0.71 |
| 1:AI:107:ASP:CG | 1:AI:107:ASP:O | 2.29 | 0.71 |
| 1:CN:107:ASP:CG | 1:CN:107:ASP:O | 2.29 | 0.71 |
| 1:AB:119:THR:HG22 | 1:AB:121:GLU:H | 1.55 | 0.71 |
| 1:BN:107:ASP:CG | 1:BN:107:ASP:O | 2.29 | 0.71 |
| 1:BS:107:ASP:O | 1:BS:107:ASP:CG | 2.29 | 0.71 |
| 1:C2:38:LYS:HZ2 | 1:C2:44:GLU:HG3 | 1.54 | 0.71 |
| 1:AD:107:ASP:CG | 1:AD:107:ASP:O | 2.29 | 0.70 |
| 1:A2:38:LYS:HZ2 | 1:A2:44:GLU:HG3 | 1.56 | 0.70 |
| 1:BR:38:LYS:HZ2 | 1:BR:44:GLU:HG3 | 1.56 | 0.70 |
| 1:B3:107:ASP:CG | 1:B3:107:ASP:O | 2.29 | 0.70 |
| 1:CX:149:SER:O | 1:CX:152:TRP:CZ2 | 2.43 | 0.70 |
| 1:BL:119:THR:HG22 | 1:BL:121:GLU:H | 1.55 | 0.70 |
| 1:AL:104:LEU:CD2 | 1:AM:60:LEU:HA | 2.17 | 0.70 |
| 1:CD:149:SER:O | 1:CD:152:TRP:CZ2 | 2.43 | 0.70 |
| 1:AG:119:THR:HG22 | 1:AG:121:GLU:H | 1.55 | 0.70 |
| 1:BI:107:ASP:CG | 1:BI:107:ASP:O | 2.29 | 0.70 |
| 1:CG:104:LEU:CD2 | 1:CH:60:LEU:HA | 2.17 | 0.70 |
| 1:CI:107:ASP:O | 1:CI:107:ASP:CG | 2.29 | 0.70 |
| 1:BX:107:ASP:CG | 1:BX:107:ASP:O | 2.29 | 0.70 |
| 1:CQ:104:LEU:CD2 | 1:CR:60:LEU:HA | 2.17 | 0.70 |
| 1:BU:124:ILE:O | 1:BU:129:THR:OG1 | 2.10 | 0.70 |
| 1:CG:119:THR:HG22 | 1:CG:121:GLU:H | 1.55 | 0.70 |
| 1:BL:104:LEU:CD2 | 1:BM:60:LEU:HA | 2.17 | 0.69 |
| 1:BG:104:LEU:CD2 | 1:BH:60:LEU:HA | 2.17 | 0.69 |
| 1:A1:104:LEU:CD2 | 1:A2:60:LEU:HA | 2.17 | 0.69 |
| 1:CX:107:ASP:CG | 1:CX:107:ASP:O | 2.29 | 0.69 |
| 1:CE:16:VAL:HG12 | 1:CE:75:ILE:HB | 1.74 | 0.69 |
| 1:BE:16:VAL:HG12 | 1:BE:75:ILE:HB | 1.74 | 0.69 |
| 1:BB:104:LEU:CD2 | 1:BC:60:LEU:HA | 2.17 | 0.69 |
| 1:A3:107:ASP:CG | 1:A3:107:ASP:O | 2.29 | 0.69 |
| 1:AE:16:VAL:HG12 | 1:AE:75:ILE:HB | 1.75 | 0.69 |
| 1:AJ:16:VAL:HG12 | 1:AJ:75:ILE:HB | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A4:16:VAL:HG12 | 1:A4:75:ILE:HB | 1.74 | 0.69 |
| 1:AQ:119:THR:HG22 | 1:AQ:121:GLU:H | 1.55 | 0.69 |
| 1:BB:144:GLU:CD | 1:BU:39:ARG:HH22 | 1.95 | 0.69 |
| 1:CY:16:VAL:HG12 | 1:CY:75:ILE:HB | 1.74 | 0.69 |
| 1:CZ:124:ILE:O | 1:CZ:129:THR:OG1 | 2.10 | 0.69 |
| 1:C1:119:THR:HG22 | 1:C1:121:GLU:H | 1.55 | 0.69 |
| 1:BD:107:ASP:O | 1:BD:107:ASP:CG | 2.29 | 0.69 |
| 1:CU:124:ILE:O | 1:CU:129:THR:OG1 | 2.10 | 0.69 |
| 1:CA:124:ILE:O | 1:CA:129:THR:OG1 | 2.10 | 0.69 |
| 1:AS:107:ASP:O | 1:AS:107:ASP:CG | 2.29 | 0.69 |
| 1:CT:16:VAL:HG12 | 1:CT:75:ILE:HB | 1.74 | 0.69 |
| 1:B1:119:THR:HG22 | 1:B1:121:GLU:H | 1.55 | 0.69 |
| 1:BR:129:THR:CG2 | 1:BR:130:LYS:H | 1.89 | 0.69 |
| 1:AC:38:LYS:HZ2 | 1:AC:44:GLU:HG3 | 1.58 | 0.69 |
| 1:BY:16:VAL:HG12 | 1:BY:75:ILE:HB | 1.75 | 0.69 |
| 1:B4:16:VAL:HG12 | 1:B4:75:ILE:HB | 1.74 | 0.69 |
| 1:BY:109:PRO:HG3 | 1:BY:149:SER:OG | 1.93 | 0.69 |
| 1:CJ:16:VAL:HG12 | 1:CJ:75:ILE:HB | 1.75 | 0.69 |
| 1:CR:106:THR:O | 1:CR:107:ASP:CB | 2.41 | 0.69 |
| 1:AM:106:THR:O | 1:AM:107:ASP:CB | 2.41 | 0.69 |
| 1:AO:109:PRO:HG3 | 1:AO:149:SER:OG | 1.93 | 0.69 |
| 1:CY:109:PRO:HG3 | 1:CY:149:SER:OG | 1.93 | 0.69 |
| 1:BJ:109:PRO:HG3 | 1:BJ:149:SER:OG | 1.93 | 0.69 |
| 1:CG:144:GLU:CD | 1:CU:39:ARG:HH22 | 1.96 | 0.69 |
| 1:CC:106:THR:O | 1:CC:107:ASP:CB | 2.41 | 0.69 |
| 1:CJ:109:PRO:HG3 | 1:CJ:149:SER:OG | 1.93 | 0.69 |
| 1:BO:16:VAL:HG12 | 1:BO:75:ILE:HB | 1.75 | 0.69 |
| 1:BT:16:VAL:HG12 | 1:BT:75:ILE:HB | 1.75 | 0.69 |
| 1:BR:106:THR:O | 1:BR:107:ASP:CB | 2.41 | 0.69 |
| 1:BJ:16:VAL:HG12 | 1:BJ:75:ILE:HB | 1.75 | 0.69 |
| 1:C2:106:THR:O | 1:C2:107:ASP:CB | 2.41 | 0.69 |
| 1:CS:107:ASP:CG | 1:CS:107:ASP:O | 2.29 | 0.68 |
| 1:AY:16:VAL:HG12 | 1:AY:75:ILE:HB | 1.75 | 0.68 |
| 1:BW:106:THR:O | 1:BW:107:ASP:CB | 2.41 | 0.68 |
| 1:CO:109:PRO:HG3 | 1:CO:149:SER:OG | 1.93 | 0.68 |
| 1:A4:109:PRO:HG3 | 1:A4:149:SER:OG | 1.93 | 0.68 |
| 1:BT:109:PRO:HG3 | 1:BT:149:SER:OG | 1.93 | 0.68 |
| 1:C4:109:PRO:HG3 | 1:C4:149:SER:OG | 1.93 | 0.68 |
| 1:AO:16:VAL:HG12 | 1:AO:75:ILE:HB | 1.74 | 0.68 |
| 1:BV:104:LEU:CD2 | 1:BW:60:LEU:HA | 2.17 | 0.68 |
| 1:CE:109:PRO:HG3 | 1:CE:149:SER:OG | 1.93 | 0.68 |
| 1:BO:109:PRO:HG3 | 1:BO:149:SER:OG | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:AW:106:THR:O | 1:AW:107:ASP:CB | 2.41 | 0.68 |
| 1:AY:109:PRO:HG3 | 1:AY:149:SER:OG | 1.93 | 0.68 |
| 1:BA:124:ILE:O | 1:BA:129:THR:OG1 | 2.10 | 0.68 |
| 1:AF:124:ILE:O | 1:AF:129:THR:OG1 | 2.10 | 0.68 |
| 1:BE:109:PRO:HG3 | 1:BE:149:SER:OG | 1.93 | 0.68 |
| 1:AT:109:PRO:HG3 | 1:AT:149:SER:OG | 1.93 | 0.68 |
| 1:AH:38:LYS:HZ2 | 1:AH:44:GLU:HG3 | 1.59 | 0.68 |
| 1:B2:106:THR:O | 1:B2:107:ASP:CB | 2.41 | 0.68 |
| 1:AJ:109:PRO:HG3 | 1:AJ:149:SER:OG | 1.93 | 0.68 |
| 1:A4:17:VAL:HG12 | 1:A4:50:ALA:HB3 | 1.76 | 0.68 |
| 1:BU:56:PHE:CZ | 1:BY:100:ALA:HB2 | 2.29 | 0.68 |
| 1:CU:56:PHE:CZ | 1:CY:100:ALA:HB2 | 2.29 | 0.68 |
| 1:CZ:152:TRP:CG | 1:CZ:153:ALA:N | 2.62 | 0.68 |
| 1:BK:56:PHE:CZ | 1:BO:100:ALA:HB2 | 2.29 | 0.68 |
| 1:CK:124:ILE:O | 1:CK:129:THR:OG1 | 2.10 | 0.68 |
| 1:AN:17:VAL:HG12 | 1:AN:50:ALA:HB3 | 1.76 | 0.68 |
| 1:AT:17:VAL:HG12 | 1:AT:50:ALA:HB3 | 1.76 | 0.68 |
| 1:BP:56:PHE:CZ | 1:BT:100:ALA:HB2 | 2.29 | 0.68 |
| 1:B4:17:VAL:HG12 | 1:B4:50:ALA:HB3 | 1.76 | 0.68 |
| 1:CM:106:THR:O | 1:CM:107:ASP:CB | 2.41 | 0.68 |
| 1:CQ:30:LEU:HA | 1:CQ:77:LEU:HD23 | 1.76 | 0.68 |
| 1:AT:16:VAL:HG12 | 1:AT:75:ILE:HB | 1.75 | 0.68 |
| 1:C4:16:VAL:HG12 | 1:C4:75:ILE:HB | 1.75 | 0.68 |
| 1:AE:17:VAL:HG12 | 1:AE:50:ALA:HB3 | 1.76 | 0.68 |
| 1:AP:152:TRP:CG | 1:AP:153:ALA:N | 2.62 | 0.68 |
| 1:CJ:17:VAL:HG12 | 1:CJ:50:ALA:HB3 | 1.76 | 0.68 |
| 1:CN:17:VAL:HG12 | 1:CN:50:ALA:HB3 | 1.76 | 0.68 |
| 1:C3:17:VAL:HG12 | 1:C3:50:ALA:HB3 | 1.76 | 0.68 |
| 1:CZ:56:PHE:CZ | 1:C4:100:ALA:HB2 | 2.29 | 0.68 |
| 1:AE:109:PRO:HG3 | 1:AE:149:SER:OG | 1.93 | 0.68 |
| 1:B4:109:PRO:HG3 | 1:B4:149:SER:OG | 1.93 | 0.68 |
| 1:BG:30:LEU:HA | 1:BG:77:LEU:HD23 | 1.76 | 0.68 |
| 1:AP:56:PHE:CZ | 1:AT:100:ALA:HB2 | 2.29 | 0.68 |
| 1:BJ:17:VAL:HG12 | 1:BJ:50:ALA:HB3 | 1.76 | 0.68 |
| 1:BF:152:TRP:CG | 1:BF:153:ALA:N | 2.62 | 0.68 |
| 1:BP:152:TRP:CG | 1:BP:153:ALA:N | 2.62 | 0.68 |
| 1:CF:152:TRP:CG | 1:CF:153:ALA:N | 2.62 | 0.68 |
| 1:B1:30:LEU:HA | 1:B1:77:LEU:HD23 | 1.76 | 0.68 |
| 1:CL:30:LEU:HA | 1:CL:77:LEU:HD23 | 1.76 | 0.68 |
| 1:AU:152:TRP:CG | 1:AU:153:ALA:N | 2.62 | 0.68 |
| 1:BZ:56:PHE:CZ | 1:B4:100:ALA:HB2 | 2.29 | 0.68 |
| 1:BQ:104:LEU:CD2 | 1:BR:60:LEU:HA | 2.17 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CT:109:PRO:HG3 | 1:CT:149:SER:OG | 1.93 | 0.68 |
| 1:AB:96:ALA:C | 1:AB:100:ALA:CB | 2.62 | 0.68 |
| 1:AQ:30:LEU:HA | 1:AQ:77:LEU:HD23 | 1.76 | 0.68 |
| 1:AK:56:PHE:CZ | 1:AO:100:ALA:HB2 | 2.29 | 0.68 |
| 1:BD:17:VAL:HG12 | 1:BD:50:ALA:HB3 | 1.76 | 0.68 |
| 1:AF:56:PHE:CZ | 1:AJ:100:ALA:HB2 | 2.29 | 0.68 |
| 1:C1:30:LEU:HA | 1:C1:77:LEU:HD23 | 1.76 | 0.68 |
| 1:CO:17:VAL:HG12 | 1:CO:50:ALA:HB3 | 1.76 | 0.68 |
| 1:C4:17:VAL:HG12 | 1:C4:50:ALA:HB3 | 1.76 | 0.68 |
| 1:BE:37:LEU:HG | 1:BE:139:ALA:HB1 | 1.77 | 0.68 |
| 1:BU:152:TRP:CG | 1:BU:153:ALA:N | 2.62 | 0.68 |
| 1:AG:96:ALA:C | 1:AG:100:ALA:CB | 2.62 | 0.67 |
| 1:BG:96:ALA:C | 1:BG:100:ALA:CB | 2.62 | 0.67 |
| 1:CP:124:ILE:O | 1:CP:129:THR:OG1 | 2.10 | 0.67 |
| 1:AP:124:ILE:O | 1:AP:129:THR:OG1 | 2.10 | 0.67 |
| 1:AX:151:HIS:CB | 1:AY:64:LYS:HB3 | 2.25 | 0.67 |
| 1:BB:30:LEU:HA | 1:BB:77:LEU:HD23 | 1.76 | 0.67 |
| 1:AX:17:VAL:HG12 | 1:AX:50:ALA:HB3 | 1.76 | 0.67 |
| 1:CA:56:PHE:CZ | 1:CE:100:ALA:HB2 | 2.29 | 0.67 |
| 1:CK:56:PHE:CZ | 1:CO:100:ALA:HB2 | 2.29 | 0.67 |
| 1:AG:104:LEU:CD2 | 1:AH:60:LEU:HA | 2.17 | 0.67 |
| 1:BQ:96:ALA:C | 1:BQ:100:ALA:CB | 2.62 | 0.67 |
| 1:BK:124:ILE:O | 1:BK:129:THR:OG1 | 2.10 | 0.67 |
| 1:AF:152:TRP:CG | 1:AF:153:ALA:N | 2.62 | 0.67 |
| 1:BF:56:PHE:CZ | 1:BJ:100:ALA:HB2 | 2.29 | 0.67 |
| 1:CF:56:PHE:CZ | 1:CJ:100:ALA:HB2 | 2.29 | 0.67 |
| 1:AO:37:LEU:HG | 1:AO:139:ALA:HB1 | 1.77 | 0.67 |
| 1:AF:7:LEU:HD23 | 1:AQ:40:HIS:CE1 | 2.28 | 0.67 |
| 1:BI:151:HIS:CB | 1:BJ:64:LYS:HB3 | 2.25 | 0.67 |
| 1:BS:151:HIS:CB | 1:BT:64:LYS:HB3 | 2.25 | 0.67 |
| 1:AU:56:PHE:CZ | 1:AY:100:ALA:HB2 | 2.29 | 0.67 |
| 1:AR:106:THR:O | 1:AR:107:ASP:CB | 2.41 | 0.67 |
| 1:A1:96:ALA:C | 1:A1:100:ALA:CB | 2.62 | 0.67 |
| 1:BB:124:ILE:HD11 | 1:BV:24:PHE:CE2 | 2.29 | 0.67 |
| 1:BD:151:HIS:CB | 1:BE:64:LYS:HB3 | 2.25 | 0.67 |
| 1:CT:17:VAL:HG12 | 1:CT:50:ALA:HB3 | 1.76 | 0.67 |
| 1:CX:151:HIS:CB | 1:CY:64:LYS:HB3 | 2.25 | 0.67 |
| 1:CS:151:HIS:CB | 1:CT:64:LYS:HB3 | 2.25 | 0.67 |
| 1:C3:151:HIS:CB | 1:C4:64:LYS:HB3 | 2.25 | 0.67 |
| 1:AB:30:LEU:HA | 1:AB:77:LEU:HD23 | 1.76 | 0.67 |
| 1:BY:17:VAL:HG12 | 1:BY:50:ALA:HB3 | 1.76 | 0.67 |
| 1:B3:151:HIS:CB | 1:B4:64:LYS:HB3 | 2.25 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:AA:152:TRP:CG | 1:AA:153:ALA:N | 2.62 | 0.67 |
| 1:AT:37:LEU:HG | 1:AT:139:ALA:HB1 | 1.77 | 0.67 |
| 1:CB:104:LEU:CD2 | 1:CC:60:LEU:HA | 2.17 | 0.67 |
| 1:BZ:124:ILE:O | 1:BZ:129:THR:OG1 | 2.10 | 0.67 |
| 1:AI:151:HIS:CB | 1:AJ:64:LYS:HB3 | 2.25 | 0.67 |
| 1:AD:151:HIS:CB | 1:AE:64:LYS:HB3 | 2.25 | 0.67 |
| 1:BM:106:THR:O | 1:BM:107:ASP:CB | 2.41 | 0.67 |
| 1:CP:56:PHE:CZ | 1:CT:100:ALA:HB2 | 2.29 | 0.67 |
| 1:CG:30:LEU:HA | 1:CG:77:LEU:HD23 | 1.76 | 0.67 |
| 1:A3:151:HIS:CB | 1:A4:64:LYS:HB3 | 2.25 | 0.67 |
| 1:BO:17:VAL:HG12 | 1:BO:50:ALA:HB3 | 1.76 | 0.67 |
| 1:B4:37:LEU:HG | 1:B4:139:ALA:HB1 | 1.77 | 0.67 |
| 1:BX:151:HIS:CB | 1:BY:64:LYS:HB3 | 2.25 | 0.67 |
| 1:A1:30:LEU:HA | 1:A1:77:LEU:HD23 | 1.76 | 0.67 |
| 1:BN:151:HIS:CB | 1:BO:64:LYS:HB3 | 2.25 | 0.67 |
| 1:BC:106:THR:O | 1:BC:107:ASP:CB | 2.41 | 0.67 |
| 1:CW:106:THR:O | 1:CW:107:ASP:CB | 2.41 | 0.67 |
| 1:CL:104:LEU:CD2 | 1:CM:60:LEU:HA | 2.17 | 0.67 |
| 1:C1:96:ALA:C | 1:C1:100:ALA:CB | 2.62 | 0.67 |
| 1:CV:96:ALA:C | 1:CV:100:ALA:CB | 2.63 | 0.67 |
| 1:CN:151:HIS:CB | 1:CO:64:LYS:HB3 | 2.25 | 0.67 |
| 1:AK:152:TRP:CG | 1:AK:153:ALA:N | 2.62 | 0.67 |
| 1:AA:56:PHE:CZ | 1:AE:100:ALA:HB2 | 2.29 | 0.67 |
| 1:AD:17:VAL:HG12 | 1:AD:50:ALA:HB3 | 1.76 | 0.67 |
| 1:BO:37:LEU:HG | 1:BO:139:ALA:HB1 | 1.77 | 0.67 |
| 1:BV:30:LEU:HA | 1:BV:77:LEU:HD23 | 1.76 | 0.67 |
| 1:AE:37:LEU:HG | 1:AE:139:ALA:HB1 | 1.77 | 0.67 |
| 1:AV:96:ALA:C | 1:AV:100:ALA:CB | 2.62 | 0.67 |
| 1:CB:96:ALA:C | 1:CB:100:ALA:CB | 2.63 | 0.67 |
| 1:CW:7:LEU:HB3 | 1:C2:39:ARG:O | 1.94 | 0.67 |
| 1:AW:38:LYS:HZ2 | 1:AW:44:GLU:HG3 | 1.60 | 0.67 |
| 1:BA:56:PHE:CZ | 1:BE:100:ALA:HB2 | 2.29 | 0.67 |
| 1:AC:106:THR:O | 1:AC:107:ASP:CB | 2.41 | 0.67 |
| 1:BZ:152:TRP:CG | 1:BZ:153:ALA:N | 2.62 | 0.67 |
| 1:AJ:17:VAL:HG12 | 1:AJ:50:ALA:HB3 | 1.76 | 0.67 |
| 1:AG:30:LEU:HA | 1:AG:77:LEU:HD23 | 1.76 | 0.67 |
| 1:CK:152:TRP:CG | 1:CK:153:ALA:N | 2.62 | 0.67 |
| 1:AS:151:HIS:CB | 1:AT:64:LYS:HB3 | 2.25 | 0.67 |
| 1:A1:148:LEU:HD13 | 1:A2:61:ILE:CD1 | 2.25 | 0.67 |
| 1:AZ:152:TRP:CG | 1:AZ:153:ALA:N | 2.62 | 0.67 |
| 1:CT:37:LEU:HG | 1:CT:139:ALA:HB1 | 1.77 | 0.67 |
| 1:A3:17:VAL:HG12 | 1:A3:50:ALA:HB3 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CY:37:LEU:HG | 1:CY:139:ALA:HB1 | 1.77 | 0.67 |
| 1:BX:17:VAL:HG12 | 1:BX:50:ALA:HB3 | 1.76 | 0.67 |
| 1:C1:104:LEU:CD2 | 1:C2:60:LEU:HA | 2.17 | 0.67 |
| 1:CQ:148:LEU:HD13 | 1:CR:61:ILE:CD1 | 2.25 | 0.67 |
| 1:BL:30:LEU:HA | 1:BL:77:LEU:HD23 | 1.76 | 0.67 |
| 1:AN:151:HIS:CB | 1:AO:64:LYS:HB3 | 2.25 | 0.67 |
| 1:BT:55:ALA:HB1 | 1:BT:95:VAL:HG21 | 1.77 | 0.67 |
| 1:BL:96:ALA:C | 1:BL:100:ALA:CB | 2.63 | 0.66 |
| 1:AG:148:LEU:HD13 | 1:AH:61:ILE:CD1 | 2.25 | 0.66 |
| 1:CO:16:VAL:HG12 | 1:CO:75:ILE:HB | 1.74 | 0.66 |
| 1:BM:106:THR:O | 1:BM:107:ASP:HB3 | 1.96 | 0.66 |
| 1:B4:55:ALA:HB1 | 1:B4:95:VAL:HG21 | 1.77 | 0.66 |
| 1:A2:106:THR:O | 1:A2:107:ASP:CB | 2.41 | 0.66 |
| 1:CD:151:HIS:CB | 1:CE:64:LYS:HB3 | 2.25 | 0.66 |
| 1:CB:148:LEU:HD13 | 1:CC:61:ILE:CD1 | 2.25 | 0.66 |
| 1:AV:148:LEU:HD13 | 1:AW:61:ILE:CD1 | 2.26 | 0.66 |
| 1:BL:148:LEU:HD13 | 1:BM:61:ILE:CD1 | 2.25 | 0.66 |
| 1:AZ:56:PHE:CZ | 1:A4:100:ALA:HB2 | 2.29 | 0.66 |
| 1:AL:30:LEU:HA | 1:AL:77:LEU:HD23 | 1.76 | 0.66 |
| 1:BB:148:LEU:HD13 | 1:BC:61:ILE:CD1 | 2.25 | 0.66 |
| 1:CV:148:LEU:HD13 | 1:CW:61:ILE:CD1 | 2.26 | 0.66 |
| 1:AU:124:ILE:O | 1:AU:129:THR:OG1 | 2.10 | 0.66 |
| 1:AM:106:THR:O | 1:AM:107:ASP:HB3 | 1.96 | 0.66 |
| 1:BW:106:THR:O | 1:BW:107:ASP:HB3 | 1.96 | 0.66 |
| 1:B2:106:THR:O | 1:B2:107:ASP:HB3 | 1.96 | 0.66 |
| 1:AY:55:ALA:HB1 | 1:AY:95:VAL:HG21 | 1.77 | 0.66 |
| 1:CS:17:VAL:HG12 | 1:CS:50:ALA:HB3 | 1.76 | 0.66 |
| 1:BA:152:TRP:CG | 1:BA:153:ALA:N | 2.62 | 0.66 |
| 1:CI:17:VAL:HG12 | 1:CI:50:ALA:HB3 | 1.76 | 0.66 |
| 1:CV:30:LEU:HA | 1:CV:77:LEU:HD23 | 1.76 | 0.66 |
| 1:CG:96:ALA:C | 1:CG:100:ALA:CB | 2.63 | 0.66 |
| 1:BG:148:LEU:HD13 | 1:BH:61:ILE:CD1 | 2.25 | 0.66 |
| 1:B1:148:LEU:HD13 | 1:B2:61:ILE:CD1 | 2.25 | 0.66 |
| 1:C1:148:LEU:HD13 | 1:C2:61:ILE:CD1 | 2.25 | 0.66 |
| 1:AZ:124:ILE:O | 1:AZ:129:THR:OG1 | 2.10 | 0.66 |
| 1:CM:106:THR:O | 1:CM:107:ASP:HB3 | 1.96 | 0.66 |
| 1:AT:55:ALA:HB1 | 1:AT:95:VAL:HG21 | 1.77 | 0.66 |
| 1:CD:17:VAL:HG12 | 1:CD:50:ALA:HB3 | 1.76 | 0.66 |
| 1:AV:104:LEU:CD2 | 1:AW:60:LEU:HA | 2.17 | 0.66 |
| 1:BR:106:THR:O | 1:BR:107:ASP:HB3 | 1.96 | 0.66 |
| 1:AC:106:THR:O | 1:AC:107:ASP:HB3 | 1.96 | 0.66 |
| 1:BS:17:VAL:HG12 | 1:BS:50:ALA:HB3 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:C4:37:LEU:HG | 1:C4:139:ALA:HB1 | 1.77 | 0.66 |
| 1:A4:55:ALA:HB1 | 1:A4:95:VAL:HG21 | 1.77 | 0.66 |
| 1:AE:55:ALA:HB1 | 1:AE:95:VAL:HG21 | 1.77 | 0.66 |
| 1:CT:55:ALA:HB1 | 1:CT:95:VAL:HG21 | 1.78 | 0.66 |
| 1:AR:106:THR:O | 1:AR:107:ASP:HB3 | 1.96 | 0.66 |
| 1:BH:106:THR:O | 1:BH:107:ASP:CB | 2.41 | 0.66 |
| 1:AS:17:VAL:HG12 | 1:AS:50:ALA:HB3 | 1.76 | 0.66 |
| 1:BI:17:VAL:HG12 | 1:BI:50:ALA:HB3 | 1.76 | 0.66 |
| 1:BT:17:VAL:HG12 | 1:BT:50:ALA:HB3 | 1.76 | 0.66 |
| 1:AY:37:LEU:HG | 1:AY:139:ALA:HB1 | 1.77 | 0.66 |
| 1:CE:17:VAL:HG12 | 1:CE:50:ALA:HB3 | 1.76 | 0.66 |
| 1:AD:120:ILE:HD11 | 1:AR:129:THR:HG21 | 1.76 | 0.66 |
| 1:AL:96:ALA:C | 1:AL:100:ALA:CB | 2.62 | 0.66 |
| 1:B1:96:ALA:C | 1:B1:100:ALA:CB | 2.62 | 0.66 |
| 1:BQ:148:LEU:HD13 | 1:BR:61:ILE:CD1 | 2.25 | 0.66 |
| 1:AC:7:LEU:HB3 | 1:AR:39:ARG:O | 1.96 | 0.66 |
| 1:CW:106:THR:O | 1:CW:107:ASP:HB3 | 1.96 | 0.66 |
| 1:BE:17:VAL:HG12 | 1:BE:50:ALA:HB3 | 1.76 | 0.66 |
| 1:CG:148:LEU:HD13 | 1:CH:61:ILE:CD1 | 2.26 | 0.66 |
| 1:B2:38:LYS:NZ | 1:B2:44:GLU:HG3 | 2.11 | 0.66 |
| 1:AV:30:LEU:HA | 1:AV:77:LEU:HD23 | 1.76 | 0.66 |
| 1:A4:37:LEU:HG | 1:A4:139:ALA:HB1 | 1.77 | 0.66 |
| 1:CJ:55:ALA:HB1 | 1:CJ:95:VAL:HG21 | 1.77 | 0.66 |
| 1:CI:151:HIS:CB | 1:CJ:64:LYS:HB3 | 2.25 | 0.66 |
| 1:CA:152:TRP:CG | 1:CA:153:ALA:N | 2.62 | 0.66 |
| 1:CV:104:LEU:CD2 | 1:CW:60:LEU:HA | 2.17 | 0.66 |
| 1:CL:148:LEU:HD13 | 1:CM:61:ILE:CD1 | 2.26 | 0.66 |
| 1:BM:38:LYS:NZ | 1:BM:44:GLU:HG3 | 2.11 | 0.66 |
| 1:BR:38:LYS:NZ | 1:BR:44:GLU:HG3 | 2.11 | 0.66 |
| 1:BC:38:LYS:NZ | 1:BC:44:GLU:HG3 | 2.11 | 0.66 |
| 1:BW:38:LYS:NZ | 1:BW:44:GLU:HG3 | 2.11 | 0.66 |
| 1:AE:75:ILE:HG22 | 1:AE:77:LEU:HD13 | 1.78 | 0.66 |
| 1:BP:124:ILE:O | 1:BP:129:THR:OG1 | 2.10 | 0.66 |
| 1:AK:124:ILE:O | 1:AK:129:THR:OG1 | 2.10 | 0.66 |
| 1:CW:128:GLY:O | 1:C3:22:ASN:HA | 1.96 | 0.66 |
| 1:CH:106:THR:O | 1:CH:107:ASP:CB | 2.41 | 0.66 |
| 1:AJ:55:ALA:HB1 | 1:AJ:95:VAL:HG21 | 1.77 | 0.66 |
| 1:AO:58:ILE:HG22 | 1:AO:58:ILE:O | 1.96 | 0.66 |
| 1:BK:152:TRP:CG | 1:BK:153:ALA:N | 2.62 | 0.66 |
| 1:AG:96:ALA:O | 1:AG:100:ALA:CB | 2.44 | 0.66 |
| 1:AB:148:LEU:HD13 | 1:AC:61:ILE:CD1 | 2.25 | 0.66 |
| 1:CW:38:LYS:NZ | 1:CW:44:GLU:HG3 | 2.11 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CC:38:LYS:NZ | 1:CC:44:GLU:HG3 | 2.11 | 0.66 |
| 1:CJ:75:ILE:HG22 | 1:CJ:77:LEU:HD13 | 1.78 | 0.66 |
| 1:C4:75:ILE:HG22 | 1:C4:77:LEU:HD13 | 1.78 | 0.66 |
| 1:AA:124:ILE:O | 1:AA:129:THR:OG1 | 2.10 | 0.66 |
| 1:CR:106:THR:O | 1:CR:107:ASP:HB3 | 1.96 | 0.66 |
| 1:BH:106:THR:O | 1:BH:107:ASP:HB3 | 1.96 | 0.66 |
| 1:BQ:4:GLU:HG2 | 1:BR:51:TRP:HD1 | 1.61 | 0.66 |
| 1:BT:37:LEU:HG | 1:BT:139:ALA:HB1 | 1.77 | 0.66 |
| 1:CO:58:ILE:O | 1:CO:58:ILE:HG22 | 1.96 | 0.66 |
| 1:BL:96:ALA:O | 1:BL:100:ALA:CB | 2.45 | 0.65 |
| 1:BT:75:ILE:HG22 | 1:BT:77:LEU:HD13 | 1.78 | 0.65 |
| 1:AW:38:LYS:NZ | 1:AW:44:GLU:HG3 | 2.11 | 0.65 |
| 1:CF:124:ILE:O | 1:CF:129:THR:OG1 | 2.10 | 0.65 |
| 1:B3:17:VAL:HG12 | 1:B3:50:ALA:HB3 | 1.76 | 0.65 |
| 1:CO:37:LEU:HG | 1:CO:139:ALA:HB1 | 1.77 | 0.65 |
| 1:BV:4:GLU:HG2 | 1:BW:51:TRP:HD1 | 1.61 | 0.65 |
| 1:CY:17:VAL:HG12 | 1:CY:50:ALA:HB3 | 1.76 | 0.65 |
| 1:AY:17:VAL:HG12 | 1:AY:50:ALA:HB3 | 1.76 | 0.65 |
| 1:AJ:37:LEU:HG | 1:AJ:139:ALA:HB1 | 1.77 | 0.65 |
| 1:AH:106:THR:O | 1:AH:107:ASP:HB3 | 1.96 | 0.65 |
| 1:BB:96:ALA:C | 1:BB:100:ALA:CB | 2.62 | 0.65 |
| 1:AQ:96:ALA:O | 1:AQ:100:ALA:CB | 2.45 | 0.65 |
| 1:BG:96:ALA:O | 1:BG:100:ALA:CB | 2.44 | 0.65 |
| 1:CF:39:ARG:HH22 | 1:CQ:144:GLU:CD | 2.00 | 0.65 |
| 1:AL:148:LEU:HD13 | 1:AM:61:ILE:CD1 | 2.26 | 0.65 |
| 1:AK:53:PRO:HD2 | 1:AK:57:GLU:HB2 | 1.79 | 0.65 |
| 1:BA:53:PRO:HD2 | 1:BA:57:GLU:HB2 | 1.79 | 0.65 |
| 1:AO:75:ILE:HG22 | 1:AO:77:LEU:HD13 | 1.78 | 0.65 |
| 1:B4:75:ILE:HG22 | 1:B4:77:LEU:HD13 | 1.78 | 0.65 |
| 1:BJ:58:ILE:HG22 | 1:BJ:58:ILE:O | 1.96 | 0.65 |
| 1:BY:55:ALA:HB1 | 1:BY:95:VAL:HG21 | 1.77 | 0.65 |
| 1:BE:55:ALA:HB1 | 1:BE:95:VAL:HG21 | 1.77 | 0.65 |
| 1:CP:152:TRP:CG | 1:CP:153:ALA:N | 2.62 | 0.65 |
| 1:CX:17:VAL:HG12 | 1:CX:50:ALA:HB3 | 1.76 | 0.65 |
| 1:BB:96:ALA:O | 1:BB:100:ALA:CB | 2.45 | 0.65 |
| 1:CP:39:ARG:O | 1:CV:7:LEU:HB3 | 1.96 | 0.65 |
| 1:AR:38:LYS:NZ | 1:AR:44:GLU:HG3 | 2.11 | 0.65 |
| 1:AC:38:LYS:NZ | 1:AC:44:GLU:HG3 | 2.11 | 0.65 |
| 1:AH:38:LYS:NZ | 1:AH:44:GLU:HG3 | 2.11 | 0.65 |
| 1:AT:58:ILE:HG22 | 1:AT:58:ILE:O | 1.96 | 0.65 |
| 1:AO:17:VAL:HG12 | 1:AO:50:ALA:HB3 | 1.76 | 0.65 |
| 1:AI:17:VAL:HG12 | 1:AI:50:ALA:HB3 | 1.76 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AL:96:ALA:O | 1:AL:100:ALA:CB | 2.45 | 0.65 |
| 1:BQ:96:ALA:O | 1:BQ:100:ALA:CB | 2.45 | 0.65 |
| 1:CG:96:ALA:O | 1:CG:100:ALA:CB | 2.45 | 0.65 |
| 1:AQ:148:LEU:HD13 | 1:AR:61:ILE:CD1 | 2.26 | 0.65 |
| 1:CY:75:ILE:HG22 | 1:CY:77:LEU:HD13 | 1.78 | 0.65 |
| 1:A4:75:ILE:HG22 | 1:A4:77:LEU:HD13 | 1.78 | 0.65 |
| 1:A2:106:THR:O | 1:A2:107:ASP:HB3 | 1.96 | 0.65 |
| 1:CU:152:TRP:CG | 1:CU:153:ALA:N | 2.62 | 0.65 |
| 1:BN:17:VAL:HG12 | 1:BN:50:ALA:HB3 | 1.76 | 0.65 |
| 1:CO:55:ALA:HB1 | 1:CO:95:VAL:HG21 | 1.77 | 0.65 |
| 1:BJ:55:ALA:HB1 | 1:BJ:95:VAL:HG21 | 1.77 | 0.65 |
| 1:CL:4:GLU:HG2 | 1:CM:51:TRP:HD1 | 1.61 | 0.65 |
| 1:CE:37:LEU:HG | 1:CE:139:ALA:HB1 | 1.77 | 0.65 |
| 1:BL:100:ALA:HA | 1:BM:56:PHE:HZ | 1.62 | 0.65 |
| 1:C1:96:ALA:O | 1:C1:100:ALA:CB | 2.44 | 0.65 |
| 1:BV:96:ALA:O | 1:BV:100:ALA:CB | 2.45 | 0.65 |
| 1:A1:96:ALA:O | 1:A1:100:ALA:CB | 2.45 | 0.65 |
| 1:BV:148:LEU:HD13 | 1:BW:61:ILE:CD1 | 2.26 | 0.65 |
| 1:CU:53:PRO:HD2 | 1:CU:57:GLU:HB2 | 1.79 | 0.65 |
| 1:AZ:53:PRO:HD2 | 1:AZ:57:GLU:HB2 | 1.79 | 0.65 |
| 1:C2:106:THR:O | 1:C2:107:ASP:HB3 | 1.96 | 0.65 |
| 1:BQ:4:GLU:HG2 | 1:BR:51:TRP:CD1 | 2.32 | 0.65 |
| 1:C1:4:GLU:HG2 | 1:C2:51:TRP:HD1 | 1.61 | 0.65 |
| 1:CB:30:LEU:HA | 1:CB:77:LEU:HD23 | 1.76 | 0.65 |
| 1:BO:58:ILE:HG22 | 1:BO:58:ILE:O | 1.96 | 0.65 |
| 1:CE:107:ASP:CG | 1:CE:107:ASP:O | 2.35 | 0.65 |
| 1:C4:55:ALA:HB1 | 1:C4:95:VAL:HG21 | 1.77 | 0.65 |
| 1:AC:129:THR:HG21 | 1:AS:120:ILE:CD1 | 2.27 | 0.65 |
| 1:CQ:96:ALA:C | 1:CQ:100:ALA:CB | 2.63 | 0.65 |
| 1:CQ:96:ALA:O | 1:CQ:100:ALA:CB | 2.45 | 0.65 |
| 1:AB:7:LEU:HB3 | 1:AU:39:ARG:O | 1.97 | 0.65 |
| 1:BF:53:PRO:HD2 | 1:BF:57:GLU:HB2 | 1.79 | 0.65 |
| 1:CZ:53:PRO:HD2 | 1:CZ:57:GLU:HB2 | 1.79 | 0.65 |
| 1:AM:38:LYS:NZ | 1:AM:44:GLU:HG3 | 2.11 | 0.65 |
| 1:CC:40:HIS:CE1 | 1:CR:7:LEU:HD23 | 2.32 | 0.65 |
| 1:CT:75:ILE:HG22 | 1:CT:77:LEU:HD13 | 1.78 | 0.65 |
| 1:C1:4:GLU:HG2 | 1:C2:51:TRP:CD1 | 2.32 | 0.65 |
| 1:BJ:37:LEU:HG | 1:BJ:139:ALA:HB1 | 1.77 | 0.65 |
| 1:BY:37:LEU:HG | 1:BY:139:ALA:HB1 | 1.77 | 0.65 |
| 1:BK:7:LEU:HD11 | 1:BK:140:VAL:HG13 | 1.79 | 0.65 |
| 1:AE:107:ASP:CG | 1:AE:107:ASP:O | 2.35 | 0.65 |
| 1:B1:96:ALA:O | 1:B1:100:ALA:CB | 2.45 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:AU:53:PRO:HD2 | 1:AU:57:GLU:HB2 | 1.79 | 0.65 |
| 1:BJ:75:ILE:HG22 | 1:BJ:77:LEU:HD13 | 1.78 | 0.65 |
| 1:CU:7:LEU:HD11 | 1:CU:140:VAL:HG13 | 1.79 | 0.65 |
| 1:CJ:37:LEU:HG | 1:CJ:139:ALA:HB1 | 1.77 | 0.65 |
| 1:CE:55:ALA:HB1 | 1:CE:95:VAL:HG21 | 1.77 | 0.65 |
| 1:BA:7:LEU:HD11 | 1:BA:140:VAL:HG13 | 1.79 | 0.65 |
| 1:BL:4:GLU:HG2 | 1:BM:51:TRP:HD1 | 1.61 | 0.65 |
| 1:CB:4:GLU:HG2 | 1:CC:51:TRP:HD1 | 1.61 | 0.65 |
| 1:AP:7:LEU:HD11 | 1:AP:140:VAL:HG13 | 1.79 | 0.65 |
| 1:BB:100:ALA:HA | 1:BC:56:PHE:HZ | 1.62 | 0.65 |
| 1:CB:96:ALA:O | 1:CB:100:ALA:CB | 2.45 | 0.65 |
| 1:CV:96:ALA:O | 1:CV:100:ALA:CB | 2.45 | 0.65 |
| 1:BO:75:ILE:HG22 | 1:BO:77:LEU:HD13 | 1.78 | 0.65 |
| 1:AW:106:THR:O | 1:AW:107:ASP:HB3 | 1.96 | 0.65 |
| 1:BL:4:GLU:HG2 | 1:BM:51:TRP:CD1 | 2.32 | 0.65 |
| 1:CF:7:LEU:HD11 | 1:CF:140:VAL:HG13 | 1.79 | 0.65 |
| 1:BB:4:GLU:HG2 | 1:BC:51:TRP:HD1 | 1.61 | 0.65 |
| 1:BZ:7:LEU:HD11 | 1:BZ:140:VAL:HG13 | 1.79 | 0.65 |
| 1:BQ:30:LEU:HA | 1:BQ:77:LEU:HD23 | 1.76 | 0.65 |
| 1:CX:120:ILE:CD1 | 1:C2:129:THR:HG21 | 2.27 | 0.65 |
| 1:BV:107:ASP:HB2 | 1:BV:152:TRP:HZ3 | 1.62 | 0.65 |
| 1:AB:100:ALA:HA | 1:AC:56:PHE:HZ | 1.62 | 0.65 |
| 1:CK:53:PRO:HD2 | 1:CK:57:GLU:HB2 | 1.79 | 0.65 |
| 1:CD:28:LYS:NZ | 1:CF:28:LYS:NZ | 2.43 | 0.65 |
| 1:BE:75:ILE:HG22 | 1:BE:77:LEU:HD13 | 1.78 | 0.65 |
| 1:CL:4:GLU:HG2 | 1:CM:51:TRP:CD1 | 2.32 | 0.65 |
| 1:CQ:4:GLU:HG2 | 1:CR:51:TRP:HD1 | 1.62 | 0.65 |
| 1:BT:107:ASP:O | 1:BT:107:ASP:CG | 2.35 | 0.65 |
| 1:CT:58:ILE:O | 1:CT:58:ILE:HG22 | 1.96 | 0.65 |
| 1:CT:107:ASP:CG | 1:CT:107:ASP:O | 2.35 | 0.65 |
| 1:CE:58:ILE:HG22 | 1:CE:58:ILE:O | 1.96 | 0.65 |
| 1:BY:107:ASP:CG | 1:BY:107:ASP:O | 2.35 | 0.65 |
| 1:CB:107:ASP:HB2 | 1:CB:152:TRP:HZ3 | 1.61 | 0.65 |
| 1:CB:100:ALA:HA | 1:CC:56:PHE:HZ | 1.62 | 0.65 |
| 1:AG:100:ALA:HA | 1:AH:56:PHE:HZ | 1.62 | 0.65 |
| 1:C1:100:ALA:HA | 1:C2:56:PHE:HZ | 1.62 | 0.65 |
| 1:B1:100:ALA:HA | 1:B2:56:PHE:HZ | 1.62 | 0.65 |
| 1:CL:96:ALA:O | 1:CL:100:ALA:CB | 2.45 | 0.65 |
| 1:CQ:100:ALA:HA | 1:CR:56:PHE:HZ | 1.62 | 0.65 |
| 1:BU:53:PRO:HD2 | 1:BU:57:GLU:HB2 | 1.79 | 0.65 |
| 1:BF:124:ILE:O | 1:BF:129:THR:OG1 | 2.10 | 0.65 |
| 1:BC:106:THR:O | 1:BC:107:ASP:HB3 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BO:55:ALA:HB1 | 1:BO:95:VAL:HG21 | 1.77 | 0.65 |
| 1:AK:7:LEU:HD11 | 1:AK:140:VAL:HG13 | 1.79 | 0.65 |
| 1:BJ:107:ASP:CG | 1:BJ:107:ASP:O | 2.35 | 0.65 |
| 1:BS:100:ALA:HB2 | 1:BT:56:PHE:CZ | 2.32 | 0.65 |
| 1:CY:55:ALA:HB1 | 1:CY:95:VAL:HG21 | 1.77 | 0.65 |
| 1:CV:4:GLU:HG2 | 1:CW:51:TRP:CD1 | 2.32 | 0.65 |
| 1:CN:100:ALA:HB2 | 1:CO:56:PHE:CZ | 2.32 | 0.65 |
| 1:BG:4:GLU:HG2 | 1:BH:51:TRP:CD1 | 2.32 | 0.65 |
| 1:BY:58:ILE:O | 1:BY:58:ILE:HG22 | 1.96 | 0.65 |
| 1:AV:100:ALA:HA | 1:AW:56:PHE:HZ | 1.62 | 0.64 |
| 1:A1:96:ALA:HB2 | 1:A1:112:PHE:CZ | 2.33 | 0.64 |
| 1:BY:75:ILE:HG22 | 1:BY:77:LEU:HD13 | 1.78 | 0.64 |
| 1:BU:7:LEU:HD11 | 1:BU:140:VAL:HG13 | 1.79 | 0.64 |
| 1:BX:149:SER:O | 1:BX:152:TRP:CE2 | 2.51 | 0.64 |
| 1:B3:149:SER:O | 1:B3:152:TRP:CE2 | 2.50 | 0.64 |
| 1:BI:149:SER:O | 1:BI:152:TRP:CE2 | 2.50 | 0.64 |
| 1:CS:149:SER:O | 1:CS:152:TRP:CE2 | 2.51 | 0.64 |
| 1:BI:100:ALA:HB2 | 1:BJ:56:PHE:CZ | 2.32 | 0.64 |
| 1:AD:100:ALA:HB2 | 1:AE:56:PHE:CZ | 2.32 | 0.64 |
| 1:AN:100:ALA:HB2 | 1:AO:56:PHE:CZ | 2.32 | 0.64 |
| 1:BN:100:ALA:HB2 | 1:BO:56:PHE:CZ | 2.33 | 0.64 |
| 1:C3:100:ALA:HB2 | 1:C4:56:PHE:CZ | 2.33 | 0.64 |
| 1:BG:96:ALA:HB2 | 1:BG:112:PHE:CZ | 2.33 | 0.64 |
| 1:CG:96:ALA:HB2 | 1:CG:112:PHE:CZ | 2.33 | 0.64 |
| 1:AP:53:PRO:HD2 | 1:AP:57:GLU:HB2 | 1.79 | 0.64 |
| 1:BH:38:LYS:NZ | 1:BH:44:GLU:HG3 | 2.11 | 0.64 |
| 1:CR:38:LYS:NZ | 1:CR:44:GLU:HG3 | 2.11 | 0.64 |
| 1:AY:75:ILE:HG22 | 1:AY:77:LEU:HD13 | 1.78 | 0.64 |
| 1:BD:149:SER:O | 1:BD:152:TRP:CE2 | 2.50 | 0.64 |
| 1:AH:106:THR:O | 1:AH:107:ASP:CB | 2.41 | 0.64 |
| 1:BB:4:GLU:HG2 | 1:BC:51:TRP:CD1 | 2.32 | 0.64 |
| 1:AA:7:LEU:HD11 | 1:AA:140:VAL:HG13 | 1.79 | 0.64 |
| 1:CY:107:ASP:O | 1:CY:107:ASP:CG | 2.35 | 0.64 |
| 1:CI:100:ALA:HB2 | 1:CJ:56:PHE:CZ | 2.32 | 0.64 |
| 1:A4:107:ASP:O | 1:A4:107:ASP:CG | 2.35 | 0.64 |
| 1:CD:100:ALA:HB2 | 1:CE:56:PHE:CZ | 2.33 | 0.64 |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:CG1 | 2.27 | 0.64 |
| 1:BD:120:ILE:HD11 | 1:BR:129:THR:HG21 | 1.79 | 0.64 |
| 1:BB:98:GLY:HA2 | 1:BB:102:LEU:HD23 | 1.80 | 0.64 |
| 1:AV:96:ALA:O | 1:AV:100:ALA:CB | 2.45 | 0.64 |
| 1:C1:96:ALA:HB2 | 1:C1:112:PHE:CZ | 2.33 | 0.64 |
| 1:BV:96:ALA:HB2 | 1:BV:112:PHE:CZ | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BV:96:ALA:C | 1:BV:100:ALA:CB | 2.63 | 0.64 |
| 1:BQ:96:ALA:HB2 | 1:BQ:112:PHE:CZ | 2.33 | 0.64 |
| 1:CG:98:GLY:HA2 | 1:CG:102:LEU:HD23 | 1.80 | 0.64 |
| 1:BP:53:PRO:HD2 | 1:BP:57:GLU:HB2 | 1.79 | 0.64 |
| 1:BK:53:PRO:HD2 | 1:BK:57:GLU:HB2 | 1.79 | 0.64 |
| 1:CH:38:LYS:NZ | 1:CH:44:GLU:HG3 | 2.11 | 0.64 |
| 1:CM:38:LYS:NZ | 1:CM:44:GLU:HG3 | 2.11 | 0.64 |
| 1:AJ:75:ILE:HG22 | 1:AJ:77:LEU:HD13 | 1.78 | 0.64 |
| 1:CO:75:ILE:HG22 | 1:CO:77:LEU:HD13 | 1.78 | 0.64 |
| 1:CE:75:ILE:HG22 | 1:CE:77:LEU:HD13 | 1.78 | 0.64 |
| 1:AT:75:ILE:HG22 | 1:AT:77:LEU:HD13 | 1.78 | 0.64 |
| 1:AN:149:SER:O | 1:AN:152:TRP:CE2 | 2.51 | 0.64 |
| 1:CC:106:THR:O | 1:CC:107:ASP:HB3 | 1.96 | 0.64 |
| 1:CH:106:THR:O | 1:CH:107:ASP:HB3 | 1.96 | 0.64 |
| 1:CF:7:LEU:HD23 | 1:CQ:40:HIS:CE1 | 2.32 | 0.64 |
| 1:CY:58:ILE:O | 1:CY:58:ILE:HG22 | 1.96 | 0.64 |
| 1:CG:4:GLU:HG2 | 1:CH:51:TRP:CD1 | 2.32 | 0.64 |
| 1:AX:100:ALA:HB2 | 1:AY:56:PHE:CZ | 2.33 | 0.64 |
| 1:BE:58:ILE:HG22 | 1:BE:58:ILE:O | 1.96 | 0.64 |
| 1:BD:119:THR:HG22 | 1:BD:121:GLU:H | 1.63 | 0.64 |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:HD11 | 1.75 | 0.64 |
| 1:AQ:100:ALA:HA | 1:AR:56:PHE:HZ | 1.62 | 0.64 |
| 1:CL:98:GLY:O | 1:CL:102:LEU:HB3 | 1.98 | 0.64 |
| 1:CL:100:ALA:HA | 1:CM:56:PHE:HZ | 1.62 | 0.64 |
| 1:AA:53:PRO:HD2 | 1:AA:57:GLU:HB2 | 1.79 | 0.64 |
| 1:A2:38:LYS:NZ | 1:A2:44:GLU:HG3 | 2.11 | 0.64 |
| 1:CI:149:SER:O | 1:CI:152:TRP:CE2 | 2.50 | 0.64 |
| 1:C3:119:THR:HG22 | 1:C3:121:GLU:H | 1.63 | 0.64 |
| 1:CX:119:THR:HG22 | 1:CX:121:GLU:H | 1.63 | 0.64 |
| 1:CS:100:ALA:HB2 | 1:CT:56:PHE:CZ | 2.32 | 0.64 |
| 1:C4:107:ASP:O | 1:C4:107:ASP:CG | 2.35 | 0.64 |
| 1:BL:98:GLY:O | 1:BL:102:LEU:HB3 | 1.98 | 0.64 |
| 1:B1:96:ALA:HB2 | 1:B1:112:PHE:CZ | 2.33 | 0.64 |
| 1:CQ:98:GLY:O | 1:CQ:102:LEU:HB3 | 1.98 | 0.64 |
| 1:AI:149:SER:O | 1:AI:152:TRP:CE2 | 2.51 | 0.64 |
| 1:BF:7:LEU:HD11 | 1:BF:140:VAL:HG13 | 1.79 | 0.64 |
| 1:BQ:18:VAL:HG22 | 1:BQ:77:LEU:HB2 | 1.80 | 0.64 |
| 1:BX:119:THR:HG22 | 1:BX:121:GLU:H | 1.63 | 0.64 |
| 1:BI:119:THR:HG22 | 1:BI:121:GLU:H | 1.63 | 0.64 |
| 1:B1:4:GLU:HG2 | 1:B2:51:TRP:HD1 | 1.61 | 0.64 |
| 1:CI:119:THR:HG22 | 1:CI:121:GLU:H | 1.63 | 0.64 |
| 1:AE:58:ILE:HG22 | 1:AE:58:ILE:O | 1.96 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B3:100:ALA:HB2 | 1:B4:56:PHE:CZ | 2.33 | 0.64 |
| 1:B4:58:ILE:O | 1:B4:58:ILE:HG22 | 1.96 | 0.64 |
| 1:BX:100:ALA:HB2 | 1:BY:56:PHE:CZ | 2.32 | 0.64 |
| 1:AX:119:THR:HG22 | 1:AX:121:GLU:H | 1.63 | 0.64 |
| 1:BB:98:GLY:O | 1:BB:102:LEU:HB3 | 1.98 | 0.64 |
| 1:AG:98:GLY:O | 1:AG:102:LEU:HB3 | 1.98 | 0.64 |
| 1:AL:98:GLY:O | 1:AL:102:LEU:HB3 | 1.98 | 0.64 |
| 1:AB:98:GLY:O | 1:AB:102:LEU:HB3 | 1.98 | 0.64 |
| 1:BG:98:GLY:O | 1:BG:102:LEU:HB3 | 1.98 | 0.64 |
| 1:BG:100:ALA:HA | 1:BH:56:PHE:HZ | 1.62 | 0.64 |
| 1:CG:100:ALA:HA | 1:CH:56:PHE:HZ | 1.62 | 0.64 |
| 1:CV:96:ALA:HB2 | 1:CV:112:PHE:CZ | 2.33 | 0.64 |
| 1:A3:149:SER:O | 1:A3:152:TRP:CE2 | 2.51 | 0.64 |
| 1:CB:4:GLU:HG2 | 1:CC:51:TRP:CD1 | 2.32 | 0.64 |
| 1:CV:4:GLU:HG2 | 1:CW:51:TRP:HD1 | 1.61 | 0.64 |
| 1:CB:98:GLY:O | 1:CB:102:LEU:HB3 | 1.98 | 0.64 |
| 1:C1:98:GLY:O | 1:C1:102:LEU:HB3 | 1.98 | 0.64 |
| 1:CL:98:GLY:HA2 | 1:CL:102:LEU:HD23 | 1.80 | 0.64 |
| 1:BV:98:GLY:O | 1:BV:102:LEU:HB3 | 1.98 | 0.64 |
| 1:BV:100:ALA:HA | 1:BW:56:PHE:HZ | 1.62 | 0.64 |
| 1:BN:149:SER:O | 1:BN:152:TRP:CE2 | 2.51 | 0.64 |
| 1:AS:149:SER:O | 1:AS:152:TRP:CE2 | 2.51 | 0.64 |
| 1:C3:149:SER:O | 1:C3:152:TRP:CE2 | 2.50 | 0.64 |
| 1:AD:149:SER:O | 1:AD:152:TRP:CE2 | 2.51 | 0.64 |
| 1:BB:18:VAL:HG22 | 1:BB:77:LEU:HB2 | 1.80 | 0.64 |
| 1:CQ:4:GLU:HG2 | 1:CR:51:TRP:CD1 | 2.32 | 0.64 |
| 1:CG:4:GLU:HG2 | 1:CH:51:TRP:HD1 | 1.61 | 0.64 |
| 1:AO:107:ASP:CG | 1:AO:107:ASP:O | 2.35 | 0.64 |
| 1:AY:58:ILE:HG22 | 1:AY:58:ILE:O | 1.96 | 0.64 |
| 1:AV:96:ALA:HB2 | 1:AV:112:PHE:CZ | 2.33 | 0.64 |
| 1:CB:96:ALA:HB2 | 1:CB:112:PHE:CZ | 2.33 | 0.64 |
| 1:AG:96:ALA:HB2 | 1:AG:112:PHE:CZ | 2.33 | 0.64 |
| 1:BL:96:ALA:HB2 | 1:BL:112:PHE:CZ | 2.33 | 0.64 |
| 1:AL:96:ALA:HB2 | 1:AL:112:PHE:CZ | 2.33 | 0.64 |
| 1:AB:96:ALA:O | 1:AB:100:ALA:CB | 2.45 | 0.64 |
| 1:B1:98:GLY:HA2 | 1:B1:102:LEU:HD23 | 1.80 | 0.64 |
| 1:BQ:100:ALA:HA | 1:BR:56:PHE:HZ | 1.62 | 0.64 |
| 1:CV:98:GLY:O | 1:CV:102:LEU:HB3 | 1.98 | 0.64 |
| 1:BR:82:ARG:HH11 | 1:BR:82:ARG:CG | 2.11 | 0.64 |
| 1:BV:4:GLU:HG2 | 1:BW:51:TRP:CD1 | 2.32 | 0.64 |
| 1:AJ:107:ASP:CG | 1:AJ:107:ASP:O | 2.35 | 0.64 |
| 1:AI:100:ALA:HB2 | 1:AJ:56:PHE:CZ | 2.32 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AL:100:ALA:HA | 1:AM:56:PHE:HZ | 1.62 | 0.64 |
| 1:CV:98:GLY:HA2 | 1:CV:102:LEU:HD23 | 1.80 | 0.64 |
| 1:CP:53:PRO:HD2 | 1:CP:57:GLU:HB2 | 1.79 | 0.64 |
| 1:CX:149:SER:O | 1:CX:152:TRP:CE2 | 2.51 | 0.64 |
| 1:C1:18:VAL:HG22 | 1:C1:77:LEU:HB2 | 1.80 | 0.64 |
| 1:AF:7:LEU:HD11 | 1:AF:140:VAL:HG13 | 1.79 | 0.64 |
| 1:AJ:58:ILE:HG22 | 1:AJ:58:ILE:O | 1.96 | 0.64 |
| 1:CX:100:ALA:HB2 | 1:CY:56:PHE:CZ | 2.32 | 0.64 |
| 1:AS:100:ALA:HB2 | 1:AT:56:PHE:CZ | 2.33 | 0.64 |
| 1:CT:7:LEU:HB3 | 1:C3:39:ARG:O | 1.98 | 0.64 |
| 1:C1:98:GLY:HA2 | 1:C1:102:LEU:HD23 | 1.80 | 0.64 |
| 1:AF:53:PRO:HD2 | 1:AF:57:GLU:HB2 | 1.79 | 0.64 |
| 1:CF:53:PRO:HD2 | 1:CF:57:GLU:HB2 | 1.79 | 0.64 |
| 1:BZ:53:PRO:HD2 | 1:BZ:57:GLU:HB2 | 1.79 | 0.64 |
| 1:C2:38:LYS:NZ | 1:C2:44:GLU:HG3 | 2.11 | 0.64 |
| 1:CQ:18:VAL:HG22 | 1:CQ:77:LEU:HB2 | 1.80 | 0.64 |
| 1:B1:18:VAL:HG22 | 1:B1:77:LEU:HB2 | 1.80 | 0.64 |
| 1:AQ:18:VAL:HG22 | 1:AQ:77:LEU:HB2 | 1.80 | 0.64 |
| 1:CG:18:VAL:HG22 | 1:CG:77:LEU:HB2 | 1.80 | 0.64 |
| 1:AL:18:VAL:HG22 | 1:AL:77:LEU:HB2 | 1.80 | 0.64 |
| 1:AV:18:VAL:HG22 | 1:AV:77:LEU:HB2 | 1.80 | 0.64 |
| 1:AT:107:ASP:CG | 1:AT:107:ASP:O | 2.35 | 0.64 |
| 1:CU:34:LEU:HD11 | 1:CU:38:LYS:HD2 | 1.80 | 0.64 |
| 1:B4:107:ASP:O | 1:B4:107:ASP:CG | 2.35 | 0.64 |
| 1:AQ:96:ALA:C | 1:AQ:100:ALA:CB | 2.63 | 0.63 |
| 1:CQ:96:ALA:HB2 | 1:CQ:112:PHE:CZ | 2.33 | 0.63 |
| 1:AC:82:ARG:CG | 1:AC:82:ARG:HH11 | 2.11 | 0.63 |
| 1:CN:149:SER:O | 1:CN:152:TRP:CE2 | 2.50 | 0.63 |
| 1:AG:18:VAL:HG22 | 1:AG:77:LEU:HB2 | 1.80 | 0.63 |
| 1:CN:119:THR:HG22 | 1:CN:121:GLU:H | 1.63 | 0.63 |
| 1:AU:34:LEU:HD11 | 1:AU:38:LYS:HD2 | 1.80 | 0.63 |
| 1:AI:119:THR:HG22 | 1:AI:121:GLU:H | 1.63 | 0.63 |
| 1:A3:100:ALA:HB2 | 1:A4:56:PHE:CZ | 2.33 | 0.63 |
| 1:BT:58:ILE:O | 1:BT:58:ILE:HG22 | 1.96 | 0.63 |
| 1:BS:119:THR:HG22 | 1:BS:121:GLU:H | 1.63 | 0.63 |
| 1:BP:34:LEU:HD11 | 1:BP:38:LYS:HD2 | 1.80 | 0.63 |
| 1:CZ:34:LEU:HD11 | 1:CZ:38:LYS:HD2 | 1.80 | 0.63 |
| 1:BB:96:ALA:HB2 | 1:BB:112:PHE:CZ | 2.33 | 0.63 |
| 1:AB:96:ALA:HB2 | 1:AB:112:PHE:CZ | 2.33 | 0.63 |
| 1:BQ:98:GLY:HA2 | 1:BQ:102:LEU:HD23 | 1.80 | 0.63 |
| 1:A1:100:ALA:HA | 1:A2:56:PHE:HZ | 1.62 | 0.63 |
| 1:BC:82:ARG:HH11 | 1:BC:82:ARG:CG | 2.11 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:AW:82:ARG:HH11 | 1:AW:82:ARG:CG | 2.11 | 0.63 |
| 1:CL:18:VAL:HG22 | 1:CL:77:LEU:HB2 | 1.80 | 0.63 |
| 1:A4:58:ILE:O | 1:A4:58:ILE:HG22 | 1.96 | 0.63 |
| 1:CA:7:LEU:HD11 | 1:CA:140:VAL:HG13 | 1.79 | 0.63 |
| 1:CJ:107:ASP:CG | 1:CJ:107:ASP:O | 2.35 | 0.63 |
| 1:CK:7:LEU:HD11 | 1:CK:140:VAL:HG13 | 1.79 | 0.63 |
| 1:AO:55:ALA:HB1 | 1:AO:95:VAL:HG21 | 1.77 | 0.63 |
| 1:BD:100:ALA:HB2 | 1:BE:56:PHE:CZ | 2.32 | 0.63 |
| 1:AI:39:ARG:O | 1:AO:7:LEU:HB3 | 1.99 | 0.63 |
| 1:AQ:96:ALA:HB2 | 1:AQ:112:PHE:CZ | 2.33 | 0.63 |
| 1:CQ:98:GLY:HA2 | 1:CQ:102:LEU:HD23 | 1.80 | 0.63 |
| 1:CV:100:ALA:HA | 1:CW:56:PHE:HZ | 1.62 | 0.63 |
| 1:AX:149:SER:O | 1:AX:152:TRP:CE2 | 2.51 | 0.63 |
| 1:AB:18:VAL:HG22 | 1:AB:77:LEU:HB2 | 1.80 | 0.63 |
| 1:BV:18:VAL:HG22 | 1:BV:77:LEU:HB2 | 1.80 | 0.63 |
| 1:B1:4:GLU:HG2 | 1:B2:51:TRP:CD1 | 2.32 | 0.63 |
| 1:BF:34:LEU:HD11 | 1:BF:38:LYS:HD2 | 1.80 | 0.63 |
| 1:CA:34:LEU:HD11 | 1:CA:38:LYS:HD2 | 1.80 | 0.63 |
| 1:AZ:7:LEU:HD11 | 1:AZ:140:VAL:HG13 | 1.79 | 0.63 |
| 1:BE:107:ASP:CG | 1:BE:107:ASP:O | 2.35 | 0.63 |
| 1:CO:107:ASP:CG | 1:CO:107:ASP:O | 2.35 | 0.63 |
| 1:AQ:98:GLY:HA2 | 1:AQ:102:LEU:HD23 | 1.80 | 0.63 |
| 1:CL:96:ALA:HB2 | 1:CL:112:PHE:CZ | 2.33 | 0.63 |
| 1:BG:98:GLY:HA2 | 1:BG:102:LEU:HD23 | 1.80 | 0.63 |
| 1:A1:98:GLY:O | 1:A1:102:LEU:HB3 | 1.98 | 0.63 |
| 1:A1:98:GLY:HA2 | 1:A1:102:LEU:HD23 | 1.80 | 0.63 |
| 1:CA:53:PRO:HD2 | 1:CA:57:GLU:HB2 | 1.79 | 0.63 |
| 1:CC:82:ARG:HH11 | 1:CC:82:ARG:CG | 2.11 | 0.63 |
| 1:BS:149:SER:O | 1:BS:152:TRP:CE2 | 2.50 | 0.63 |
| 1:CD:149:SER:O | 1:CD:152:TRP:CE2 | 2.51 | 0.63 |
| 1:BG:4:GLU:HG2 | 1:BH:51:TRP:HD1 | 1.61 | 0.63 |
| 1:AY:107:ASP:O | 1:AY:107:ASP:CG | 2.35 | 0.63 |
| 1:BO:107:ASP:O | 1:BO:107:ASP:CG | 2.35 | 0.63 |
| 1:C4:58:ILE:O | 1:C4:58:ILE:HG22 | 1.96 | 0.63 |
| 1:BQ:98:GLY:O | 1:BQ:102:LEU:HB3 | 1.98 | 0.63 |
| 1:CG:7:LEU:HB3 | 1:CU:39:ARG:O | 1.98 | 0.63 |
| 1:AF:39:ARG:HH22 | 1:AQ:144:GLU:CD | 2.02 | 0.63 |
| 1:CW:82:ARG:HH11 | 1:CW:82:ARG:CG | 2.11 | 0.63 |
| 1:A2:82:ARG:CG | 1:A2:82:ARG:HH11 | 2.11 | 0.63 |
| 1:BA:34:LEU:HD11 | 1:BA:38:LYS:HD2 | 1.80 | 0.63 |
| 1:CZ:7:LEU:HD11 | 1:CZ:140:VAL:HG13 | 1.79 | 0.63 |
| 1:BP:7:LEU:HD11 | 1:BP:140:VAL:HG13 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CJ:58:ILE:O | 1:CJ:58:ILE:HG22 | 1.96 | 0.63 |
| 1:CP:7:LEU:HD11 | 1:CP:140:VAL:HG13 | 1.79 | 0.63 |
| 1:AZ:34:LEU:HD11 | 1:AZ:38:LYS:HD2 | 1.80 | 0.63 |
| 1:A3:119:THR:HG22 | 1:A3:121:GLU:H | 1.63 | 0.63 |
| 1:CD:119:THR:HG22 | 1:CD:121:GLU:H | 1.63 | 0.63 |
| 1:AV:98:GLY:O | 1:AV:102:LEU:HB3 | 1.98 | 0.63 |
| 1:AQ:98:GLY:O | 1:AQ:102:LEU:HB3 | 1.98 | 0.63 |
| 1:BV:98:GLY:HA2 | 1:BV:102:LEU:HD23 | 1.80 | 0.63 |
| 1:AF:34:LEU:HD11 | 1:AF:38:LYS:HD2 | 1.80 | 0.63 |
| 1:AG:98:GLY:HA2 | 1:AG:102:LEU:HD23 | 1.80 | 0.63 |
| 1:B1:98:GLY:O | 1:B1:102:LEU:HB3 | 1.98 | 0.63 |
| 1:AM:82:ARG:CG | 1:AM:82:ARG:HH11 | 2.11 | 0.63 |
| 1:CM:82:ARG:HH11 | 1:CM:82:ARG:CG | 2.11 | 0.63 |
| 1:BD:40:HIS:CE1 | 1:BJ:7:LEU:HD23 | 2.34 | 0.63 |
| 1:AV:58:ILE:N | 1:AV:59:PRO:HD2 | 2.14 | 0.63 |
| 1:AR:82:ARG:HH11 | 1:AR:82:ARG:CG | 2.11 | 0.63 |
| 1:BB:107:ASP:HB2 | 1:BB:152:TRP:HZ3 | 1.62 | 0.63 |
| 1:BB:58:ILE:N | 1:BB:59:PRO:HD2 | 2.14 | 0.63 |
| 1:BL:98:GLY:HA2 | 1:BL:102:LEU:HD23 | 1.80 | 0.63 |
| 1:CL:96:ALA:C | 1:CL:100:ALA:CB | 2.63 | 0.63 |
| 1:BG:58:ILE:N | 1:BG:59:PRO:HD2 | 2.14 | 0.63 |
| 1:CV:58:ILE:N | 1:CV:59:PRO:HD2 | 2.14 | 0.63 |
| 1:A1:58:ILE:N | 1:A1:59:PRO:HD2 | 2.14 | 0.63 |
| 1:CR:82:ARG:HH11 | 1:CR:82:ARG:CG | 2.11 | 0.63 |
| 1:AF:58:ILE:N | 1:AF:59:PRO:HD2 | 2.14 | 0.63 |
| 1:CB:18:VAL:HG22 | 1:CB:77:LEU:HB2 | 1.80 | 0.63 |
| 1:BD:7:LEU:HD23 | 1:BJ:40:HIS:CE1 | 2.34 | 0.63 |
| 1:CP:34:LEU:HD11 | 1:CP:38:LYS:HD2 | 1.80 | 0.63 |
| 1:AQ:13:LYS:HZ1 | 1:BU:43:GLU:CG | 2.10 | 0.62 |
| 1:AL:98:GLY:HA2 | 1:AL:102:LEU:HD23 | 1.80 | 0.62 |
| 1:C1:58:ILE:N | 1:C1:59:PRO:HD2 | 2.14 | 0.62 |
| 1:CH:82:ARG:HH11 | 1:CH:82:ARG:CG | 2.11 | 0.62 |
| 1:CU:58:ILE:N | 1:CU:59:PRO:HD2 | 2.14 | 0.62 |
| 1:A1:18:VAL:HG22 | 1:A1:77:LEU:HB2 | 1.80 | 0.62 |
| 1:BK:34:LEU:HD11 | 1:BK:38:LYS:HD2 | 1.80 | 0.62 |
| 1:AN:119:THR:HG22 | 1:AN:121:GLU:H | 1.63 | 0.62 |
| 1:BZ:34:LEU:HD11 | 1:BZ:38:LYS:HD2 | 1.80 | 0.62 |
| 1:B3:119:THR:HG22 | 1:B3:121:GLU:H | 1.63 | 0.62 |
| 1:AW:97:LYS:HG3 | 1:AX:97:LYS:HZ3 | 1.65 | 0.62 |
| 1:BL:58:ILE:N | 1:BL:59:PRO:HD2 | 2.14 | 0.62 |
| 1:AQ:58:ILE:N | 1:AQ:59:PRO:HD2 | 2.14 | 0.62 |
| 1:AB:98:GLY:HA2 | 1:AB:102:LEU:HD23 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BL:18:VAL:HG22 | 1:BL:77:LEU:HB2 | 1.80 | 0.62 |
| 1:CT:7:LEU:HD23 | 1:C3:40:HIS:CE1 | 2.34 | 0.62 |
| 1:BG:18:VAL:HG22 | 1:BG:77:LEU:HB2 | 1.80 | 0.62 |
| 1:BX:151:HIS:HB3 | 1:BY:64:LYS:HB3 | 1.82 | 0.62 |
| 1:CN:151:HIS:HB3 | 1:CO:64:LYS:HB3 | 1.82 | 0.62 |
| 1:CS:119:THR:HG22 | 1:CS:121:GLU:H | 1.63 | 0.62 |
| 1:CF:34:LEU:HD11 | 1:CF:38:LYS:HD2 | 1.80 | 0.62 |
| 1:BN:119:THR:HG22 | 1:BN:121:GLU:H | 1.63 | 0.62 |
| 1:CD:120:ILE:CD1 | 1:CR:129:THR:HG21 | 2.30 | 0.62 |
| 1:CB:58:ILE:N | 1:CB:59:PRO:HD2 | 2.14 | 0.62 |
| 1:AB:58:ILE:N | 1:AB:59:PRO:HD2 | 2.14 | 0.62 |
| 1:C2:82:ARG:CG | 1:C2:82:ARG:HH11 | 2.11 | 0.62 |
| 1:AK:58:ILE:N | 1:AK:59:PRO:HD2 | 2.14 | 0.62 |
| 1:BP:58:ILE:N | 1:BP:59:PRO:HD2 | 2.14 | 0.62 |
| 1:CF:58:ILE:N | 1:CF:59:PRO:HD2 | 2.14 | 0.62 |
| 1:BK:58:ILE:N | 1:BK:59:PRO:HD2 | 2.14 | 0.62 |
| 1:CD:151:HIS:HB3 | 1:CE:64:LYS:HB3 | 1.82 | 0.62 |
| 1:AU:7:LEU:HD11 | 1:AU:140:VAL:HG13 | 1.79 | 0.62 |
| 1:AG:58:ILE:N | 1:AG:59:PRO:HD2 | 2.14 | 0.62 |
| 1:BH:82:ARG:HH11 | 1:BH:82:ARG:CG | 2.11 | 0.62 |
| 1:CK:58:ILE:N | 1:CK:59:PRO:HD2 | 2.15 | 0.62 |
| 1:AP:58:ILE:N | 1:AP:59:PRO:HD2 | 2.14 | 0.62 |
| 1:AS:151:HIS:HB3 | 1:AT:64:LYS:HB3 | 1.81 | 0.62 |
| 1:B4:152:TRP:HE3 | 1:B4:153:ALA:H | 1.48 | 0.62 |
| 1:C4:152:TRP:HE3 | 1:C4:153:ALA:H | 1.47 | 0.62 |
| 1:AT:152:TRP:HE3 | 1:AT:153:ALA:H | 1.48 | 0.62 |
| 1:CX:22:ASN:HA | 1:C2:128:GLY:O | 2.00 | 0.62 |
| 1:CQ:58:ILE:N | 1:CQ:59:PRO:HD2 | 2.14 | 0.62 |
| 1:CG:98:GLY:O | 1:CG:102:LEU:HB3 | 1.98 | 0.62 |
| 1:B2:82:ARG:CG | 1:B2:82:ARG:HH11 | 2.11 | 0.62 |
| 1:CS:151:HIS:HB3 | 1:CT:64:LYS:HB3 | 1.82 | 0.62 |
| 1:A3:151:HIS:HB3 | 1:A4:64:LYS:HB3 | 1.82 | 0.62 |
| 1:BN:151:HIS:HB3 | 1:BO:64:LYS:HB3 | 1.82 | 0.62 |
| 1:CV:18:VAL:HG22 | 1:CV:77:LEU:HB2 | 1.80 | 0.62 |
| 1:BU:34:LEU:HD11 | 1:BU:38:LYS:HD2 | 1.80 | 0.62 |
| 1:CK:34:LEU:HD11 | 1:CK:38:LYS:HD2 | 1.80 | 0.62 |
| 1:AD:119:THR:HG22 | 1:AD:121:GLU:H | 1.63 | 0.62 |
| 1:AK:34:LEU:HD11 | 1:AK:38:LYS:HD2 | 1.80 | 0.62 |
| 1:C1:107:ASP:HB2 | 1:C1:152:TRP:HZ3 | 1.62 | 0.62 |
| 1:CB:98:GLY:HA2 | 1:CB:102:LEU:HD23 | 1.80 | 0.62 |
| 1:CG:58:ILE:N | 1:CG:59:PRO:HD2 | 2.14 | 0.62 |
| 1:AH:82:ARG:CG | 1:AH:82:ARG:HH11 | 2.11 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BC:38:LYS:HZ2 | 1:BC:44:GLU:HG3 | 1.64 | 0.62 |
| 1:AI:151:HIS:HB3 | 1:AJ:64:LYS:HB3 | 1.82 | 0.62 |
| 1:CE:152:TRP:HE3 | 1:CE:153:ALA:H | 1.48 | 0.62 |
| 1:CC:8:VAL:HG13 | 1:CR:8:VAL:HG21 | 1.81 | 0.62 |
| 1:AV:98:GLY:HA2 | 1:AV:102:LEU:HD23 | 1.80 | 0.62 |
| 1:CT:58:ILE:N | 1:CT:59:PRO:HD2 | 2.15 | 0.62 |
| 1:A4:58:ILE:N | 1:A4:59:PRO:HD2 | 2.15 | 0.62 |
| 1:BQ:58:ILE:N | 1:BQ:59:PRO:HD2 | 2.14 | 0.62 |
| 1:CP:58:ILE:N | 1:CP:59:PRO:HD2 | 2.14 | 0.62 |
| 1:BD:151:HIS:HB3 | 1:BE:64:LYS:HB3 | 1.82 | 0.62 |
| 1:BJ:152:TRP:HE3 | 1:BJ:153:ALA:H | 1.47 | 0.62 |
| 1:CC:129:THR:O | 1:CC:132:GLY:N | 2.25 | 0.62 |
| 1:BU:58:ILE:N | 1:BU:59:PRO:HD2 | 2.14 | 0.62 |
| 1:B4:58:ILE:N | 1:B4:59:PRO:HD2 | 2.15 | 0.62 |
| 1:BT:152:TRP:HE3 | 1:BT:153:ALA:H | 1.48 | 0.62 |
| 1:AU:58:ILE:N | 1:AU:59:PRO:HD2 | 2.14 | 0.61 |
| 1:CZ:58:ILE:N | 1:CZ:59:PRO:HD2 | 2.14 | 0.61 |
| 1:AZ:58:ILE:N | 1:AZ:59:PRO:HD2 | 2.14 | 0.61 |
| 1:BI:151:HIS:HB3 | 1:BJ:64:LYS:HB3 | 1.82 | 0.61 |
| 1:AY:58:ILE:N | 1:AY:59:PRO:HD2 | 2.15 | 0.61 |
| 1:BO:152:TRP:HE3 | 1:BO:153:ALA:H | 1.48 | 0.61 |
| 1:CR:129:THR:O | 1:CR:132:GLY:N | 2.25 | 0.61 |
| 1:AA:58:ILE:N | 1:AA:59:PRO:HD2 | 2.14 | 0.61 |
| 1:BF:58:ILE:N | 1:BF:59:PRO:HD2 | 2.14 | 0.61 |
| 1:AD:151:HIS:HB3 | 1:AE:64:LYS:HB3 | 1.82 | 0.61 |
| 1:CI:151:HIS:HB3 | 1:CJ:64:LYS:HB3 | 1.81 | 0.61 |
| 1:AE:58:ILE:N | 1:AE:59:PRO:HD2 | 2.15 | 0.61 |
| 1:AA:34:LEU:HD11 | 1:AA:38:LYS:HD2 | 1.80 | 0.61 |
| 1:BT:58:ILE:N | 1:BT:59:PRO:HD2 | 2.15 | 0.61 |
| 1:B2:6:HIS:HE1 | 1:B2:8:VAL:HB | 1.66 | 0.61 |
| 1:BL:97:LYS:HE3 | 1:BM:97:LYS:HZ3 | 1.64 | 0.61 |
| 1:A1:148:LEU:HD13 | 1:A2:61:ILE:HD11 | 1.83 | 0.61 |
| 1:BA:58:ILE:N | 1:BA:59:PRO:HD2 | 2.14 | 0.61 |
| 1:AX:151:HIS:HB3 | 1:AY:64:LYS:HB3 | 1.82 | 0.61 |
| 1:CE:58:ILE:N | 1:CE:59:PRO:HD2 | 2.15 | 0.61 |
| 1:C4:58:ILE:N | 1:C4:59:PRO:HD2 | 2.15 | 0.61 |
| 1:CJ:58:ILE:N | 1:CJ:59:PRO:HD2 | 2.15 | 0.61 |
| 1:AA:34:LEU:HD12 | 1:AA:38:LYS:HB2 | 1.83 | 0.61 |
| 1:CW:100:ALA:HB2 | 1:CX:56:PHE:CZ | 2.36 | 0.61 |
| 1:AE:152:TRP:HE3 | 1:AE:153:ALA:H | 1.48 | 0.61 |
| 1:B1:58:ILE:N | 1:B1:59:PRO:HD2 | 2.14 | 0.61 |
| 1:CL:58:ILE:N | 1:CL:59:PRO:HD2 | 2.14 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BS:151:HIS:HB3 | 1:BT:64:LYS:HB3 | 1.82 | 0.61 |
| 1:BJ:58:ILE:N | 1:BJ:59:PRO:HD2 | 2.15 | 0.61 |
| 1:AJ:58:ILE:N | 1:AJ:59:PRO:HD2 | 2.15 | 0.61 |
| 1:CZ:34:LEU:HD12 | 1:CZ:38:LYS:HB2 | 1.83 | 0.61 |
| 1:CC:6:HIS:HE1 | 1:CC:8:VAL:HB | 1.66 | 0.61 |
| 1:AS:119:THR:HG22 | 1:AS:121:GLU:H | 1.63 | 0.61 |
| 1:AR:6:HIS:HE1 | 1:AR:8:VAL:HB | 1.66 | 0.61 |
| 1:B2:100:ALA:HB2 | 1:B3:56:PHE:CZ | 2.36 | 0.61 |
| 1:CT:152:TRP:HE3 | 1:CT:153:ALA:H | 1.47 | 0.61 |
| 1:CO:53:PRO:CD | 1:CO:57:GLU:HG3 | 2.29 | 0.61 |
| 1:AW:129:THR:O | 1:AW:132:GLY:N | 2.25 | 0.61 |
| 1:BV:58:ILE:N | 1:BV:59:PRO:HD2 | 2.14 | 0.61 |
| 1:CQ:148:LEU:HD13 | 1:CR:61:ILE:HD11 | 1.83 | 0.61 |
| 1:BQ:148:LEU:HD13 | 1:BR:61:ILE:HD11 | 1.83 | 0.61 |
| 1:AQ:148:LEU:HD13 | 1:AR:61:ILE:HD11 | 1.83 | 0.61 |
| 1:CA:58:ILE:N | 1:CA:59:PRO:HD2 | 2.14 | 0.61 |
| 1:B3:151:HIS:HB3 | 1:B4:64:LYS:HB3 | 1.82 | 0.61 |
| 1:BP:34:LEU:HD12 | 1:BP:38:LYS:HB2 | 1.83 | 0.61 |
| 1:BF:34:LEU:HD12 | 1:BF:38:LYS:HB2 | 1.83 | 0.61 |
| 1:BA:34:LEU:HD12 | 1:BA:38:LYS:HB2 | 1.83 | 0.61 |
| 1:BU:34:LEU:HD12 | 1:BU:38:LYS:HB2 | 1.83 | 0.61 |
| 1:AR:100:ALA:HB2 | 1:AS:56:PHE:CZ | 2.36 | 0.61 |
| 1:BM:100:ALA:HB2 | 1:BN:56:PHE:CZ | 2.36 | 0.61 |
| 1:AW:6:HIS:HE1 | 1:AW:8:VAL:HB | 1.66 | 0.61 |
| 1:BW:100:ALA:HB2 | 1:BX:56:PHE:CZ | 2.36 | 0.61 |
| 1:CM:6:HIS:HE1 | 1:CM:8:VAL:HB | 1.66 | 0.61 |
| 1:BV:148:LEU:HD13 | 1:BW:61:ILE:HD11 | 1.83 | 0.61 |
| 1:CG:24:PHE:CE2 | 1:CQ:124:ILE:HD11 | 2.35 | 0.61 |
| 1:CO:58:ILE:N | 1:CO:59:PRO:HD2 | 2.15 | 0.61 |
| 1:AT:58:ILE:N | 1:AT:59:PRO:HD2 | 2.15 | 0.61 |
| 1:BO:58:ILE:N | 1:BO:59:PRO:HD2 | 2.15 | 0.61 |
| 1:AU:34:LEU:HD12 | 1:AU:38:LYS:HB2 | 1.83 | 0.61 |
| 1:CH:100:ALA:HB2 | 1:CI:56:PHE:CZ | 2.36 | 0.61 |
| 1:A2:100:ALA:HB2 | 1:A3:56:PHE:CZ | 2.36 | 0.61 |
| 1:AW:100:ALA:HB2 | 1:AX:56:PHE:CZ | 2.36 | 0.61 |
| 1:AP:34:LEU:HD11 | 1:AP:38:LYS:HD2 | 1.80 | 0.61 |
| 1:AY:53:PRO:CD | 1:AY:57:GLU:HG3 | 2.29 | 0.61 |
| 1:BH:129:THR:O | 1:BH:132:GLY:N | 2.25 | 0.61 |
| 1:C1:148:LEU:HD13 | 1:C2:61:ILE:HD11 | 1.83 | 0.61 |
| 1:BW:82:ARG:HH11 | 1:BW:82:ARG:CG | 2.11 | 0.61 |
| 1:BR:63:LYS:O | 1:BR:67:ASN:HB2 | 2.01 | 0.61 |
| 1:AO:58:ILE:N | 1:AO:59:PRO:HD2 | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:AP:34:LEU:HD12 | 1:AP:38:LYS:HB2 | 1.83 | 0.61 |
| 1:CH:6:HIS:HE1 | 1:CH:8:VAL:HB | 1.66 | 0.61 |
| 1:B2:63:LYS:O | 1:B2:67:ASN:HB2 | 2.01 | 0.61 |
| 1:B4:53:PRO:CD | 1:B4:57:GLU:HG3 | 2.29 | 0.61 |
| 1:CH:129:THR:O | 1:CH:132:GLY:N | 2.25 | 0.61 |
| 1:B2:97:LYS:HG3 | 1:B3:97:LYS:HZ3 | 1.65 | 0.61 |
| 1:AB:148:LEU:HD13 | 1:AC:61:ILE:HD11 | 1.83 | 0.61 |
| 1:AG:148:LEU:HD13 | 1:AH:61:ILE:HD11 | 1.83 | 0.61 |
| 1:AV:148:LEU:HD13 | 1:AW:61:ILE:HD11 | 1.83 | 0.61 |
| 1:B1:148:LEU:HD13 | 1:B2:61:ILE:HD11 | 1.83 | 0.61 |
| 1:CV:148:LEU:HD13 | 1:CW:61:ILE:HD11 | 1.83 | 0.61 |
| 1:AW:63:LYS:O | 1:AW:67:ASN:HB2 | 2.01 | 0.61 |
| 1:BM:63:LYS:O | 1:BM:67:ASN:HB2 | 2.01 | 0.61 |
| 1:CM:63:LYS:O | 1:CM:67:ASN:HB2 | 2.01 | 0.61 |
| 1:CH:63:LYS:O | 1:CH:67:ASN:HB2 | 2.01 | 0.61 |
| 1:BE:58:ILE:N | 1:BE:59:PRO:HD2 | 2.15 | 0.61 |
| 1:BZ:34:LEU:HD12 | 1:BZ:38:LYS:HB2 | 1.83 | 0.61 |
| 1:AC:100:ALA:HB2 | 1:AD:56:PHE:CZ | 2.36 | 0.61 |
| 1:AM:6:HIS:HE1 | 1:AM:8:VAL:HB | 1.66 | 0.61 |
| 1:BC:6:HIS:HE1 | 1:BC:8:VAL:HB | 1.66 | 0.61 |
| 1:CI:124:ILE:O | 1:CI:129:THR:OG1 | 2.16 | 0.61 |
| 1:BN:124:ILE:O | 1:BN:129:THR:OG1 | 2.16 | 0.61 |
| 1:CY:152:TRP:HE3 | 1:CY:153:ALA:H | 1.48 | 0.61 |
| 1:AL:58:ILE:N | 1:AL:59:PRO:HD2 | 2.14 | 0.61 |
| 1:BG:148:LEU:HD13 | 1:BH:61:ILE:HD11 | 1.83 | 0.61 |
| 1:CB:148:LEU:HD13 | 1:CC:61:ILE:HD11 | 1.83 | 0.61 |
| 1:AF:39:ARG:O | 1:AQ:7:LEU:HB3 | 2.01 | 0.61 |
| 1:BZ:58:ILE:N | 1:BZ:59:PRO:HD2 | 2.14 | 0.61 |
| 1:C3:151:HIS:HB3 | 1:C4:64:LYS:HB3 | 1.82 | 0.61 |
| 1:AN:151:HIS:HB3 | 1:AO:64:LYS:HB3 | 1.82 | 0.61 |
| 1:CY:58:ILE:N | 1:CY:59:PRO:HD2 | 2.15 | 0.61 |
| 1:AZ:34:LEU:HD12 | 1:AZ:38:LYS:HB2 | 1.83 | 0.61 |
| 1:CK:34:LEU:HD12 | 1:CK:38:LYS:HB2 | 1.83 | 0.61 |
| 1:BH:100:ALA:HB2 | 1:BI:56:PHE:CZ | 2.36 | 0.61 |
| 1:C2:6:HIS:HE1 | 1:C2:8:VAL:HB | 1.66 | 0.61 |
| 1:AD:124:ILE:O | 1:AD:129:THR:OG1 | 2.16 | 0.61 |
| 1:BW:6:HIS:HE1 | 1:BW:8:VAL:HB | 1.66 | 0.61 |
| 1:AH:100:ALA:HB2 | 1:AI:56:PHE:CZ | 2.36 | 0.61 |
| 1:AJ:152:TRP:HE3 | 1:AJ:153:ALA:H | 1.48 | 0.61 |
| 1:BM:82:ARG:CG | 1:BM:82:ARG:HH11 | 2.11 | 0.60 |
| 1:AK:34:LEU:HD12 | 1:AK:38:LYS:HB2 | 1.83 | 0.60 |
| 1:A2:6:HIS:HE1 | 1:A2:8:VAL:HB | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:CM:100:ALA:HB2 | 1:CN:56:PHE:CZ | 2.36 | 0.60 |
| 1:CR:97:LYS:HG3 | 1:CS:97:LYS:HZ1 | 1.66 | 0.60 |
| 1:BR:20:ARG:HG3 | 1:BR:52:VAL:O | 2.01 | 0.60 |
| 1:AR:63:LYS:O | 1:AR:67:ASN:HB2 | 2.01 | 0.60 |
| 1:C2:63:LYS:O | 1:C2:67:ASN:HB2 | 2.01 | 0.60 |
| 1:BY:58:ILE:N | 1:BY:59:PRO:HD2 | 2.15 | 0.60 |
| 1:CA:34:LEU:HD12 | 1:CA:38:LYS:HB2 | 1.83 | 0.60 |
| 1:CP:34:LEU:HD12 | 1:CP:38:LYS:HB2 | 1.83 | 0.60 |
| 1:C2:100:ALA:HB2 | 1:C3:56:PHE:CZ | 2.36 | 0.60 |
| 1:CD:124:ILE:O | 1:CD:129:THR:OG1 | 2.16 | 0.60 |
| 1:CW:129:THR:O | 1:CW:132:GLY:N | 2.25 | 0.60 |
| 1:BC:20:ARG:HG3 | 1:BC:52:VAL:O | 2.01 | 0.60 |
| 1:CX:151:HIS:HB3 | 1:CY:64:LYS:HB3 | 1.82 | 0.60 |
| 1:AF:34:LEU:HD12 | 1:AF:38:LYS:HB2 | 1.83 | 0.60 |
| 1:BC:63:LYS:O | 1:BC:67:ASN:HB2 | 2.01 | 0.60 |
| 1:AM:100:ALA:HB2 | 1:AN:56:PHE:CZ | 2.36 | 0.60 |
| 1:CP:28:LYS:HD2 | 1:CW:24:PHE:CD1 | 2.36 | 0.60 |
| 1:BH:6:HIS:HE1 | 1:BH:8:VAL:HB | 1.66 | 0.60 |
| 1:CR:20:ARG:HG3 | 1:CR:52:VAL:O | 2.02 | 0.60 |
| 1:CC:20:ARG:HG3 | 1:CC:52:VAL:O | 2.01 | 0.60 |
| 1:CW:63:LYS:O | 1:CW:67:ASN:HB2 | 2.01 | 0.60 |
| 1:BR:6:HIS:HE1 | 1:BR:8:VAL:HB | 1.66 | 0.60 |
| 1:CO:152:TRP:HE3 | 1:CO:153:ALA:H | 1.47 | 0.60 |
| 1:CY:53:PRO:CD | 1:CY:57:GLU:HG3 | 2.29 | 0.60 |
| 1:AH:63:LYS:O | 1:AH:67:ASN:HB2 | 2.01 | 0.60 |
| 1:BE:152:TRP:HE3 | 1:BE:153:ALA:H | 1.48 | 0.60 |
| 1:CR:100:ALA:HB2 | 1:CS:56:PHE:CZ | 2.36 | 0.60 |
| 1:CC:100:ALA:HB2 | 1:CD:56:PHE:CZ | 2.36 | 0.60 |
| 1:BM:6:HIS:HE1 | 1:BM:8:VAL:HB | 1.66 | 0.60 |
| 1:CJ:152:TRP:HE3 | 1:CJ:153:ALA:H | 1.47 | 0.60 |
| 1:AM:63:LYS:O | 1:AM:67:ASN:HB2 | 2.01 | 0.60 |
| 1:AC:63:LYS:O | 1:AC:67:ASN:HB2 | 2.01 | 0.60 |
| 1:BC:100:ALA:HB2 | 1:BD:56:PHE:CZ | 2.36 | 0.60 |
| 1:CW:6:HIS:HE1 | 1:CW:8:VAL:HB | 1.66 | 0.60 |
| 1:AH:20:ARG:HG3 | 1:AH:52:VAL:O | 2.02 | 0.60 |
| 1:AW:20:ARG:HG3 | 1:AW:52:VAL:O | 2.01 | 0.60 |
| 1:C2:20:ARG:HG3 | 1:C2:52:VAL:O | 2.01 | 0.60 |
| 1:BH:63:LYS:O | 1:BH:67:ASN:HB2 | 2.01 | 0.60 |
| 1:CK:95:VAL:HG12 | 1:CK:112:PHE:HE1 | 1.67 | 0.60 |
| 1:AP:95:VAL:HG12 | 1:AP:112:PHE:HE1 | 1.67 | 0.60 |
| 1:BK:34:LEU:HD12 | 1:BK:38:LYS:HB2 | 1.83 | 0.60 |
| 1:BD:124:ILE:O | 1:BD:129:THR:OG1 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BH:20:ARG:HG3 | 1:BH:52:VAL:O | 2.01 | 0.60 |
| 1:CW:20:ARG:HG3 | 1:CW:52:VAL:O | 2.01 | 0.60 |
| 1:BA:95:VAL:HG12 | 1:BA:112:PHE:HE1 | 1.67 | 0.60 |
| 1:A2:63:LYS:O | 1:A2:67:ASN:HB2 | 2.01 | 0.60 |
| 1:BZ:95:VAL:HG12 | 1:BZ:112:PHE:HE1 | 1.67 | 0.60 |
| 1:A4:152:TRP:HE3 | 1:A4:153:ALA:H | 1.48 | 0.60 |
| 1:AN:124:ILE:O | 1:AN:129:THR:OG1 | 2.16 | 0.60 |
| 1:AH:6:HIS:HE1 | 1:AH:8:VAL:HB | 1.66 | 0.60 |
| 1:BF:39:ARG:HH22 | 1:BQ:144:GLU:CD | 2.05 | 0.60 |
| 1:CC:63:LYS:O | 1:CC:67:ASN:HB2 | 2.01 | 0.60 |
| 1:AM:20:ARG:HG3 | 1:AM:52:VAL:O | 2.02 | 0.60 |
| 1:AL:148:LEU:HD13 | 1:AM:61:ILE:HD11 | 1.83 | 0.60 |
| 1:BW:20:ARG:HG3 | 1:BW:52:VAL:O | 2.01 | 0.60 |
| 1:AR:20:ARG:HG3 | 1:AR:52:VAL:O | 2.01 | 0.60 |
| 1:CA:95:VAL:HG12 | 1:CA:112:PHE:HE1 | 1.67 | 0.60 |
| 1:BK:95:VAL:HG12 | 1:BK:112:PHE:HE1 | 1.67 | 0.60 |
| 1:BR:100:ALA:HB2 | 1:BS:56:PHE:CZ | 2.36 | 0.60 |
| 1:AC:6:HIS:HE1 | 1:AC:8:VAL:HB | 1.66 | 0.60 |
| 1:AT:53:PRO:CD | 1:AT:57:GLU:HG3 | 2.29 | 0.59 |
| 1:AG:97:LYS:HE3 | 1:AH:97:LYS:NZ | 2.17 | 0.59 |
| 1:CL:97:LYS:HE3 | 1:CM:97:LYS:HZ3 | 1.67 | 0.59 |
| 1:BQ:97:LYS:HE3 | 1:BR:97:LYS:NZ | 2.17 | 0.59 |
| 1:CG:148:LEU:HD13 | 1:CH:61:ILE:HD11 | 1.83 | 0.59 |
| 1:CZ:95:VAL:HG12 | 1:CZ:112:PHE:HE1 | 1.67 | 0.59 |
| 1:BA:58:ILE:O | 1:BA:58:ILE:CG2 | 2.50 | 0.59 |
| 1:CF:95:VAL:HG12 | 1:CF:112:PHE:HE1 | 1.67 | 0.59 |
| 1:AE:58:ILE:CG2 | 1:AE:58:ILE:O | 2.50 | 0.59 |
| 1:CR:63:LYS:O | 1:CR:67:ASN:HB2 | 2.01 | 0.59 |
| 1:BY:152:TRP:HE3 | 1:BY:153:ALA:H | 1.48 | 0.59 |
| 1:BW:63:LYS:O | 1:BW:67:ASN:HB2 | 2.01 | 0.59 |
| 1:B3:124:ILE:O | 1:B3:129:THR:OG1 | 2.16 | 0.59 |
| 1:AL:97:LYS:HE3 | 1:AM:97:LYS:NZ | 2.17 | 0.59 |
| 1:AQ:97:LYS:HE3 | 1:AR:97:LYS:NZ | 2.17 | 0.59 |
| 1:A1:97:LYS:HE3 | 1:A2:97:LYS:NZ | 2.18 | 0.59 |
| 1:B2:20:ARG:HG3 | 1:B2:52:VAL:O | 2.01 | 0.59 |
| 1:BM:20:ARG:HG3 | 1:BM:52:VAL:O | 2.02 | 0.59 |
| 1:CW:39:ARG:O | 1:C2:7:LEU:HB3 | 2.02 | 0.59 |
| 1:AA:95:VAL:HG12 | 1:AA:112:PHE:HE1 | 1.67 | 0.59 |
| 1:AO:58:ILE:O | 1:AO:58:ILE:CG2 | 2.51 | 0.59 |
| 1:CP:83:GLY:HA3 | 2:CP:201:PO4:O2 | 2.03 | 0.59 |
| 1:BD:33:ALA:O | 1:BD:37:LEU:HB2 | 2.03 | 0.59 |
| 1:AP:83:GLY:HA3 | 2:AP:1001:PO4:O2 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CU:83:GLY:HA3 | 2:CU:201:PO4:O2 | 2.02 | 0.59 |
| 1:AF:83:GLY:HA3 | 2:AF:1001:PO4:O2 | 2.03 | 0.59 |
| 1:AZ:83:GLY:HA3 | 2:AZ:1001:PO4:O2 | 2.03 | 0.59 |
| 1:AS:33:ALA:O | 1:AS:37:LEU:HB2 | 2.03 | 0.59 |
| 1:AU:83:GLY:HA3 | 2:AU:1001:PO4:O2 | 2.03 | 0.59 |
| 1:C1:97:LYS:HE3 | 1:C2:97:LYS:NZ | 2.18 | 0.59 |
| 1:AB:97:LYS:HE3 | 1:AC:97:LYS:NZ | 2.18 | 0.59 |
| 1:BV:97:LYS:HE3 | 1:BW:97:LYS:NZ | 2.18 | 0.59 |
| 1:BH:97:LYS:HG3 | 1:BI:97:LYS:HZ3 | 1.66 | 0.59 |
| 1:AF:95:VAL:HG12 | 1:AF:112:PHE:HE1 | 1.67 | 0.59 |
| 1:AO:152:TRP:HE3 | 1:AO:153:ALA:H | 1.48 | 0.59 |
| 1:AB:107:ASP:CB | 1:AB:152:TRP:CZ3 | 2.86 | 0.59 |
| 1:AY:152:TRP:HE3 | 1:AY:153:ALA:H | 1.48 | 0.59 |
| 1:AN:33:ALA:O | 1:AN:37:LEU:HB2 | 2.03 | 0.59 |
| 1:B1:6:HIS:HE1 | 1:B1:8:VAL:HB | 1.68 | 0.59 |
| 1:AV:107:ASP:CB | 1:AV:152:TRP:CZ3 | 2.86 | 0.59 |
| 1:BZ:83:GLY:HA3 | 2:BZ:1001:PO4:O2 | 2.02 | 0.59 |
| 1:CV:97:LYS:HE3 | 1:CW:97:LYS:NZ | 2.18 | 0.59 |
| 1:CH:20:ARG:HG3 | 1:CH:52:VAL:O | 2.02 | 0.59 |
| 1:CK:58:ILE:CG2 | 1:CK:58:ILE:O | 2.50 | 0.59 |
| 1:AZ:148:LEU:HD23 | 1:AZ:148:LEU:O | 2.03 | 0.59 |
| 1:AL:6:HIS:HE1 | 1:AL:8:VAL:HB | 1.68 | 0.59 |
| 1:BP:148:LEU:O | 1:BP:148:LEU:HD23 | 2.03 | 0.59 |
| 1:CA:83:GLY:HA3 | 2:CA:1001:PO4:O2 | 2.03 | 0.59 |
| 1:AQ:107:ASP:CB | 1:AQ:152:TRP:CZ3 | 2.86 | 0.59 |
| 1:CN:33:ALA:O | 1:CN:37:LEU:HB2 | 2.03 | 0.59 |
| 1:AU:148:LEU:HD23 | 1:AU:148:LEU:O | 2.03 | 0.59 |
| 1:AI:33:ALA:O | 1:AI:37:LEU:HB2 | 2.03 | 0.59 |
| 1:BK:148:LEU:HD23 | 1:BK:148:LEU:O | 2.03 | 0.59 |
| 1:AL:107:ASP:CB | 1:AL:152:TRP:CZ3 | 2.86 | 0.59 |
| 1:BG:107:ASP:HB2 | 1:BG:152:TRP:HZ3 | 1.62 | 0.59 |
| 1:BG:97:LYS:HE3 | 1:BH:97:LYS:NZ | 2.18 | 0.59 |
| 1:CM:20:ARG:HG3 | 1:CM:52:VAL:O | 2.01 | 0.59 |
| 1:BB:148:LEU:HD13 | 1:BC:61:ILE:HD11 | 1.83 | 0.59 |
| 1:A2:20:ARG:HG3 | 1:A2:52:VAL:O | 2.01 | 0.59 |
| 1:AK:95:VAL:HG12 | 1:AK:112:PHE:HE1 | 1.67 | 0.59 |
| 1:CO:58:ILE:CG2 | 1:CO:58:ILE:O | 2.51 | 0.59 |
| 1:BX:33:ALA:O | 1:BX:37:LEU:HB2 | 2.03 | 0.59 |
| 1:AK:148:LEU:HD23 | 1:AK:148:LEU:O | 2.03 | 0.59 |
| 1:AG:107:ASP:CB | 1:AG:152:TRP:CZ3 | 2.86 | 0.59 |
| 1:CA:148:LEU:O | 1:CA:148:LEU:HD23 | 2.03 | 0.59 |
| 1:BP:83:GLY:HA3 | 2:BP:1001:PO4:O2 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CK:148:LEU:HD23 | 1:CK:148:LEU:O | 2.03 | 0.59 |
| 1:BJ:53:PRO:CD | 1:BJ:57:GLU:HG3 | 2.29 | 0.59 |
| 1:AO:53:PRO:CD | 1:AO:57:GLU:HG3 | 2.29 | 0.59 |
| 1:AH:97:LYS:HG3 | 1:AI:97:LYS:HZ1 | 1.67 | 0.59 |
| 1:B1:97:LYS:HE3 | 1:B2:97:LYS:NZ | 2.17 | 0.59 |
| 1:AC:20:ARG:HG3 | 1:AC:52:VAL:O | 2.01 | 0.59 |
| 1:AZ:95:VAL:HG12 | 1:AZ:112:PHE:HE1 | 1.67 | 0.59 |
| 1:CR:6:HIS:HE1 | 1:CR:8:VAL:HB | 1.66 | 0.59 |
| 1:BU:83:GLY:HA3 | 2:BU:1001:PO4:O2 | 2.03 | 0.59 |
| 1:CD:33:ALA:O | 1:CD:37:LEU:HB2 | 2.03 | 0.59 |
| 1:BU:148:LEU:HD23 | 1:BU:148:LEU:O | 2.03 | 0.59 |
| 1:CL:148:LEU:HD13 | 1:CM:61:ILE:HD11 | 1.83 | 0.59 |
| 1:CC:65:MET:HE3 | 1:CC:71:TYR:CE1 | 2.38 | 0.59 |
| 1:AA:58:ILE:CG2 | 1:AA:58:ILE:O | 2.50 | 0.59 |
| 1:AK:83:GLY:HA3 | 2:AK:1001:PO4:O2 | 2.03 | 0.59 |
| 1:AP:148:LEU:O | 1:AP:148:LEU:HD23 | 2.03 | 0.59 |
| 1:AB:6:HIS:HE1 | 1:AB:8:VAL:HB | 1.68 | 0.59 |
| 1:CB:6:HIS:HE1 | 1:CB:8:VAL:HB | 1.68 | 0.59 |
| 1:BF:83:GLY:HA3 | 2:BF:1001:PO4:O2 | 2.03 | 0.59 |
| 1:A1:107:ASP:CB | 1:A1:152:TRP:CZ3 | 2.86 | 0.59 |
| 1:AM:129:THR:O | 1:AM:132:GLY:N | 2.25 | 0.59 |
| 1:BR:129:THR:O | 1:BR:132:GLY:N | 2.25 | 0.59 |
| 1:CB:97:LYS:HE3 | 1:CC:97:LYS:NZ | 2.18 | 0.59 |
| 1:BL:148:LEU:HD13 | 1:BM:61:ILE:HD11 | 1.83 | 0.59 |
| 1:CM:65:MET:HE3 | 1:CM:71:TYR:CE1 | 2.38 | 0.59 |
| 1:BY:58:ILE:O | 1:BY:58:ILE:CG2 | 2.51 | 0.59 |
| 1:AX:33:ALA:O | 1:AX:37:LEU:HB2 | 2.03 | 0.59 |
| 1:B3:33:ALA:O | 1:B3:37:LEU:HB2 | 2.03 | 0.59 |
| 1:AW:116:THR:O | 1:AX:85:THR:HB | 2.03 | 0.59 |
| 1:CX:33:ALA:O | 1:CX:37:LEU:HB2 | 2.03 | 0.59 |
| 1:BI:33:ALA:O | 1:BI:37:LEU:HB2 | 2.03 | 0.59 |
| 1:B2:129:THR:O | 1:B2:132:GLY:N | 2.25 | 0.59 |
| 1:CQ:97:LYS:HE3 | 1:CR:97:LYS:NZ | 2.18 | 0.59 |
| 1:BU:95:VAL:HG12 | 1:BU:112:PHE:HE1 | 1.67 | 0.59 |
| 1:BP:95:VAL:HG12 | 1:BP:112:PHE:HE1 | 1.67 | 0.59 |
| 1:BE:58:ILE:CG2 | 1:BE:58:ILE:O | 2.50 | 0.59 |
| 1:CF:34:LEU:HD12 | 1:CF:38:LYS:HB2 | 1.83 | 0.59 |
| 1:CQ:6:HIS:HE1 | 1:CQ:8:VAL:HB | 1.68 | 0.59 |
| 1:CZ:148:LEU:HD23 | 1:CZ:148:LEU:O | 2.03 | 0.59 |
| 1:A3:33:ALA:O | 1:A3:37:LEU:HB2 | 2.03 | 0.59 |
| 1:BH:116:THR:O | 1:BI:85:THR:HB | 2.03 | 0.59 |
| 1:BZ:148:LEU:O | 1:BZ:148:LEU:HD23 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CK:83:GLY:HA3 | 2:CK:201:PO4:O2 | 2.03 | 0.59 |
| 1:CH:116:THR:O | 1:CI:85:THR:HB | 2.03 | 0.59 |
| 1:AQ:6:HIS:HE1 | 1:AQ:8:VAL:HB | 1.68 | 0.59 |
| 1:BV:6:HIS:HE1 | 1:BV:8:VAL:HB | 1.68 | 0.59 |
| 1:CW:65:MET:HE3 | 1:CW:71:TYR:CE1 | 2.38 | 0.59 |
| 1:CU:34:LEU:HD12 | 1:CU:38:LYS:HB2 | 1.83 | 0.59 |
| 1:BF:148:LEU:O | 1:BF:148:LEU:HD23 | 2.03 | 0.59 |
| 1:CF:148:LEU:HD23 | 1:CF:148:LEU:O | 2.03 | 0.59 |
| 1:CL:6:HIS:HE1 | 1:CL:8:VAL:HB | 1.68 | 0.59 |
| 1:C3:33:ALA:O | 1:C3:37:LEU:HB2 | 2.03 | 0.59 |
| 1:BA:148:LEU:HD23 | 1:BA:148:LEU:O | 2.03 | 0.59 |
| 1:B2:116:THR:O | 1:B3:85:THR:HB | 2.03 | 0.59 |
| 1:CC:116:THR:O | 1:CD:85:THR:HB | 2.03 | 0.59 |
| 1:BW:116:THR:O | 1:BX:85:THR:HB | 2.03 | 0.59 |
| 1:BG:6:HIS:HE1 | 1:BG:8:VAL:HB | 1.68 | 0.59 |
| 1:BL:97:LYS:HE3 | 1:BM:97:LYS:NZ | 2.17 | 0.58 |
| 1:CG:97:LYS:HE3 | 1:CH:97:LYS:NZ | 2.18 | 0.58 |
| 1:AR:65:MET:HE3 | 1:AR:71:TYR:CE1 | 2.38 | 0.58 |
| 1:AU:95:VAL:HG12 | 1:AU:112:PHE:HE1 | 1.67 | 0.58 |
| 1:CY:58:ILE:O | 1:CY:58:ILE:CG2 | 2.50 | 0.58 |
| 1:C2:116:THR:O | 1:C3:85:THR:HB | 2.03 | 0.58 |
| 1:AI:124:ILE:O | 1:AI:129:THR:OG1 | 2.16 | 0.58 |
| 1:CS:33:ALA:O | 1:CS:37:LEU:HB2 | 2.02 | 0.58 |
| 1:CP:148:LEU:O | 1:CP:148:LEU:HD23 | 2.03 | 0.58 |
| 1:BN:33:ALA:O | 1:BN:37:LEU:HB2 | 2.03 | 0.58 |
| 1:BM:116:THR:O | 1:BN:85:THR:HB | 2.03 | 0.58 |
| 1:CV:6:HIS:HE1 | 1:CV:8:VAL:HB | 1.68 | 0.58 |
| 1:AM:116:THR:O | 1:AN:85:THR:HB | 2.03 | 0.58 |
| 1:AH:116:THR:O | 1:AI:85:THR:HB | 2.03 | 0.58 |
| 1:BU:58:ILE:O | 1:BU:58:ILE:CG2 | 2.50 | 0.58 |
| 1:BF:95:VAL:HG12 | 1:BF:112:PHE:HE1 | 1.67 | 0.58 |
| 1:BD:39:ARG:O | 1:BJ:7:LEU:HB3 | 2.02 | 0.58 |
| 1:AF:148:LEU:HD23 | 1:AF:148:LEU:O | 2.03 | 0.58 |
| 1:AD:33:ALA:O | 1:AD:37:LEU:HB2 | 2.03 | 0.58 |
| 1:CJ:53:PRO:CD | 1:CJ:57:GLU:HG3 | 2.29 | 0.58 |
| 1:AE:53:PRO:CD | 1:AE:57:GLU:HG3 | 2.29 | 0.58 |
| 1:BB:97:LYS:HE3 | 1:BC:97:LYS:NZ | 2.17 | 0.58 |
| 1:AV:97:LYS:HE3 | 1:AW:97:LYS:NZ | 2.18 | 0.58 |
| 1:BM:65:MET:HE3 | 1:BM:71:TYR:CE1 | 2.38 | 0.58 |
| 1:BJ:58:ILE:CG2 | 1:BJ:58:ILE:O | 2.51 | 0.58 |
| 1:CT:58:ILE:O | 1:CT:58:ILE:CG2 | 2.50 | 0.58 |
| 1:BA:83:GLY:HA3 | 2:BA:1001:PO4:O2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CF:83:GLY:HA3 | 2:CF:201:PO4:O2 | 2.03 | 0.58 |
| 1:A1:6:HIS:HE1 | 1:A1:8:VAL:HB | 1.68 | 0.58 |
| 1:BR:116:THR:O | 1:BS:85:THR:HB | 2.03 | 0.58 |
| 1:BC:97:LYS:HG3 | 1:BD:97:LYS:HZ3 | 1.68 | 0.58 |
| 1:CD:28:LYS:HZ3 | 1:CF:28:LYS:NZ | 2.00 | 0.58 |
| 1:AZ:58:ILE:O | 1:AZ:58:ILE:CG2 | 2.50 | 0.58 |
| 1:CP:95:VAL:HG12 | 1:CP:112:PHE:HE1 | 1.67 | 0.58 |
| 1:C3:124:ILE:O | 1:C3:129:THR:OG1 | 2.16 | 0.58 |
| 1:CI:33:ALA:O | 1:CI:37:LEU:HB2 | 2.03 | 0.58 |
| 1:C1:6:HIS:HE1 | 1:C1:8:VAL:HB | 1.68 | 0.58 |
| 1:BK:83:GLY:HA3 | 2:BK:1001:PO4:O2 | 2.03 | 0.58 |
| 1:A2:116:THR:O | 1:A3:85:THR:HB | 2.03 | 0.58 |
| 1:CM:116:THR:O | 1:CN:85:THR:HB | 2.03 | 0.58 |
| 1:CM:129:THR:O | 1:CM:132:GLY:N | 2.25 | 0.58 |
| 1:CZ:58:ILE:O | 1:CZ:58:ILE:CG2 | 2.50 | 0.58 |
| 1:AM:65:MET:HE3 | 1:AM:71:TYR:CE1 | 2.39 | 0.58 |
| 1:B4:58:ILE:O | 1:B4:58:ILE:CG2 | 2.51 | 0.58 |
| 1:CZ:83:GLY:HA3 | 2:CZ:201:PO4:O2 | 2.03 | 0.58 |
| 1:BQ:6:HIS:HE1 | 1:BQ:8:VAL:HB | 1.68 | 0.58 |
| 1:A4:53:PRO:CD | 1:A4:57:GLU:HG3 | 2.29 | 0.58 |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:HG12 | 1.85 | 0.58 |
| 1:CL:97:LYS:HE3 | 1:CM:97:LYS:NZ | 2.17 | 0.58 |
| 1:CU:95:VAL:HG12 | 1:CU:112:PHE:HE1 | 1.67 | 0.58 |
| 1:BO:58:ILE:CG2 | 1:BO:58:ILE:O | 2.51 | 0.58 |
| 1:CE:58:ILE:O | 1:CE:58:ILE:CG2 | 2.50 | 0.58 |
| 1:C4:58:ILE:O | 1:C4:58:ILE:CG2 | 2.50 | 0.58 |
| 1:BB:6:HIS:HE1 | 1:BB:8:VAL:HB | 1.68 | 0.58 |
| 1:BC:116:THR:O | 1:BD:85:THR:HB | 2.03 | 0.58 |
| 1:CL:107:ASP:HB2 | 1:CL:152:TRP:HZ3 | 1.62 | 0.58 |
| 1:BL:107:ASP:HB2 | 1:BL:152:TRP:HZ3 | 1.62 | 0.58 |
| 1:CG:107:ASP:HB2 | 1:CG:152:TRP:HZ3 | 1.62 | 0.58 |
| 1:CF:58:ILE:CG2 | 1:CF:58:ILE:O | 2.50 | 0.58 |
| 1:AT:58:ILE:CG2 | 1:AT:58:ILE:O | 2.51 | 0.58 |
| 1:AJ:58:ILE:CG2 | 1:AJ:58:ILE:O | 2.50 | 0.58 |
| 1:CJ:58:ILE:O | 1:CJ:58:ILE:CG2 | 2.50 | 0.58 |
| 1:CU:148:LEU:O | 1:CU:148:LEU:HD23 | 2.03 | 0.58 |
| 1:CG:6:HIS:HE1 | 1:CG:8:VAL:HB | 1.68 | 0.58 |
| 1:CD:20:ARG:CZ | 1:CR:39:ARG:CZ | 2.81 | 0.58 |
| 1:CW:116:THR:O | 1:CX:85:THR:HB | 2.03 | 0.58 |
| 1:BO:53:PRO:CD | 1:BO:57:GLU:HG3 | 2.29 | 0.58 |
| 1:AQ:13:LYS:HZ1 | 1:BU:43:GLU:HG2 | 1.63 | 0.58 |
| 1:CW:40:HIS:CE1 | 1:C2:7:LEU:HD23 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AF:125:GLU:O | 1:AF:131:ALA:HB3 | 2.04 | 0.58 |
| 1:AA:125:GLU:O | 1:AA:131:ALA:HB3 | 2.04 | 0.58 |
| 1:AF:58:ILE:CG2 | 1:AF:58:ILE:O | 2.50 | 0.58 |
| 1:CL:121:GLU:O | 1:CL:124:ILE:HG22 | 2.04 | 0.58 |
| 1:BT:53:PRO:HG2 | 1:BT:57:GLU:HG3 | 0.65 | 0.58 |
| 1:AU:125:GLU:O | 1:AU:131:ALA:HB3 | 2.04 | 0.58 |
| 1:BZ:125:GLU:O | 1:BZ:131:ALA:HB3 | 2.04 | 0.58 |
| 1:AC:65:MET:HE3 | 1:AC:71:TYR:CE1 | 2.39 | 0.58 |
| 1:AY:58:ILE:CG2 | 1:AY:58:ILE:O | 2.50 | 0.58 |
| 1:BS:33:ALA:O | 1:BS:37:LEU:HB2 | 2.03 | 0.58 |
| 1:AA:83:GLY:HA3 | 2:AA:1001:PO4:O2 | 2.03 | 0.58 |
| 1:AA:148:LEU:O | 1:AA:148:LEU:HD23 | 2.03 | 0.58 |
| 1:CT:53:PRO:CD | 1:CT:57:GLU:HG3 | 2.29 | 0.58 |
| 1:CP:125:GLU:O | 1:CP:131:ALA:HB3 | 2.04 | 0.58 |
| 1:CU:125:GLU:O | 1:CU:131:ALA:HB3 | 2.04 | 0.58 |
| 1:CA:125:GLU:O | 1:CA:131:ALA:HB3 | 2.04 | 0.58 |
| 1:A1:121:GLU:O | 1:A1:124:ILE:HG22 | 2.04 | 0.58 |
| 1:BG:121:GLU:O | 1:BG:124:ILE:HG22 | 2.04 | 0.58 |
| 1:BQ:121:GLU:O | 1:BQ:124:ILE:HG22 | 2.04 | 0.58 |
| 1:B1:121:GLU:O | 1:B1:124:ILE:HG22 | 2.04 | 0.58 |
| 1:AR:116:THR:O | 1:AS:85:THR:HB | 2.03 | 0.58 |
| 1:AC:116:THR:O | 1:AD:85:THR:HB | 2.03 | 0.58 |
| 1:CU:102:LEU:HD22 | 1:CY:104:LEU:HD13 | 1.86 | 0.58 |
| 1:CQ:107:ASP:HB2 | 1:CQ:152:TRP:HZ3 | 1.62 | 0.57 |
| 1:AH:65:MET:HE3 | 1:AH:71:TYR:CE1 | 2.38 | 0.57 |
| 1:CF:125:GLU:O | 1:CF:131:ALA:HB3 | 2.04 | 0.57 |
| 1:BU:125:GLU:O | 1:BU:131:ALA:HB3 | 2.04 | 0.57 |
| 1:CK:125:GLU:O | 1:CK:131:ALA:HB3 | 2.04 | 0.57 |
| 1:AZ:125:GLU:O | 1:AZ:131:ALA:HB3 | 2.04 | 0.57 |
| 1:CP:58:ILE:CG2 | 1:CP:58:ILE:O | 2.50 | 0.57 |
| 1:AK:125:GLU:O | 1:AK:131:ALA:HB3 | 2.04 | 0.57 |
| 1:AG:121:GLU:O | 1:AG:124:ILE:HG22 | 2.04 | 0.57 |
| 1:BA:102:LEU:HD22 | 1:BE:104:LEU:HD13 | 1.86 | 0.57 |
| 1:AV:6:HIS:HE1 | 1:AV:8:VAL:HB | 1.68 | 0.57 |
| 1:C4:53:PRO:HG2 | 1:C4:57:GLU:HG3 | 0.65 | 0.57 |
| 1:BZ:58:ILE:CG2 | 1:BZ:58:ILE:O | 2.50 | 0.57 |
| 1:BS:7:LEU:HB3 | 1:BY:39:ARG:O | 2.04 | 0.57 |
| 1:AG:6:HIS:HE1 | 1:AG:8:VAL:HB | 1.68 | 0.57 |
| 1:BK:125:GLU:O | 1:BK:131:ALA:HB3 | 2.04 | 0.57 |
| 1:BF:125:GLU:O | 1:BF:131:ALA:HB3 | 2.04 | 0.57 |
| 1:A4:58:ILE:O | 1:A4:58:ILE:CG2 | 2.50 | 0.57 |
| 1:BZ:102:LEU:HD22 | 1:B4:104:LEU:HD13 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CP:102:LEU:HD22 | 1:CT:104:LEU:HD13 | 1.87 | 0.57 |
| 1:BL:6:HIS:HE1 | 1:BL:8:VAL:HB | 1.68 | 0.57 |
| 1:CR:116:THR:O | 1:CS:85:THR:HB | 2.03 | 0.57 |
| 1:AF:102:LEU:HD22 | 1:AJ:104:LEU:HD13 | 1.86 | 0.57 |
| 1:BK:58:ILE:O | 1:BK:58:ILE:CG2 | 2.50 | 0.57 |
| 1:CQ:121:GLU:O | 1:CQ:124:ILE:HG22 | 2.04 | 0.57 |
| 1:CB:121:GLU:O | 1:CB:124:ILE:HG22 | 2.04 | 0.57 |
| 1:AF:73:ALA:HB2 | 1:AF:146:ALA:HB2 | 1.87 | 0.57 |
| 1:CZ:102:LEU:HD22 | 1:C4:104:LEU:HD13 | 1.86 | 0.57 |
| 1:AI:48:ASP:HB2 | 1:AI:71:TYR:HE1 | 1.70 | 0.57 |
| 1:CK:102:LEU:HD22 | 1:CO:104:LEU:HD13 | 1.86 | 0.57 |
| 1:AK:58:ILE:O | 1:AK:58:ILE:CG2 | 2.50 | 0.57 |
| 1:BB:121:GLU:O | 1:BB:124:ILE:HG22 | 2.04 | 0.57 |
| 1:CV:121:GLU:O | 1:CV:124:ILE:HG22 | 2.04 | 0.57 |
| 1:CG:121:GLU:O | 1:CG:124:ILE:HG22 | 2.04 | 0.57 |
| 1:CD:48:ASP:HB2 | 1:CD:71:TYR:HE1 | 1.70 | 0.57 |
| 1:CD:63:LYS:O | 1:CD:67:ASN:HB2 | 2.05 | 0.57 |
| 1:AP:73:ALA:HB2 | 1:AP:146:ALA:HB2 | 1.87 | 0.57 |
| 1:BP:102:LEU:HD22 | 1:BT:104:LEU:HD13 | 1.86 | 0.57 |
| 1:AC:24:PHE:CE1 | 1:AU:28:LYS:HD2 | 2.40 | 0.57 |
| 1:A2:65:MET:HE3 | 1:A2:71:TYR:CE1 | 2.39 | 0.57 |
| 1:CZ:125:GLU:O | 1:CZ:131:ALA:HB3 | 2.04 | 0.57 |
| 1:C2:65:MET:HE3 | 1:C2:71:TYR:CE1 | 2.38 | 0.57 |
| 1:AP:125:GLU:O | 1:AP:131:ALA:HB3 | 2.04 | 0.57 |
| 1:BT:58:ILE:O | 1:BT:58:ILE:CG2 | 2.50 | 0.57 |
| 1:AA:102:LEU:HD22 | 1:AE:104:LEU:HD13 | 1.86 | 0.57 |
| 1:AN:63:LYS:O | 1:AN:67:ASN:HB2 | 2.05 | 0.57 |
| 1:CP:73:ALA:HB2 | 1:CP:146:ALA:HB2 | 1.87 | 0.57 |
| 1:CW:58:ILE:N | 1:CW:59:PRO:HD2 | 2.20 | 0.57 |
| 1:CA:102:LEU:HD22 | 1:CE:104:LEU:HD13 | 1.87 | 0.57 |
| 1:C4:53:PRO:CD | 1:C4:57:GLU:HG3 | 2.29 | 0.57 |
| 1:CY:53:PRO:HG2 | 1:CY:57:GLU:HG3 | 0.65 | 0.57 |
| 1:BW:129:THR:O | 1:BW:132:GLY:N | 2.25 | 0.57 |
| 1:BA:125:GLU:O | 1:BA:131:ALA:HB3 | 2.04 | 0.57 |
| 1:BL:121:GLU:O | 1:BL:124:ILE:HG22 | 2.04 | 0.57 |
| 1:CC:8:VAL:HG21 | 1:CR:8:VAL:HG13 | 1.86 | 0.57 |
| 1:BR:58:ILE:N | 1:BR:59:PRO:HD2 | 2.20 | 0.57 |
| 1:CZ:73:ALA:HB2 | 1:CZ:146:ALA:HB2 | 1.87 | 0.57 |
| 1:AU:102:LEU:HD22 | 1:AY:104:LEU:HD13 | 1.86 | 0.57 |
| 1:BS:124:ILE:O | 1:BS:129:THR:OG1 | 2.16 | 0.57 |
| 1:CA:73:ALA:HB2 | 1:CA:146:ALA:HB2 | 1.87 | 0.57 |
| 1:CU:73:ALA:HB2 | 1:CU:146:ALA:HB2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BM:58:ILE:N | 1:BM:59:PRO:HD2 | 2.20 | 0.57 |
| 1:BU:73:ALA:HB2 | 1:BU:146:ALA:HB2 | 1.87 | 0.57 |
| 1:CS:48:ASP:HB2 | 1:CS:71:TYR:HE1 | 1.70 | 0.57 |
| 1:C2:129:THR:O | 1:C2:132:GLY:N | 2.25 | 0.57 |
| 1:BV:97:LYS:HE3 | 1:BW:97:LYS:HZ3 | 1.69 | 0.57 |
| 1:CP:39:ARG:HH22 | 1:CV:144:GLU:CD | 2.08 | 0.57 |
| 1:BP:125:GLU:O | 1:BP:131:ALA:HB3 | 2.04 | 0.57 |
| 1:BR:65:MET:HE3 | 1:BR:71:TYR:CE1 | 2.40 | 0.57 |
| 1:AV:121:GLU:O | 1:AV:124:ILE:HG22 | 2.04 | 0.57 |
| 1:CX:63:LYS:O | 1:CX:67:ASN:HB2 | 2.05 | 0.57 |
| 1:BI:63:LYS:O | 1:BI:67:ASN:HB2 | 2.05 | 0.57 |
| 1:A2:58:ILE:N | 1:A2:59:PRO:HD2 | 2.20 | 0.57 |
| 1:CN:48:ASP:HB2 | 1:CN:71:TYR:HE1 | 1.70 | 0.57 |
| 1:CF:102:LEU:HD22 | 1:CJ:104:LEU:HD13 | 1.86 | 0.57 |
| 1:BH:58:ILE:N | 1:BH:59:PRO:HD2 | 2.20 | 0.57 |
| 1:AJ:53:PRO:CD | 1:AJ:57:GLU:HG3 | 2.29 | 0.57 |
| 1:BW:97:LYS:HG3 | 1:BX:97:LYS:HZ1 | 1.70 | 0.57 |
| 1:BF:39:ARG:O | 1:BQ:7:LEU:HB3 | 2.04 | 0.57 |
| 1:BN:48:ASP:HB2 | 1:BN:71:TYR:HE1 | 1.70 | 0.57 |
| 1:AP:102:LEU:HD22 | 1:AT:104:LEU:HD13 | 1.86 | 0.57 |
| 1:BS:63:LYS:O | 1:BS:67:ASN:HB2 | 2.05 | 0.57 |
| 1:AK:73:ALA:HB2 | 1:AK:146:ALA:HB2 | 1.87 | 0.57 |
| 1:CX:7:LEU:HD11 | 1:CX:140:VAL:HG22 | 1.87 | 0.57 |
| 1:BM:37:LEU:HD12 | 1:BM:47:ILE:HD13 | 1.87 | 0.57 |
| 1:AM:58:ILE:N | 1:AM:59:PRO:HD2 | 2.20 | 0.57 |
| 1:AX:63:LYS:O | 1:AX:67:ASN:HB2 | 2.05 | 0.57 |
| 1:B3:63:LYS:O | 1:B3:67:ASN:HB2 | 2.05 | 0.57 |
| 1:CC:8:VAL:HG13 | 1:CR:8:VAL:CG2 | 2.34 | 0.57 |
| 1:BR:6:HIS:CE1 | 1:BR:8:VAL:HB | 2.40 | 0.57 |
| 1:BC:58:ILE:N | 1:BC:59:PRO:HD2 | 2.20 | 0.57 |
| 1:CS:63:LYS:O | 1:CS:67:ASN:HB2 | 2.05 | 0.57 |
| 1:BX:48:ASP:HB2 | 1:BX:71:TYR:HE1 | 1.70 | 0.57 |
| 1:CT:52:VAL:CB | 1:CT:53:PRO:HD2 | 2.34 | 0.56 |
| 1:B4:53:PRO:HG2 | 1:B4:57:GLU:HG3 | 0.65 | 0.56 |
| 1:BF:58:ILE:O | 1:BF:58:ILE:CG2 | 2.50 | 0.56 |
| 1:CA:58:ILE:O | 1:CA:58:ILE:CG2 | 2.50 | 0.56 |
| 1:AL:121:GLU:O | 1:AL:124:ILE:HG22 | 2.04 | 0.56 |
| 1:AB:121:GLU:O | 1:AB:124:ILE:HG22 | 2.04 | 0.56 |
| 1:AQ:121:GLU:O | 1:AQ:124:ILE:HG22 | 2.04 | 0.56 |
| 1:BW:6:HIS:CE1 | 1:BW:8:VAL:HB | 2.40 | 0.56 |
| 1:AM:37:LEU:HD12 | 1:AM:47:ILE:HD13 | 1.87 | 0.56 |
| 1:AC:58:ILE:N | 1:AC:59:PRO:HD2 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AS:124:ILE:O | 1:AS:129:THR:OG1 | 2.16 | 0.56 |
| 1:BP:73:ALA:HB2 | 1:BP:146:ALA:HB2 | 1.87 | 0.56 |
| 1:CC:37:LEU:HD12 | 1:CC:47:ILE:HD13 | 1.87 | 0.56 |
| 1:BK:73:ALA:HB2 | 1:BK:146:ALA:HB2 | 1.87 | 0.56 |
| 1:CK:73:ALA:HB2 | 1:CK:146:ALA:HB2 | 1.87 | 0.56 |
| 1:AR:58:ILE:N | 1:AR:59:PRO:HD2 | 2.20 | 0.56 |
| 1:BF:73:ALA:HB2 | 1:BF:146:ALA:HB2 | 1.87 | 0.56 |
| 1:AP:82:ARG:HG3 | 1:AP:118:GLU:OE2 | 2.06 | 0.56 |
| 1:BQ:107:ASP:HB2 | 1:BQ:152:TRP:HZ3 | 1.62 | 0.56 |
| 1:AP:58:ILE:CG2 | 1:AP:58:ILE:O | 2.50 | 0.56 |
| 1:CH:6:HIS:CE1 | 1:CH:8:VAL:HB | 2.40 | 0.56 |
| 1:BC:6:HIS:CE1 | 1:BC:8:VAL:HB | 2.41 | 0.56 |
| 1:BS:48:ASP:HB2 | 1:BS:71:TYR:HE1 | 1.70 | 0.56 |
| 1:CF:82:ARG:HG3 | 1:CF:118:GLU:OE2 | 2.06 | 0.56 |
| 1:BC:37:LEU:HD12 | 1:BC:47:ILE:HD13 | 1.87 | 0.56 |
| 1:BZ:82:ARG:HG3 | 1:BZ:118:GLU:OE2 | 2.05 | 0.56 |
| 1:AD:48:ASP:HB2 | 1:AD:71:TYR:HE1 | 1.70 | 0.56 |
| 1:BZ:73:ALA:HB2 | 1:BZ:146:ALA:HB2 | 1.87 | 0.56 |
| 1:B2:58:ILE:N | 1:B2:59:PRO:HD2 | 2.20 | 0.56 |
| 1:CA:82:ARG:HG3 | 1:CA:118:GLU:OE2 | 2.06 | 0.56 |
| 1:BW:58:ILE:N | 1:BW:59:PRO:HD2 | 2.20 | 0.56 |
| 1:BU:102:LEU:HD22 | 1:BY:104:LEU:HD13 | 1.86 | 0.56 |
| 1:AY:53:PRO:CG | 1:AY:57:GLU:CG | 2.46 | 0.56 |
| 1:AW:6:HIS:CE1 | 1:AW:8:VAL:HB | 2.41 | 0.56 |
| 1:C2:6:HIS:CE1 | 1:C2:8:VAL:HB | 2.41 | 0.56 |
| 1:CH:58:ILE:N | 1:CH:59:PRO:HD2 | 2.20 | 0.56 |
| 1:AU:100:ALA:HB2 | 1:AV:56:PHE:CZ | 2.41 | 0.56 |
| 1:BK:100:ALA:HB2 | 1:BL:56:PHE:CZ | 2.41 | 0.56 |
| 1:AA:73:ALA:HB2 | 1:AA:146:ALA:HB2 | 1.87 | 0.56 |
| 1:CM:58:ILE:N | 1:CM:59:PRO:HD2 | 2.20 | 0.56 |
| 1:CE:83:GLY:HA3 | 2:CE:1001:PO4:P | 2.46 | 0.56 |
| 1:AR:37:LEU:HD12 | 1:AR:47:ILE:HD13 | 1.87 | 0.56 |
| 1:AX:48:ASP:HB2 | 1:AX:71:TYR:HE1 | 1.70 | 0.56 |
| 1:AH:58:ILE:N | 1:AH:59:PRO:HD2 | 2.20 | 0.56 |
| 1:AN:7:LEU:HD11 | 1:AN:140:VAL:HG22 | 1.87 | 0.56 |
| 1:AS:48:ASP:HB2 | 1:AS:71:TYR:HE1 | 1.70 | 0.56 |
| 1:CI:48:ASP:HB2 | 1:CI:71:TYR:HE1 | 1.70 | 0.56 |
| 1:AA:82:ARG:HG3 | 1:AA:118:GLU:OE2 | 2.06 | 0.56 |
| 1:CC:58:ILE:N | 1:CC:59:PRO:HD2 | 2.20 | 0.56 |
| 1:AK:82:ARG:HG3 | 1:AK:118:GLU:OE2 | 2.06 | 0.56 |
| 1:CZ:82:ARG:HG3 | 1:CZ:118:GLU:OE2 | 2.06 | 0.56 |
| 1:BD:48:ASP:HB2 | 1:BD:71:TYR:HE1 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:BA:82:ARG:HG3 | 1:BA:118:GLU:OE2 | 2.06 | 0.56 |
| 1:C2:58:ILE:N | 1:C2:59:PRO:HD2 | 2.20 | 0.56 |
| 1:BE:83:GLY:HA3 | 2:BE:1001:PO4:P | 2.46 | 0.56 |
| 1:C3:48:ASP:HB2 | 1:C3:71:TYR:HE1 | 1.70 | 0.56 |
| 1:AE:53:PRO:HG2 | 1:AE:57:GLU:HG3 | 0.65 | 0.56 |
| 1:CG:96:ALA:O | 1:CG:100:ALA:HB2 | 2.06 | 0.56 |
| 1:BV:121:GLU:O | 1:BV:124:ILE:HG22 | 2.04 | 0.56 |
| 1:CM:6:HIS:CE1 | 1:CM:8:VAL:HB | 2.40 | 0.56 |
| 1:A3:63:LYS:O | 1:A3:67:ASN:HB2 | 2.05 | 0.56 |
| 1:CZ:100:ALA:HB2 | 1:C1:56:PHE:CZ | 2.41 | 0.56 |
| 1:CX:48:ASP:HB2 | 1:CX:71:TYR:HE1 | 1.70 | 0.56 |
| 1:AZ:100:ALA:HB2 | 1:A1:56:PHE:CZ | 2.40 | 0.56 |
| 1:BI:48:ASP:HB2 | 1:BI:71:TYR:HE1 | 1.70 | 0.56 |
| 1:CW:37:LEU:HD12 | 1:CW:47:ILE:HD13 | 1.87 | 0.56 |
| 1:CU:100:ALA:HB2 | 1:CV:56:PHE:CZ | 2.41 | 0.56 |
| 1:BN:7:LEU:HD11 | 1:BN:140:VAL:HG22 | 1.87 | 0.56 |
| 1:AU:82:ARG:HG3 | 1:AU:118:GLU:OE2 | 2.05 | 0.56 |
| 1:CJ:53:PRO:CG | 1:CJ:57:GLU:CG | 2.46 | 0.56 |
| 1:BJ:53:PRO:HG2 | 1:BJ:57:GLU:HG3 | 0.65 | 0.56 |
| 1:AV:96:ALA:O | 1:AV:100:ALA:HB2 | 2.06 | 0.56 |
| 1:BG:97:LYS:HE3 | 1:BH:97:LYS:HZ3 | 1.70 | 0.56 |
| 1:BC:39:ARG:O | 1:BR:7:LEU:HB3 | 2.06 | 0.56 |
| 1:BM:6:HIS:CE1 | 1:BM:8:VAL:HB | 2.40 | 0.56 |
| 1:AS:63:LYS:O | 1:AS:67:ASN:HB2 | 2.05 | 0.56 |
| 1:CI:63:LYS:O | 1:CI:67:ASN:HB2 | 2.05 | 0.56 |
| 1:CS:7:LEU:HD11 | 1:CS:140:VAL:HG22 | 1.87 | 0.56 |
| 1:BJ:83:GLY:HA3 | 2:BJ:1001:PO4:P | 2.46 | 0.56 |
| 1:CS:124:ILE:O | 1:CS:129:THR:OG1 | 2.16 | 0.56 |
| 1:BN:63:LYS:O | 1:BN:67:ASN:HB2 | 2.05 | 0.56 |
| 1:AE:83:GLY:HA3 | 2:AE:1001:PO4:P | 2.46 | 0.56 |
| 1:AQ:70:LYS:HE3 | 1:BU:43:GLU:OE2 | 2.05 | 0.56 |
| 1:AV:97:LYS:HE3 | 1:AW:97:LYS:HZ3 | 1.70 | 0.56 |
| 1:C1:121:GLU:O | 1:C1:124:ILE:HG22 | 2.04 | 0.56 |
| 1:AH:6:HIS:CE1 | 1:AH:8:VAL:HB | 2.41 | 0.56 |
| 1:CP:100:ALA:HB2 | 1:CQ:56:PHE:CZ | 2.41 | 0.56 |
| 1:AK:100:ALA:HB2 | 1:AL:56:PHE:CZ | 2.41 | 0.56 |
| 1:AZ:73:ALA:HB2 | 1:AZ:146:ALA:HB2 | 1.87 | 0.56 |
| 1:CY:83:GLY:HA3 | 2:CY:4201:PO4:P | 2.46 | 0.56 |
| 1:A3:48:ASP:HB2 | 1:A3:71:TYR:HE1 | 1.70 | 0.56 |
| 1:CA:100:ALA:HB2 | 1:CB:56:PHE:CZ | 2.41 | 0.56 |
| 1:BK:82:ARG:HG3 | 1:BK:118:GLU:OE2 | 2.06 | 0.56 |
| 1:AU:73:ALA:HB2 | 1:AU:146:ALA:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AD:63:LYS:O | 1:AD:67:ASN:HB2 | 2.05 | 0.56 |
| 1:A3:7:LEU:HD11 | 1:A3:140:VAL:HG22 | 1.87 | 0.56 |
| 1:AX:7:LEU:HD11 | 1:AX:140:VAL:HG22 | 1.87 | 0.56 |
| 1:AF:100:ALA:HB2 | 1:AG:56:PHE:CZ | 2.41 | 0.56 |
| 1:BU:100:ALA:HB2 | 1:BV:56:PHE:CZ | 2.41 | 0.56 |
| 1:BM:129:THR:O | 1:BM:132:GLY:N | 2.25 | 0.56 |
| 1:CU:58:ILE:O | 1:CU:58:ILE:CG2 | 2.50 | 0.56 |
| 1:C3:7:LEU:HD11 | 1:C3:140:VAL:HG22 | 1.87 | 0.56 |
| 1:C4:83:GLY:HA3 | 2:C4:4201:PO4:P | 2.46 | 0.56 |
| 1:AY:83:GLY:HA3 | 2:AY:1001:PO4:P | 2.46 | 0.56 |
| 1:BH:37:LEU:HD12 | 1:BH:47:ILE:HD13 | 1.87 | 0.56 |
| 1:AO:83:GLY:HA3 | 2:AO:1001:PO4:P | 2.46 | 0.56 |
| 1:C3:63:LYS:O | 1:C3:67:ASN:HB2 | 2.05 | 0.56 |
| 1:CJ:52:VAL:CB | 1:CJ:53:PRO:HD2 | 2.34 | 0.56 |
| 1:AJ:53:PRO:HG2 | 1:AJ:57:GLU:HG3 | 0.65 | 0.56 |
| 1:BC:38:LYS:HZ2 | 1:BC:44:GLU:HA | 1.69 | 0.56 |
| 1:CR:6:HIS:CE1 | 1:CR:8:VAL:HB | 2.40 | 0.56 |
| 1:CW:6:HIS:CE1 | 1:CW:8:VAL:HB | 2.41 | 0.56 |
| 1:AI:63:LYS:O | 1:AI:67:ASN:HB2 | 2.05 | 0.56 |
| 1:BI:7:LEU:HD11 | 1:BI:140:VAL:HG22 | 1.87 | 0.56 |
| 1:AA:100:ALA:HB2 | 1:AB:56:PHE:CZ | 2.41 | 0.56 |
| 1:CO:83:GLY:HA3 | 2:CO:4201:PO4:P | 2.46 | 0.56 |
| 1:AK:102:LEU:HD22 | 1:AO:104:LEU:HD13 | 1.86 | 0.56 |
| 1:CR:58:ILE:N | 1:CR:59:PRO:HD2 | 2.20 | 0.56 |
| 1:AD:7:LEU:HD11 | 1:AD:140:VAL:HG22 | 1.87 | 0.56 |
| 1:C2:37:LEU:HD12 | 1:C2:47:ILE:HD13 | 1.87 | 0.56 |
| 1:BO:83:GLY:HA3 | 2:BO:1001:PO4:P | 2.46 | 0.56 |
| 1:AI:7:LEU:HD11 | 1:AI:140:VAL:HG22 | 1.87 | 0.56 |
| 1:CV:96:ALA:O | 1:CV:100:ALA:HB2 | 2.06 | 0.56 |
| 1:AU:58:ILE:CG2 | 1:AU:58:ILE:O | 2.50 | 0.56 |
| 1:BP:58:ILE:CG2 | 1:BP:58:ILE:O | 2.50 | 0.56 |
| 1:BF:102:LEU:HD22 | 1:BJ:104:LEU:HD13 | 1.86 | 0.56 |
| 1:BY:83:GLY:HA3 | 2:BY:1001:PO4:P | 2.46 | 0.56 |
| 1:B2:37:LEU:HD12 | 1:B2:47:ILE:HD13 | 1.87 | 0.56 |
| 1:BZ:100:ALA:HB2 | 1:B1:56:PHE:CZ | 2.41 | 0.56 |
| 1:CK:82:ARG:HG3 | 1:CK:118:GLU:OE2 | 2.06 | 0.56 |
| 1:B3:48:ASP:HB2 | 1:B3:71:TYR:HE1 | 1.70 | 0.56 |
| 1:A3:95:VAL:HG12 | 1:A3:112:PHE:HE1 | 1.71 | 0.56 |
| 1:AF:82:ARG:HG3 | 1:AF:118:GLU:OE2 | 2.06 | 0.56 |
| 1:AJ:53:PRO:CG | 1:AJ:57:GLU:CG | 2.46 | 0.56 |
| 1:BJ:52:VAL:CB | 1:BJ:53:PRO:HD2 | 2.34 | 0.56 |
| 1:BD:151:HIS:HB2 | 1:BE:64:LYS:HB3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CS:151:HIS:HB2 | 1:CT:64:LYS:HB3 | 1.88 | 0.56 |
| 1:AD:151:HIS:HB2 | 1:AE:64:LYS:HB3 | 1.88 | 0.56 |
| 1:AO:107:ASP:OD1 | 1:AO:107:ASP:O | 2.24 | 0.56 |
| 1:B2:6:HIS:CE1 | 1:B2:8:VAL:HB | 2.41 | 0.56 |
| 1:CD:7:LEU:HD11 | 1:CD:140:VAL:HG22 | 1.87 | 0.56 |
| 1:CR:37:LEU:HD12 | 1:CR:47:ILE:HD13 | 1.87 | 0.56 |
| 1:CP:82:ARG:HG3 | 1:CP:118:GLU:OE2 | 2.06 | 0.56 |
| 1:BA:100:ALA:HB2 | 1:BB:56:PHE:CZ | 2.41 | 0.56 |
| 1:AW:58:ILE:N | 1:AW:59:PRO:HD2 | 2.20 | 0.56 |
| 1:AZ:102:LEU:HD22 | 1:A4:104:LEU:HD13 | 1.87 | 0.56 |
| 1:BA:73:ALA:HB2 | 1:BA:146:ALA:HB2 | 1.87 | 0.56 |
| 1:CJ:83:GLY:HA3 | 2:CJ:4201:PO4:P | 2.46 | 0.56 |
| 1:AP:100:ALA:HB2 | 1:AQ:56:PHE:CZ | 2.41 | 0.56 |
| 1:AE:53:PRO:CG | 1:AE:57:GLU:CG | 2.46 | 0.55 |
| 1:CY:53:PRO:CG | 1:CY:57:GLU:CG | 2.46 | 0.55 |
| 1:AV:95:VAL:HG12 | 1:AV:112:PHE:HE1 | 1.72 | 0.55 |
| 1:AI:151:HIS:HB2 | 1:AJ:64:LYS:HB3 | 1.88 | 0.55 |
| 1:AS:151:HIS:HB2 | 1:AT:64:LYS:HB3 | 1.89 | 0.55 |
| 1:CT:107:ASP:OD1 | 1:CT:107:ASP:O | 2.24 | 0.55 |
| 1:C4:107:ASP:O | 1:C4:107:ASP:OD1 | 2.24 | 0.55 |
| 1:BF:85:THR:HB | 1:BJ:116:THR:O | 2.07 | 0.55 |
| 1:CM:37:LEU:HD12 | 1:CM:47:ILE:HD13 | 1.87 | 0.55 |
| 1:CK:100:ALA:HB2 | 1:CL:56:PHE:CZ | 2.41 | 0.55 |
| 1:AN:48:ASP:HB2 | 1:AN:71:TYR:HE1 | 1.70 | 0.55 |
| 1:BD:63:LYS:O | 1:BD:67:ASN:HB2 | 2.05 | 0.55 |
| 1:CU:82:ARG:HG3 | 1:CU:118:GLU:OE2 | 2.06 | 0.55 |
| 1:BF:100:ALA:HB2 | 1:BG:56:PHE:CZ | 2.40 | 0.55 |
| 1:A4:83:GLY:HA3 | 2:A4:1001:PO4:P | 2.46 | 0.55 |
| 1:CH:37:LEU:HD12 | 1:CH:47:ILE:HD13 | 1.87 | 0.55 |
| 1:BX:124:ILE:O | 1:BX:129:THR:OG1 | 2.16 | 0.55 |
| 1:AR:129:THR:O | 1:AR:132:GLY:N | 2.25 | 0.55 |
| 1:BB:95:VAL:HG12 | 1:BB:112:PHE:HE1 | 1.72 | 0.55 |
| 1:CB:96:ALA:O | 1:CB:100:ALA:HB2 | 2.06 | 0.55 |
| 1:AC:97:LYS:HE3 | 1:AD:97:LYS:HZ3 | 1.69 | 0.55 |
| 1:BS:7:LEU:HD11 | 1:BS:140:VAL:HG22 | 1.87 | 0.55 |
| 1:BF:82:ARG:HG3 | 1:BF:118:GLU:OE2 | 2.06 | 0.55 |
| 1:CN:124:ILE:O | 1:CN:129:THR:OG1 | 2.16 | 0.55 |
| 1:BP:82:ARG:HG3 | 1:BP:118:GLU:OE2 | 2.05 | 0.55 |
| 1:CF:85:THR:HB | 1:CJ:116:THR:O | 2.07 | 0.55 |
| 1:CF:73:ALA:HB2 | 1:CF:146:ALA:HB2 | 1.87 | 0.55 |
| 1:AK:85:THR:HB | 1:AO:116:THR:O | 2.07 | 0.55 |
| 1:BW:37:LEU:HD12 | 1:BW:47:ILE:HD13 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BA:85:THR:HB | 1:BE:116:THR:O | 2.07 | 0.55 |
| 1:CT:83:GLY:HA3 | 2:CT:4201:PO4:P | 2.46 | 0.55 |
| 1:BK:102:LEU:HD22 | 1:BO:104:LEU:HD13 | 1.86 | 0.55 |
| 1:CQ:96:ALA:O | 1:CQ:100:ALA:HB2 | 2.06 | 0.55 |
| 1:CQ:100:ALA:HA | 1:CR:56:PHE:CZ | 2.42 | 0.55 |
| 1:CV:95:VAL:HG12 | 1:CV:112:PHE:HE1 | 1.72 | 0.55 |
| 1:CV:97:LYS:O | 1:CV:102:LEU:HB2 | 2.07 | 0.55 |
| 1:AX:151:HIS:HB2 | 1:AY:64:LYS:HB3 | 1.88 | 0.55 |
| 1:BN:151:HIS:HB2 | 1:BO:64:LYS:HB3 | 1.88 | 0.55 |
| 1:BE:107:ASP:OD1 | 1:BE:107:ASP:O | 2.24 | 0.55 |
| 1:CC:6:HIS:CE1 | 1:CC:8:VAL:HB | 2.41 | 0.55 |
| 1:AR:6:HIS:CE1 | 1:AR:8:VAL:HB | 2.40 | 0.55 |
| 1:AM:6:HIS:CE1 | 1:AM:8:VAL:HB | 2.41 | 0.55 |
| 1:A2:6:HIS:CE1 | 1:A2:8:VAL:HB | 2.40 | 0.55 |
| 1:CH:152:TRP:HD1 | 1:CI:68:SER:HB2 | 1.72 | 0.55 |
| 1:AZ:85:THR:HB | 1:A4:116:THR:O | 2.07 | 0.55 |
| 1:BU:85:THR:HB | 1:BY:116:THR:O | 2.07 | 0.55 |
| 1:CF:100:ALA:HB2 | 1:CG:56:PHE:CZ | 2.41 | 0.55 |
| 1:AP:85:THR:HB | 1:AT:116:THR:O | 2.07 | 0.55 |
| 1:CO:53:PRO:HG2 | 1:CO:57:GLU:HG3 | 0.65 | 0.55 |
| 1:CV:107:ASP:HB2 | 1:CV:152:TRP:HZ3 | 1.62 | 0.55 |
| 1:AQ:100:ALA:HA | 1:AR:56:PHE:CZ | 2.42 | 0.55 |
| 1:BV:96:ALA:O | 1:BV:100:ALA:HB2 | 2.06 | 0.55 |
| 1:BV:97:LYS:O | 1:BV:102:LEU:HB2 | 2.07 | 0.55 |
| 1:AW:38:LYS:HZ2 | 1:AW:44:GLU:HA | 1.71 | 0.55 |
| 1:CY:107:ASP:O | 1:CY:107:ASP:OD1 | 2.24 | 0.55 |
| 1:AC:6:HIS:CE1 | 1:AC:8:VAL:HB | 2.40 | 0.55 |
| 1:B3:95:VAL:HG12 | 1:B3:112:PHE:HE1 | 1.71 | 0.55 |
| 1:CU:3:PHE:CD2 | 1:CU:150:LYS:HE2 | 2.42 | 0.55 |
| 1:AZ:3:PHE:CD2 | 1:AZ:150:LYS:HE2 | 2.42 | 0.55 |
| 1:CF:3:PHE:CD2 | 1:CF:150:LYS:HE2 | 2.42 | 0.55 |
| 1:CZ:85:THR:HB | 1:C4:116:THR:O | 2.07 | 0.55 |
| 1:CR:152:TRP:HD1 | 1:CS:68:SER:HB2 | 1.72 | 0.55 |
| 1:CK:3:PHE:CD2 | 1:CK:150:LYS:HE2 | 2.42 | 0.55 |
| 1:CI:7:LEU:HD11 | 1:CI:140:VAL:HG22 | 1.87 | 0.55 |
| 1:AC:152:TRP:HD1 | 1:AD:68:SER:HB2 | 1.72 | 0.55 |
| 1:BX:63:LYS:O | 1:BX:67:ASN:HB2 | 2.05 | 0.55 |
| 1:BR:37:LEU:HD12 | 1:BR:47:ILE:HD13 | 1.87 | 0.55 |
| 1:BY:53:PRO:CD | 1:BY:57:GLU:HG3 | 2.29 | 0.55 |
| 1:AY:53:PRO:HG2 | 1:AY:57:GLU:HG3 | 0.65 | 0.55 |
| 1:AL:96:ALA:O | 1:AL:100:ALA:HB2 | 2.06 | 0.55 |
| 1:AL:97:LYS:O | 1:AL:102:LEU:HB2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B1:100:ALA:HA | 1:B2:56:PHE:CZ | 2.42 | 0.55 |
| 1:BQ:96:ALA:O | 1:BQ:100:ALA:HB2 | 2.06 | 0.55 |
| 1:CG:97:LYS:O | 1:CG:102:LEU:HB2 | 2.07 | 0.55 |
| 1:BH:6:HIS:CE1 | 1:BH:8:VAL:HB | 2.41 | 0.55 |
| 1:CW:152:TRP:HD1 | 1:CX:68:SER:HB2 | 1.72 | 0.55 |
| 1:CX:124:ILE:O | 1:CX:129:THR:OG1 | 2.16 | 0.55 |
| 1:AA:85:THR:HB | 1:AE:116:THR:O | 2.07 | 0.55 |
| 1:BU:3:PHE:CD2 | 1:BU:150:LYS:HE2 | 2.42 | 0.55 |
| 1:AT:83:GLY:HA3 | 2:AT:1001:PO4:P | 2.46 | 0.55 |
| 1:BK:85:THR:HB | 1:BO:116:THR:O | 2.07 | 0.55 |
| 1:A3:124:ILE:O | 1:A3:129:THR:OG1 | 2.16 | 0.55 |
| 1:AA:3:PHE:CD2 | 1:AA:150:LYS:HE2 | 2.42 | 0.55 |
| 1:BP:100:ALA:HB2 | 1:BQ:56:PHE:CZ | 2.41 | 0.55 |
| 1:CN:63:LYS:O | 1:CN:67:ASN:HB2 | 2.05 | 0.55 |
| 1:CM:152:TRP:HD1 | 1:CN:68:SER:HB2 | 1.72 | 0.55 |
| 1:AJ:83:GLY:HA3 | 2:AJ:1001:PO4:P | 2.46 | 0.55 |
| 1:CC:97:LYS:HG3 | 1:CD:97:LYS:HZ3 | 1.71 | 0.55 |
| 1:C1:95:VAL:HG12 | 1:C1:112:PHE:HE1 | 1.72 | 0.55 |
| 1:B1:95:VAL:HG12 | 1:B1:112:PHE:HE1 | 1.72 | 0.55 |
| 1:CG:95:VAL:HG12 | 1:CG:112:PHE:HE1 | 1.72 | 0.55 |
| 1:A1:97:LYS:O | 1:A1:102:LEU:HB2 | 2.07 | 0.55 |
| 1:CO:107:ASP:OD1 | 1:CO:107:ASP:O | 2.25 | 0.55 |
| 1:AZ:82:ARG:HG3 | 1:AZ:118:GLU:OE2 | 2.06 | 0.55 |
| 1:BH:152:TRP:HD1 | 1:BI:68:SER:HB2 | 1.72 | 0.55 |
| 1:CN:95:VAL:HG12 | 1:CN:112:PHE:HE1 | 1.71 | 0.55 |
| 1:BZ:85:THR:HB | 1:B4:116:THR:O | 2.07 | 0.55 |
| 1:BP:3:PHE:CD2 | 1:BP:150:LYS:HE2 | 2.42 | 0.55 |
| 1:BP:85:THR:HB | 1:BT:116:THR:O | 2.07 | 0.55 |
| 1:AH:37:LEU:HD12 | 1:AH:47:ILE:HD13 | 1.87 | 0.55 |
| 1:CI:95:VAL:HG12 | 1:CI:112:PHE:HE1 | 1.71 | 0.55 |
| 1:AK:3:PHE:CD2 | 1:AK:150:LYS:HE2 | 2.42 | 0.55 |
| 1:CZ:3:PHE:CD2 | 1:CZ:150:LYS:HE2 | 2.42 | 0.55 |
| 1:B4:83:GLY:HA3 | 2:B4:1001:PO4:P | 2.46 | 0.55 |
| 1:AD:95:VAL:HG12 | 1:AD:112:PHE:HE1 | 1.71 | 0.55 |
| 1:BK:3:PHE:CD2 | 1:BK:150:LYS:HE2 | 2.42 | 0.55 |
| 1:CP:3:PHE:CD2 | 1:CP:150:LYS:HE2 | 2.42 | 0.55 |
| 1:AX:95:VAL:HG12 | 1:AX:112:PHE:HE1 | 1.71 | 0.55 |
| 1:CQ:95:VAL:HG12 | 1:CQ:112:PHE:HE1 | 1.72 | 0.55 |
| 1:BQ:97:LYS:O | 1:BQ:102:LEU:HB2 | 2.07 | 0.55 |
| 1:CW:39:ARG:CZ | 1:C3:20:ARG:NH1 | 2.69 | 0.55 |
| 1:AN:151:HIS:HB2 | 1:AO:64:LYS:HB3 | 1.88 | 0.55 |
| 1:AE:107:ASP:OD1 | 1:AE:107:ASP:O | 2.24 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AC:37:LEU:HD12 | 1:AC:47:ILE:HD13 | 1.87 | 0.55 |
| 1:CN:7:LEU:HD11 | 1:CN:140:VAL:HG22 | 1.87 | 0.55 |
| 1:AS:95:VAL:HG12 | 1:AS:112:PHE:HE1 | 1.71 | 0.55 |
| 1:BM:152:TRP:HD1 | 1:BN:68:SER:HB2 | 1.72 | 0.55 |
| 1:AG:129:THR:HG22 | 1:AG:130:LYS:H | 1.72 | 0.55 |
| 1:CE:53:PRO:HG2 | 1:CE:57:GLU:HG3 | 0.65 | 0.55 |
| 1:CB:97:LYS:O | 1:CB:102:LEU:HB2 | 2.07 | 0.55 |
| 1:AQ:96:ALA:O | 1:AQ:100:ALA:HB2 | 2.06 | 0.55 |
| 1:CL:95:VAL:HG12 | 1:CL:112:PHE:HE1 | 1.72 | 0.55 |
| 1:CV:100:ALA:HA | 1:CW:56:PHE:CZ | 2.42 | 0.55 |
| 1:CE:107:ASP:OD1 | 1:CE:107:ASP:O | 2.25 | 0.55 |
| 1:BY:107:ASP:OD1 | 1:BY:107:ASP:O | 2.24 | 0.55 |
| 1:BJ:107:ASP:OD1 | 1:BJ:107:ASP:O | 2.24 | 0.55 |
| 1:CV:129:THR:HG22 | 1:CV:130:LYS:H | 1.72 | 0.55 |
| 1:AW:37:LEU:HD12 | 1:AW:47:ILE:HD13 | 1.87 | 0.55 |
| 1:BC:152:TRP:HD1 | 1:BD:68:SER:HB2 | 1.72 | 0.55 |
| 1:CS:95:VAL:HG12 | 1:CS:112:PHE:HE1 | 1.71 | 0.55 |
| 1:CA:3:PHE:CD2 | 1:CA:150:LYS:HE2 | 2.42 | 0.55 |
| 1:BD:95:VAL:HG12 | 1:BD:112:PHE:HE1 | 1.71 | 0.55 |
| 1:CT:53:PRO:HG2 | 1:CT:57:GLU:HG3 | 0.65 | 0.55 |
| 1:BL:97:LYS:O | 1:BL:102:LEU:HB2 | 2.07 | 0.55 |
| 1:BM:97:LYS:HG3 | 1:BN:97:LYS:HZ3 | 1.71 | 0.55 |
| 1:BG:100:ALA:HA | 1:BH:56:PHE:CZ | 2.42 | 0.55 |
| 1:BE:18:VAL:HG12 | 1:BE:77:LEU:CB | 2.37 | 0.55 |
| 1:CH:65:MET:HE3 | 1:CH:71:TYR:CE1 | 2.41 | 0.55 |
| 1:AT:107:ASP:OD1 | 1:AT:107:ASP:O | 2.25 | 0.55 |
| 1:AS:7:LEU:HD11 | 1:AS:140:VAL:HG22 | 1.87 | 0.55 |
| 1:C3:95:VAL:HG12 | 1:C3:112:PHE:HE1 | 1.71 | 0.55 |
| 1:A2:37:LEU:HD12 | 1:A2:47:ILE:HD13 | 1.87 | 0.55 |
| 1:B3:7:LEU:HD11 | 1:B3:140:VAL:HG22 | 1.87 | 0.55 |
| 1:AW:152:TRP:HD1 | 1:AX:68:SER:HB2 | 1.72 | 0.55 |
| 1:BU:82:ARG:HG3 | 1:BU:118:GLU:OE2 | 2.06 | 0.55 |
| 1:BL:129:THR:HG22 | 1:BL:130:LYS:H | 1.72 | 0.55 |
| 1:AU:3:PHE:CD2 | 1:AU:150:LYS:HE2 | 2.42 | 0.55 |
| 1:CB:129:THR:HG22 | 1:CB:130:LYS:H | 1.72 | 0.55 |
| 1:CT:52:VAL:HB | 1:CT:53:PRO:CD | 2.35 | 0.55 |
| 1:BE:53:PRO:HG2 | 1:BE:57:GLU:HG3 | 0.65 | 0.55 |
| 1:A2:129:THR:O | 1:A2:132:GLY:N | 2.25 | 0.55 |
| 1:AG:95:VAL:HG12 | 1:AG:112:PHE:HE1 | 1.72 | 0.55 |
| 1:AQ:95:VAL:HG12 | 1:AQ:112:PHE:HE1 | 1.72 | 0.55 |
| 1:BG:95:VAL:HG12 | 1:BG:112:PHE:HE1 | 1.72 | 0.55 |
| 1:AY:18:VAL:HG12 | 1:AY:77:LEU:CB | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BI:151:HIS:HB2 | 1:BJ:64:LYS:HB3 | 1.88 | 0.55 |
| 1:BO:107:ASP:O | 1:BO:107:ASP:OD1 | 2.24 | 0.55 |
| 1:BD:7:LEU:HD11 | 1:BD:140:VAL:HG22 | 1.87 | 0.55 |
| 1:BC:18:VAL:HG21 | 1:BC:30:LEU:HD13 | 1.89 | 0.55 |
| 1:BX:7:LEU:HD11 | 1:BX:140:VAL:HG22 | 1.87 | 0.55 |
| 1:CX:95:VAL:HG12 | 1:CX:112:PHE:HE1 | 1.71 | 0.55 |
| 1:CQ:129:THR:HG22 | 1:CQ:130:LYS:H | 1.72 | 0.55 |
| 1:BI:95:VAL:HG12 | 1:BI:112:PHE:HE1 | 1.71 | 0.55 |
| 1:BZ:75:ILE:HG22 | 1:BZ:77:LEU:HD13 | 1.90 | 0.55 |
| 1:AV:129:THR:HG22 | 1:AV:130:LYS:H | 1.72 | 0.55 |
| 1:AO:52:VAL:CB | 1:AO:53:PRO:HD2 | 2.34 | 0.54 |
| 1:BB:97:LYS:O | 1:BB:102:LEU:HB2 | 2.07 | 0.54 |
| 1:CB:95:VAL:HG12 | 1:CB:112:PHE:HE1 | 1.72 | 0.54 |
| 1:C1:96:ALA:O | 1:C1:100:ALA:HB2 | 2.06 | 0.54 |
| 1:BQ:95:VAL:HG12 | 1:BQ:112:PHE:HE1 | 1.72 | 0.54 |
| 1:C4:18:VAL:HG12 | 1:C4:77:LEU:CB | 2.37 | 0.54 |
| 1:BX:151:HIS:HB2 | 1:BY:64:LYS:HB3 | 1.88 | 0.54 |
| 1:CI:151:HIS:HB2 | 1:CJ:64:LYS:HB3 | 1.88 | 0.54 |
| 1:AE:39:ARG:O | 1:AN:7:LEU:HB3 | 2.05 | 0.54 |
| 1:BX:95:VAL:HG12 | 1:BX:112:PHE:HE1 | 1.71 | 0.54 |
| 1:BZ:3:PHE:CD2 | 1:BZ:150:LYS:HE2 | 2.42 | 0.54 |
| 1:CP:85:THR:HB | 1:CT:116:THR:O | 2.07 | 0.54 |
| 1:CT:128:GLY:O | 1:C4:22:ASN:HA | 2.07 | 0.54 |
| 1:CK:85:THR:HB | 1:CO:116:THR:O | 2.07 | 0.54 |
| 1:AG:97:LYS:O | 1:AG:102:LEU:HB2 | 2.07 | 0.54 |
| 1:CW:97:LYS:HE3 | 1:CX:97:LYS:HZ1 | 1.73 | 0.54 |
| 1:CW:7:LEU:HD23 | 1:C2:40:HIS:CE1 | 2.42 | 0.54 |
| 1:AH:38:LYS:HZ2 | 1:AH:44:GLU:HA | 1.72 | 0.54 |
| 1:BS:151:HIS:HB2 | 1:BT:64:LYS:HB3 | 1.88 | 0.54 |
| 1:BG:129:THR:HG22 | 1:BG:130:LYS:H | 1.72 | 0.54 |
| 1:BT:83:GLY:HA3 | 2:BT:1001:PO4:P | 2.46 | 0.54 |
| 1:BR:18:VAL:HG21 | 1:BR:30:LEU:HD13 | 1.89 | 0.54 |
| 1:AI:95:VAL:HG12 | 1:AI:112:PHE:HE1 | 1.71 | 0.54 |
| 1:BH:18:VAL:HG21 | 1:BH:30:LEU:HD13 | 1.89 | 0.54 |
| 1:BR:152:TRP:HD1 | 1:BS:68:SER:HB2 | 1.72 | 0.54 |
| 1:BW:18:VAL:HG21 | 1:BW:30:LEU:HD13 | 1.89 | 0.54 |
| 1:AF:85:THR:HB | 1:AJ:116:THR:O | 2.07 | 0.54 |
| 1:CM:18:VAL:HG21 | 1:CM:30:LEU:HD13 | 1.89 | 0.54 |
| 1:A4:53:PRO:HG2 | 1:A4:57:GLU:HG3 | 0.65 | 0.54 |
| 1:B1:107:ASP:HB2 | 1:B1:152:TRP:HZ3 | 1.62 | 0.54 |
| 1:AB:97:LYS:O | 1:AB:102:LEU:HB2 | 2.07 | 0.54 |
| 1:BV:95:VAL:HG12 | 1:BV:112:PHE:HE1 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BG:97:LYS:O | 1:BG:102:LEU:HB2 | 2.07 | 0.54 |
| 1:AJ:18:VAL:HG12 | 1:AJ:77:LEU:CB | 2.37 | 0.54 |
| 1:A4:107:ASP:OD1 | 1:A4:107:ASP:O | 2.24 | 0.54 |
| 1:CJ:107:ASP:OD1 | 1:CJ:107:ASP:O | 2.25 | 0.54 |
| 1:A1:129:THR:HG22 | 1:A1:130:LYS:H | 1.72 | 0.54 |
| 1:C2:18:VAL:HG21 | 1:C2:30:LEU:HD13 | 1.89 | 0.54 |
| 1:BP:75:ILE:HG22 | 1:BP:77:LEU:HD13 | 1.90 | 0.54 |
| 1:BB:129:THR:HG22 | 1:BB:130:LYS:H | 1.72 | 0.54 |
| 1:AA:75:ILE:HG22 | 1:AA:77:LEU:HD13 | 1.90 | 0.54 |
| 1:CC:152:TRP:HD1 | 1:CD:68:SER:HB2 | 1.72 | 0.54 |
| 1:AU:85:THR:HB | 1:AY:116:THR:O | 2.07 | 0.54 |
| 1:CJ:52:VAL:HB | 1:CJ:53:PRO:CD | 2.35 | 0.54 |
| 1:BJ:52:VAL:HB | 1:BJ:53:PRO:CD | 2.35 | 0.54 |
| 1:AT:52:VAL:HB | 1:AT:53:PRO:CD | 2.35 | 0.54 |
| 1:AC:129:THR:O | 1:AC:132:GLY:N | 2.25 | 0.54 |
| 1:CL:100:ALA:HA | 1:CM:56:PHE:CZ | 2.42 | 0.54 |
| 1:C1:75:ILE:HG22 | 1:C1:77:LEU:HD13 | 1.90 | 0.54 |
| 1:C3:151:HIS:HB2 | 1:C4:64:LYS:HB3 | 1.88 | 0.54 |
| 1:AR:18:VAL:HG21 | 1:AR:30:LEU:HD13 | 1.89 | 0.54 |
| 1:AF:3:PHE:CD2 | 1:AF:150:LYS:HE2 | 2.42 | 0.54 |
| 1:AW:18:VAL:HG21 | 1:AW:30:LEU:HD13 | 1.89 | 0.54 |
| 1:AP:75:ILE:HG22 | 1:AP:77:LEU:HD13 | 1.89 | 0.54 |
| 1:AC:18:VAL:HG21 | 1:AC:30:LEU:HD13 | 1.89 | 0.54 |
| 1:AZ:75:ILE:HG22 | 1:AZ:77:LEU:HD13 | 1.90 | 0.54 |
| 1:CP:75:ILE:HG22 | 1:CP:77:LEU:HD13 | 1.90 | 0.54 |
| 1:B2:18:VAL:HG21 | 1:B2:30:LEU:HD13 | 1.89 | 0.54 |
| 1:CJ:53:PRO:HG2 | 1:CJ:57:GLU:HG3 | 0.65 | 0.54 |
| 1:A4:52:VAL:CB | 1:A4:53:PRO:HD2 | 2.33 | 0.54 |
| 1:BN:18:VAL:HG12 | 1:BN:77:LEU:CB | 2.37 | 0.54 |
| 1:CL:75:ILE:HG22 | 1:CL:77:LEU:HD13 | 1.90 | 0.54 |
| 1:B3:151:HIS:HB2 | 1:B4:64:LYS:HB3 | 1.88 | 0.54 |
| 1:CD:151:HIS:HB2 | 1:CE:64:LYS:HB3 | 1.88 | 0.54 |
| 1:AM:18:VAL:HG21 | 1:AM:30:LEU:HD13 | 1.89 | 0.54 |
| 1:AU:75:ILE:HG22 | 1:AU:77:LEU:HD13 | 1.89 | 0.54 |
| 1:AP:3:PHE:CD2 | 1:AP:150:LYS:HE2 | 2.42 | 0.54 |
| 1:BF:3:PHE:CD2 | 1:BF:150:LYS:HE2 | 2.42 | 0.54 |
| 1:C4:53:PRO:CG | 1:C4:57:GLU:CG | 2.46 | 0.54 |
| 1:CL:97:LYS:O | 1:CL:102:LEU:HB2 | 2.07 | 0.54 |
| 1:BQ:100:ALA:HA | 1:BR:56:PHE:CZ | 2.42 | 0.54 |
| 1:B3:18:VAL:HG12 | 1:B3:77:LEU:CB | 2.37 | 0.54 |
| 1:AO:18:VAL:HG12 | 1:AO:77:LEU:CB | 2.37 | 0.54 |
| 1:BH:65:MET:HE3 | 1:BH:71:TYR:CE1 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A3:151:HIS:HB2 | 1:A4:64:LYS:HB3 | 1.88 | 0.54 |
| 1:CW:18:VAL:HG21 | 1:CW:30:LEU:HD13 | 1.89 | 0.54 |
| 1:AH:152:TRP:HD1 | 1:AI:68:SER:HB2 | 1.72 | 0.54 |
| 1:AQ:129:THR:HG22 | 1:AQ:130:LYS:H | 1.72 | 0.54 |
| 1:CD:95:VAL:HG12 | 1:CD:112:PHE:HE1 | 1.71 | 0.54 |
| 1:BS:39:ARG:O | 1:BY:7:LEU:HB3 | 2.07 | 0.54 |
| 1:CZ:75:ILE:HG22 | 1:CZ:77:LEU:HD13 | 1.90 | 0.54 |
| 1:BL:95:VAL:HG12 | 1:BL:112:PHE:HE1 | 1.72 | 0.54 |
| 1:AL:100:ALA:HA | 1:AM:56:PHE:CZ | 2.42 | 0.54 |
| 1:B1:97:LYS:O | 1:B1:102:LEU:HB2 | 2.07 | 0.54 |
| 1:CH:97:LYS:HE3 | 1:CI:97:LYS:HZ3 | 1.73 | 0.54 |
| 1:BT:107:ASP:OD1 | 1:BT:107:ASP:O | 2.24 | 0.54 |
| 1:CA:75:ILE:HG22 | 1:CA:77:LEU:HD13 | 1.90 | 0.54 |
| 1:AM:152:TRP:HD1 | 1:AN:68:SER:HB2 | 1.72 | 0.54 |
| 1:CI:39:ARG:O | 1:CO:7:LEU:HB3 | 2.08 | 0.54 |
| 1:CD:22:ASN:HA | 1:CR:128:GLY:O | 2.07 | 0.54 |
| 1:BN:95:VAL:HG12 | 1:BN:112:PHE:HE1 | 1.71 | 0.54 |
| 1:BE:53:PRO:CD | 1:BE:57:GLU:HG3 | 2.29 | 0.54 |
| 1:AC:129:THR:HG21 | 1:AS:120:ILE:HD11 | 1.89 | 0.54 |
| 1:AV:97:LYS:O | 1:AV:102:LEU:HB2 | 2.07 | 0.54 |
| 1:CQ:97:LYS:O | 1:CQ:102:LEU:HB2 | 2.07 | 0.54 |
| 1:CG:100:ALA:HA | 1:CH:56:PHE:CZ | 2.42 | 0.54 |
| 1:AI:18:VAL:HG12 | 1:AI:77:LEU:CB | 2.37 | 0.54 |
| 1:CN:151:HIS:HB2 | 1:CO:64:LYS:HB3 | 1.88 | 0.54 |
| 1:BV:75:ILE:HG22 | 1:BV:77:LEU:HD13 | 1.90 | 0.54 |
| 1:BA:3:PHE:CD2 | 1:BA:150:LYS:HE2 | 2.42 | 0.54 |
| 1:AL:129:THR:HG22 | 1:AL:130:LYS:H | 1.72 | 0.54 |
| 1:BF:75:ILE:HG22 | 1:BF:77:LEU:HD13 | 1.90 | 0.54 |
| 1:BS:95:VAL:HG12 | 1:BS:112:PHE:HE1 | 1.71 | 0.54 |
| 1:AB:129:THR:HG22 | 1:AB:130:LYS:H | 1.72 | 0.54 |
| 1:C2:152:TRP:HD1 | 1:C3:68:SER:HB2 | 1.72 | 0.54 |
| 1:BE:52:VAL:HB | 1:BE:53:PRO:CD | 2.35 | 0.54 |
| 1:C1:100:ALA:HA | 1:C2:56:PHE:CZ | 2.42 | 0.54 |
| 1:A1:100:ALA:HA | 1:A2:56:PHE:CZ | 2.42 | 0.54 |
| 1:BW:70:LYS:HB2 | 1:BW:71:TYR:CE1 | 2.43 | 0.54 |
| 1:CX:151:HIS:HB2 | 1:CY:64:LYS:HB3 | 1.88 | 0.54 |
| 1:AJ:107:ASP:OD1 | 1:AJ:107:ASP:O | 2.25 | 0.54 |
| 1:AY:107:ASP:O | 1:AY:107:ASP:OD1 | 2.24 | 0.54 |
| 1:CR:18:VAL:HG21 | 1:CR:30:LEU:HD13 | 1.89 | 0.54 |
| 1:BK:75:ILE:HG22 | 1:BK:77:LEU:HD13 | 1.90 | 0.54 |
| 1:AN:95:VAL:HG12 | 1:AN:112:PHE:HE1 | 1.71 | 0.54 |
| 1:BV:129:THR:HG22 | 1:BV:130:LYS:H | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BA:75:ILE:HG22 | 1:BA:77:LEU:HD13 | 1.90 | 0.54 |
| 1:BE:53:PRO:CG | 1:BE:57:GLU:CG | 2.46 | 0.54 |
| 1:AQ:13:LYS:HZ1 | 1:BU:43:GLU:HB2 | 1.72 | 0.54 |
| 1:AQ:97:LYS:O | 1:AQ:102:LEU:HB2 | 2.07 | 0.54 |
| 1:A2:70:LYS:HB2 | 1:A2:71:TYR:CE1 | 2.43 | 0.54 |
| 1:BG:75:ILE:HG22 | 1:BG:77:LEU:HD13 | 1.90 | 0.54 |
| 1:AQ:75:ILE:HG22 | 1:AQ:77:LEU:HD13 | 1.90 | 0.54 |
| 1:CI:7:LEU:HB3 | 1:CO:39:ARG:O | 2.08 | 0.54 |
| 1:CH:18:VAL:HG21 | 1:CH:30:LEU:HD13 | 1.89 | 0.54 |
| 1:BM:18:VAL:HG21 | 1:BM:30:LEU:HD13 | 1.89 | 0.54 |
| 1:CK:75:ILE:HG22 | 1:CK:77:LEU:HD13 | 1.90 | 0.54 |
| 1:CP:22:ASN:HA | 1:C3:128:GLY:O | 2.08 | 0.54 |
| 1:C1:97:LYS:O | 1:C1:102:LEU:HB2 | 2.07 | 0.53 |
| 1:AB:100:ALA:HA | 1:AC:56:PHE:CZ | 2.42 | 0.53 |
| 1:CH:70:LYS:HB2 | 1:CH:71:TYR:CE1 | 2.43 | 0.53 |
| 1:AH:18:VAL:HG21 | 1:AH:30:LEU:HD13 | 1.89 | 0.53 |
| 1:A2:152:TRP:HD1 | 1:A3:68:SER:HB2 | 1.72 | 0.53 |
| 1:CZ:143:ILE:O | 1:CZ:147:HIS:HB2 | 2.09 | 0.53 |
| 1:AX:124:ILE:O | 1:AX:129:THR:OG1 | 2.16 | 0.53 |
| 1:BW:152:TRP:HD1 | 1:BX:68:SER:HB2 | 1.72 | 0.53 |
| 1:CU:85:THR:HB | 1:CY:116:THR:O | 2.07 | 0.53 |
| 1:BY:53:PRO:CG | 1:BY:57:GLU:CG | 2.46 | 0.53 |
| 1:BY:53:PRO:HG2 | 1:BY:57:GLU:HG3 | 0.65 | 0.53 |
| 1:AY:52:VAL:HB | 1:AY:53:PRO:CD | 2.35 | 0.53 |
| 1:BT:52:VAL:HB | 1:BT:53:PRO:CD | 2.35 | 0.53 |
| 1:AL:95:VAL:HG12 | 1:AL:112:PHE:HE1 | 1.72 | 0.53 |
| 1:AB:95:VAL:HG12 | 1:AB:112:PHE:HE1 | 1.72 | 0.53 |
| 1:CR:70:LYS:HB2 | 1:CR:71:TYR:CE1 | 2.43 | 0.53 |
| 1:CM:70:LYS:HB2 | 1:CM:71:TYR:CE1 | 2.43 | 0.53 |
| 1:BQ:129:THR:HG22 | 1:BQ:130:LYS:H | 1.72 | 0.53 |
| 1:BQ:75:ILE:HG22 | 1:BQ:77:LEU:HD13 | 1.90 | 0.53 |
| 1:CO:152:TRP:HE3 | 1:CO:153:ALA:N | 2.07 | 0.53 |
| 1:CJ:152:TRP:HE3 | 1:CJ:153:ALA:N | 2.07 | 0.53 |
| 1:AI:7:LEU:HD23 | 1:AO:40:HIS:CE1 | 2.43 | 0.53 |
| 1:AA:6:HIS:HB2 | 1:AA:147:HIS:ND1 | 2.24 | 0.53 |
| 1:B1:129:THR:HG22 | 1:B1:130:LYS:H | 1.72 | 0.53 |
| 1:B2:152:TRP:HD1 | 1:B3:68:SER:HB2 | 1.72 | 0.53 |
| 1:BF:6:HIS:HB2 | 1:BF:147:HIS:ND1 | 2.24 | 0.53 |
| 1:CF:75:ILE:HG22 | 1:CF:77:LEU:HD13 | 1.90 | 0.53 |
| 1:BU:6:HIS:HB2 | 1:BU:147:HIS:ND1 | 2.23 | 0.53 |
| 1:CY:52:VAL:HB | 1:CY:53:PRO:CD | 2.35 | 0.53 |
| 1:AJ:52:VAL:CB | 1:AJ:53:PRO:HD2 | 2.34 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CG:97:LYS:HE3 | 1:CH:97:LYS:HZ3 | 1.71 | 0.53 |
| 1:AW:70:LYS:HB2 | 1:AW:71:TYR:CE1 | 2.43 | 0.53 |
| 1:B4:18:VAL:HG12 | 1:B4:77:LEU:CB | 2.37 | 0.53 |
| 1:BG:121:GLU:O | 1:BG:125:GLU:HG3 | 2.09 | 0.53 |
| 1:BV:121:GLU:O | 1:BV:125:GLU:HG3 | 2.09 | 0.53 |
| 1:AY:152:TRP:HE3 | 1:AY:153:ALA:N | 2.07 | 0.53 |
| 1:BP:3:PHE:HD2 | 1:BP:150:LYS:HE2 | 1.74 | 0.53 |
| 1:AK:6:HIS:HB2 | 1:AK:147:HIS:ND1 | 2.23 | 0.53 |
| 1:CP:6:HIS:HB2 | 1:CP:147:HIS:ND1 | 2.24 | 0.53 |
| 1:AK:75:ILE:HG22 | 1:AK:77:LEU:HD13 | 1.90 | 0.53 |
| 1:CA:143:ILE:O | 1:CA:147:HIS:HB2 | 2.09 | 0.53 |
| 1:CU:75:ILE:HG22 | 1:CU:77:LEU:HD13 | 1.89 | 0.53 |
| 1:C3:104:LEU:HD13 | 1:C4:102:LEU:HG | 1.91 | 0.53 |
| 1:CN:104:LEU:HD13 | 1:CO:102:LEU:HG | 1.91 | 0.53 |
| 1:AO:52:VAL:HB | 1:AO:53:PRO:CD | 2.35 | 0.53 |
| 1:AR:97:LYS:HE3 | 1:AS:97:LYS:HZ1 | 1.74 | 0.53 |
| 1:AR:70:LYS:HB2 | 1:AR:71:TYR:CE1 | 2.43 | 0.53 |
| 1:B4:107:ASP:O | 1:B4:107:ASP:OD1 | 2.24 | 0.53 |
| 1:AJ:152:TRP:HE3 | 1:AJ:153:ALA:N | 2.07 | 0.53 |
| 1:CK:3:PHE:HD2 | 1:CK:150:LYS:HE2 | 1.74 | 0.53 |
| 1:AF:143:ILE:O | 1:AF:147:HIS:HB2 | 2.09 | 0.53 |
| 1:CI:104:LEU:HD13 | 1:CJ:102:LEU:HG | 1.91 | 0.53 |
| 1:BK:143:ILE:O | 1:BK:147:HIS:HB2 | 2.09 | 0.53 |
| 1:CK:6:HIS:HB2 | 1:CK:147:HIS:ND1 | 2.24 | 0.53 |
| 1:BV:100:ALA:HA | 1:BW:56:PHE:CZ | 2.42 | 0.53 |
| 1:CF:28:LYS:HZ1 | 1:CR:28:LYS:HZ3 | 1.57 | 0.53 |
| 1:BT:18:VAL:HG12 | 1:BT:77:LEU:CB | 2.37 | 0.53 |
| 1:CT:18:VAL:HG12 | 1:CT:77:LEU:CB | 2.37 | 0.53 |
| 1:C2:70:LYS:HB2 | 1:C2:71:TYR:CE1 | 2.43 | 0.53 |
| 1:CL:121:GLU:O | 1:CL:125:GLU:HG3 | 2.09 | 0.53 |
| 1:AL:121:GLU:O | 1:AL:125:GLU:HG3 | 2.09 | 0.53 |
| 1:AB:124:ILE:HD11 | 1:AV:24:PHE:CE2 | 2.43 | 0.53 |
| 1:B1:75:ILE:HG22 | 1:B1:77:LEU:HD13 | 1.90 | 0.53 |
| 1:BL:75:ILE:HG22 | 1:BL:77:LEU:HD13 | 1.90 | 0.53 |
| 1:CV:75:ILE:HG22 | 1:CV:77:LEU:HD13 | 1.90 | 0.53 |
| 1:C4:152:TRP:HE3 | 1:C4:153:ALA:N | 2.07 | 0.53 |
| 1:CF:3:PHE:HD2 | 1:CF:150:LYS:HE2 | 1.74 | 0.53 |
| 1:CA:3:PHE:HD2 | 1:CA:150:LYS:HE2 | 1.74 | 0.53 |
| 1:BA:6:HIS:HB2 | 1:BA:147:HIS:ND1 | 2.24 | 0.53 |
| 1:AU:6:HIS:HB2 | 1:AU:147:HIS:ND1 | 2.24 | 0.53 |
| 1:BD:128:GLY:O | 1:BF:22:ASN:HA | 2.09 | 0.53 |
| 1:BL:100:ALA:HA | 1:BM:56:PHE:CZ | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BR:97:LYS:HG3 | 1:BS:97:LYS:HZ1 | 1.74 | 0.53 |
| 1:A1:95:VAL:HG12 | 1:A1:112:PHE:HE1 | 1.72 | 0.53 |
| 1:CC:70:LYS:HB2 | 1:CC:71:TYR:CE1 | 2.43 | 0.53 |
| 1:A4:18:VAL:HG12 | 1:A4:77:LEU:CB | 2.37 | 0.53 |
| 1:B1:121:GLU:O | 1:B1:125:GLU:HG3 | 2.09 | 0.53 |
| 1:AG:75:ILE:HG22 | 1:AG:77:LEU:HD13 | 1.90 | 0.53 |
| 1:CZ:3:PHE:HD2 | 1:CZ:150:LYS:HE2 | 1.74 | 0.53 |
| 1:AU:3:PHE:HD2 | 1:AU:150:LYS:HE2 | 1.74 | 0.53 |
| 1:BA:3:PHE:HD2 | 1:BA:150:LYS:HE2 | 1.74 | 0.53 |
| 1:BA:143:ILE:O | 1:BA:147:HIS:HB2 | 2.09 | 0.53 |
| 1:AR:152:TRP:HD1 | 1:AS:68:SER:HB2 | 1.72 | 0.53 |
| 1:CG:129:THR:HG22 | 1:CG:130:LYS:H | 1.72 | 0.53 |
| 1:C1:129:THR:HG22 | 1:C1:130:LYS:H | 1.72 | 0.53 |
| 1:CD:104:LEU:HD13 | 1:CE:102:LEU:HG | 1.91 | 0.53 |
| 1:CD:28:LYS:HZ3 | 1:CF:28:LYS:HZ2 | 1.55 | 0.53 |
| 1:BR:70:LYS:HB2 | 1:BR:71:TYR:CE1 | 2.43 | 0.53 |
| 1:AG:121:GLU:O | 1:AG:125:GLU:HG3 | 2.09 | 0.53 |
| 1:A1:75:ILE:HG22 | 1:A1:77:LEU:HD13 | 1.90 | 0.53 |
| 1:BE:152:TRP:HE3 | 1:BE:153:ALA:N | 2.07 | 0.53 |
| 1:CD:20:ARG:NH1 | 1:CR:39:ARG:CZ | 2.72 | 0.53 |
| 1:AF:75:ILE:HG22 | 1:AF:77:LEU:HD13 | 1.90 | 0.53 |
| 1:AZ:6:HIS:HB2 | 1:AZ:147:HIS:ND1 | 2.24 | 0.53 |
| 1:BP:143:ILE:O | 1:BP:147:HIS:HB2 | 2.09 | 0.53 |
| 1:A2:18:VAL:HG21 | 1:A2:30:LEU:HD13 | 1.89 | 0.53 |
| 1:AE:52:VAL:HB | 1:AE:53:PRO:CD | 2.35 | 0.53 |
| 1:AG:100:ALA:HA | 1:AH:56:PHE:CZ | 2.42 | 0.53 |
| 1:C2:97:LYS:HG3 | 1:C3:97:LYS:HZ3 | 1.74 | 0.53 |
| 1:A2:97:LYS:HG3 | 1:A3:97:LYS:HZ1 | 1.74 | 0.53 |
| 1:CS:18:VAL:HG12 | 1:CS:77:LEU:CB | 2.37 | 0.53 |
| 1:BO:18:VAL:HG12 | 1:BO:77:LEU:CB | 2.37 | 0.53 |
| 1:AM:70:LYS:HB2 | 1:AM:71:TYR:CE1 | 2.43 | 0.53 |
| 1:A1:121:GLU:O | 1:A1:125:GLU:HG3 | 2.09 | 0.53 |
| 1:CB:121:GLU:O | 1:CB:125:GLU:HG3 | 2.09 | 0.53 |
| 1:BE:37:LEU:HD12 | 1:BE:47:ILE:HD11 | 1.91 | 0.53 |
| 1:BB:75:ILE:HG22 | 1:BB:77:LEU:HD13 | 1.90 | 0.53 |
| 1:AV:75:ILE:HG22 | 1:AV:77:LEU:HD13 | 1.90 | 0.53 |
| 1:CT:152:TRP:HE3 | 1:CT:153:ALA:N | 2.07 | 0.53 |
| 1:CU:3:PHE:HD2 | 1:CU:150:LYS:HE2 | 1.74 | 0.53 |
| 1:BZ:3:PHE:HD2 | 1:BZ:150:LYS:HE2 | 1.74 | 0.53 |
| 1:CA:6:HIS:HB2 | 1:CA:147:HIS:ND1 | 2.24 | 0.53 |
| 1:BK:6:HIS:HB2 | 1:BK:147:HIS:ND1 | 2.23 | 0.53 |
| 1:AU:143:ILE:O | 1:AU:147:HIS:HB2 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CU:6:HIS:HB2 | 1:CU:147:HIS:ND1 | 2.24 | 0.53 |
| 1:CX:104:LEU:HD13 | 1:CY:102:LEU:HG | 1.91 | 0.53 |
| 1:AD:104:LEU:HD13 | 1:AE:102:LEU:HG | 1.91 | 0.53 |
| 1:B4:52:VAL:HB | 1:B4:53:PRO:CD | 2.35 | 0.53 |
| 1:C4:52:VAL:CB | 1:C4:53:PRO:HD2 | 2.34 | 0.53 |
| 1:AT:53:PRO:HG2 | 1:AT:57:GLU:HG3 | 0.65 | 0.53 |
| 1:BB:100:ALA:HA | 1:BC:56:PHE:CZ | 2.42 | 0.53 |
| 1:AV:100:ALA:HA | 1:AW:56:PHE:CZ | 2.42 | 0.53 |
| 1:AC:38:LYS:HZ2 | 1:AC:44:GLU:HA | 1.73 | 0.53 |
| 1:B2:70:LYS:HB2 | 1:B2:71:TYR:CE1 | 2.43 | 0.53 |
| 1:CQ:121:GLU:O | 1:CQ:125:GLU:HG3 | 2.09 | 0.53 |
| 1:C1:121:GLU:O | 1:C1:125:GLU:HG3 | 2.09 | 0.53 |
| 1:AB:40:HIS:CE1 | 1:AU:7:LEU:HD23 | 2.44 | 0.53 |
| 1:BV:6:HIS:CE1 | 1:BV:8:VAL:HB | 2.44 | 0.53 |
| 1:AK:3:PHE:HD2 | 1:AK:150:LYS:HE2 | 1.74 | 0.53 |
| 1:CU:143:ILE:O | 1:CU:147:HIS:HB2 | 2.09 | 0.53 |
| 1:CA:85:THR:HB | 1:CE:116:THR:O | 2.07 | 0.53 |
| 1:AX:104:LEU:HD13 | 1:AY:102:LEU:HG | 1.91 | 0.53 |
| 1:C2:97:LYS:HG3 | 1:C3:97:LYS:NZ | 2.24 | 0.53 |
| 1:A2:38:LYS:HZ2 | 1:A2:44:GLU:HA | 1.74 | 0.53 |
| 1:BR:38:LYS:HZ2 | 1:BR:44:GLU:HA | 1.74 | 0.53 |
| 1:AC:70:LYS:HB2 | 1:AC:71:TYR:CE1 | 2.43 | 0.53 |
| 1:BL:121:GLU:O | 1:BL:125:GLU:HG3 | 2.09 | 0.53 |
| 1:CP:3:PHE:HD2 | 1:CP:150:LYS:HE2 | 1.74 | 0.53 |
| 1:AN:104:LEU:HD13 | 1:AO:102:LEU:HG | 1.91 | 0.53 |
| 1:AT:52:VAL:CB | 1:AT:53:PRO:HD2 | 2.34 | 0.52 |
| 1:BT:53:PRO:CD | 1:BT:57:GLU:HG3 | 2.29 | 0.52 |
| 1:AM:97:LYS:HG3 | 1:AN:97:LYS:NZ | 2.24 | 0.52 |
| 1:BB:144:GLU:CD | 1:BU:39:ARG:NH2 | 2.61 | 0.52 |
| 1:BY:18:VAL:HG12 | 1:BY:77:LEU:CB | 2.37 | 0.52 |
| 1:BM:70:LYS:HB2 | 1:BM:71:TYR:CE1 | 2.43 | 0.52 |
| 1:AQ:121:GLU:O | 1:AQ:125:GLU:HG3 | 2.09 | 0.52 |
| 1:AO:37:LEU:HD12 | 1:AO:47:ILE:HD11 | 1.91 | 0.52 |
| 1:A4:37:LEU:HD12 | 1:A4:47:ILE:HD11 | 1.91 | 0.52 |
| 1:AT:152:TRP:HE3 | 1:AT:153:ALA:N | 2.07 | 0.52 |
| 1:BT:152:TRP:HE3 | 1:BT:153:ALA:N | 2.07 | 0.52 |
| 1:BR:6:HIS:HB3 | 1:BR:147:HIS:CG | 2.45 | 0.52 |
| 1:BF:143:ILE:O | 1:BF:147:HIS:HB2 | 2.09 | 0.52 |
| 1:AK:143:ILE:O | 1:AK:147:HIS:HB2 | 2.09 | 0.52 |
| 1:CP:143:ILE:O | 1:CP:147:HIS:HB2 | 2.09 | 0.52 |
| 1:BU:75:ILE:HG22 | 1:BU:77:LEU:HD13 | 1.90 | 0.52 |
| 1:BZ:6:HIS:HB2 | 1:BZ:147:HIS:ND1 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BF:28:LYS:CE | 1:BR:28:LYS:HZ3 | 2.22 | 0.52 |
| 1:BW:97:LYS:HG3 | 1:BX:97:LYS:NZ | 2.24 | 0.52 |
| 1:A2:97:LYS:HG3 | 1:A3:97:LYS:NZ | 2.24 | 0.52 |
| 1:BJ:18:VAL:HG12 | 1:BJ:77:LEU:CB | 2.37 | 0.52 |
| 1:BK:125:GLU:CA | 1:BK:129:THR:OG1 | 2.57 | 0.52 |
| 1:CU:125:GLU:CA | 1:CU:129:THR:OG1 | 2.57 | 0.52 |
| 1:CW:70:LYS:HB2 | 1:CW:71:TYR:CE1 | 2.43 | 0.52 |
| 1:AK:125:GLU:CA | 1:AK:129:THR:OG1 | 2.57 | 0.52 |
| 1:AB:121:GLU:O | 1:AB:125:GLU:HG3 | 2.09 | 0.52 |
| 1:CG:121:GLU:O | 1:CG:125:GLU:HG3 | 2.09 | 0.52 |
| 1:CQ:75:ILE:HG22 | 1:CQ:77:LEU:HD13 | 1.90 | 0.52 |
| 1:AB:75:ILE:HG22 | 1:AB:77:LEU:HD13 | 1.90 | 0.52 |
| 1:AL:75:ILE:HG22 | 1:AL:77:LEU:HD13 | 1.90 | 0.52 |
| 1:AY:37:LEU:HD12 | 1:AY:47:ILE:HD11 | 1.91 | 0.52 |
| 1:BJ:37:LEU:HD12 | 1:BJ:47:ILE:HD11 | 1.91 | 0.52 |
| 1:BY:37:LEU:HD12 | 1:BY:47:ILE:HD11 | 1.91 | 0.52 |
| 1:BM:6:HIS:HB3 | 1:BM:147:HIS:CG | 2.45 | 0.52 |
| 1:AA:3:PHE:HD2 | 1:AA:150:LYS:HE2 | 1.74 | 0.52 |
| 1:BU:143:ILE:O | 1:BU:147:HIS:HB2 | 2.09 | 0.52 |
| 1:AP:143:ILE:O | 1:AP:147:HIS:HB2 | 2.09 | 0.52 |
| 1:A3:104:LEU:HD13 | 1:A4:102:LEU:HG | 1.91 | 0.52 |
| 1:CS:104:LEU:HD13 | 1:CT:102:LEU:HG | 1.91 | 0.52 |
| 1:CU:109:PRO:HB3 | 1:CU:145:MET:HB3 | 1.91 | 0.52 |
| 1:CC:18:VAL:HG21 | 1:CC:30:LEU:HD13 | 1.89 | 0.52 |
| 1:CF:143:ILE:O | 1:CF:147:HIS:HB2 | 2.09 | 0.52 |
| 1:CE:53:PRO:CD | 1:CE:57:GLU:HG3 | 2.29 | 0.52 |
| 1:BC:129:THR:O | 1:BC:132:GLY:N | 2.25 | 0.52 |
| 1:AH:97:LYS:HG3 | 1:AI:97:LYS:NZ | 2.24 | 0.52 |
| 1:AR:97:LYS:HG3 | 1:AS:97:LYS:NZ | 2.24 | 0.52 |
| 1:AC:97:LYS:HG3 | 1:AD:97:LYS:NZ | 2.24 | 0.52 |
| 1:BR:97:LYS:HG3 | 1:BS:97:LYS:NZ | 2.24 | 0.52 |
| 1:CH:97:LYS:HG3 | 1:CI:97:LYS:NZ | 2.24 | 0.52 |
| 1:BS:18:VAL:HG12 | 1:BS:77:LEU:CB | 2.37 | 0.52 |
| 1:BC:7:LEU:HB3 | 1:BR:39:ARG:O | 2.09 | 0.52 |
| 1:AH:70:LYS:HB2 | 1:AH:71:TYR:CE1 | 2.43 | 0.52 |
| 1:BC:70:LYS:HB2 | 1:BC:71:TYR:CE1 | 2.43 | 0.52 |
| 1:BQ:121:GLU:O | 1:BQ:125:GLU:HG3 | 2.09 | 0.52 |
| 1:BB:121:GLU:O | 1:BB:125:GLU:HG3 | 2.09 | 0.52 |
| 1:CC:6:HIS:HB3 | 1:CC:147:HIS:CG | 2.45 | 0.52 |
| 1:AM:6:HIS:HB3 | 1:AM:147:HIS:CG | 2.45 | 0.52 |
| 1:AC:6:HIS:HB3 | 1:AC:147:HIS:CG | 2.45 | 0.52 |
| 1:AQ:6:HIS:CE1 | 1:AQ:8:VAL:HB | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BG:6:HIS:CE1 | 1:BG:8:VAL:HB | 2.45 | 0.52 |
| 1:BU:3:PHE:HD2 | 1:BU:150:LYS:HE2 | 1.74 | 0.52 |
| 1:BK:3:PHE:HD2 | 1:BK:150:LYS:HE2 | 1.74 | 0.52 |
| 1:AZ:143:ILE:O | 1:AZ:147:HIS:HB2 | 2.09 | 0.52 |
| 1:CF:6:HIS:HB2 | 1:CF:147:HIS:ND1 | 2.24 | 0.52 |
| 1:AX:35:ASP:O | 1:AX:39:ARG:HG3 | 2.10 | 0.52 |
| 1:CK:109:PRO:HB3 | 1:CK:145:MET:HB3 | 1.91 | 0.52 |
| 1:CT:53:PRO:CG | 1:CT:57:GLU:CG | 2.46 | 0.52 |
| 1:CM:97:LYS:HG3 | 1:CN:97:LYS:HZ1 | 1.73 | 0.52 |
| 1:CM:97:LYS:HG3 | 1:CN:97:LYS:NZ | 2.24 | 0.52 |
| 1:AD:18:VAL:HG12 | 1:AD:77:LEU:CB | 2.37 | 0.52 |
| 1:AE:18:VAL:HG12 | 1:AE:77:LEU:CB | 2.37 | 0.52 |
| 1:CJ:18:VAL:HG12 | 1:CJ:77:LEU:CB | 2.37 | 0.52 |
| 1:BP:125:GLU:CA | 1:BP:129:THR:OG1 | 2.57 | 0.52 |
| 1:AW:6:HIS:HB3 | 1:AW:147:HIS:CG | 2.45 | 0.52 |
| 1:CY:152:TRP:HE3 | 1:CY:153:ALA:N | 2.07 | 0.52 |
| 1:BW:6:HIS:HB3 | 1:BW:147:HIS:CG | 2.45 | 0.52 |
| 1:BS:35:ASP:O | 1:BS:39:ARG:HG3 | 2.10 | 0.52 |
| 1:CZ:6:HIS:HB2 | 1:CZ:147:HIS:ND1 | 2.24 | 0.52 |
| 1:AA:143:ILE:O | 1:AA:147:HIS:HB2 | 2.09 | 0.52 |
| 1:BZ:109:PRO:HB3 | 1:BZ:145:MET:HB3 | 1.91 | 0.52 |
| 1:CZ:109:PRO:HB3 | 1:CZ:145:MET:HB3 | 1.91 | 0.52 |
| 1:BI:124:ILE:O | 1:BI:129:THR:OG1 | 2.16 | 0.52 |
| 1:BD:104:LEU:HD13 | 1:BE:102:LEU:HG | 1.91 | 0.52 |
| 1:CY:52:VAL:CB | 1:CY:53:PRO:HD2 | 2.34 | 0.52 |
| 1:CO:18:VAL:HG12 | 1:CO:77:LEU:CB | 2.37 | 0.52 |
| 1:CE:18:VAL:HG12 | 1:CE:77:LEU:CB | 2.37 | 0.52 |
| 1:AT:18:VAL:HG12 | 1:AT:77:LEU:CB | 2.37 | 0.52 |
| 1:AA:125:GLU:CA | 1:AA:129:THR:OG1 | 2.57 | 0.52 |
| 1:AV:121:GLU:O | 1:AV:125:GLU:HG3 | 2.09 | 0.52 |
| 1:CY:37:LEU:HD12 | 1:CY:47:ILE:HD11 | 1.91 | 0.52 |
| 1:CB:75:ILE:HG22 | 1:CB:77:LEU:HD13 | 1.90 | 0.52 |
| 1:B4:152:TRP:HE3 | 1:B4:153:ALA:N | 2.07 | 0.52 |
| 1:BO:152:TRP:HE3 | 1:BO:153:ALA:N | 2.07 | 0.52 |
| 1:B2:6:HIS:HB3 | 1:B2:147:HIS:CG | 2.45 | 0.52 |
| 1:BC:6:HIS:HB3 | 1:BC:147:HIS:CG | 2.45 | 0.52 |
| 1:BY:152:TRP:HE3 | 1:BY:153:ALA:N | 2.07 | 0.52 |
| 1:AG:6:HIS:CE1 | 1:AG:8:VAL:HB | 2.44 | 0.52 |
| 1:AI:104:LEU:HD13 | 1:AJ:102:LEU:HG | 1.91 | 0.52 |
| 1:BX:35:ASP:O | 1:BX:39:ARG:HG3 | 2.10 | 0.52 |
| 1:AS:6:HIS:HE1 | 1:AS:8:VAL:HB | 1.75 | 0.52 |
| 1:BJ:53:PRO:CG | 1:BJ:57:GLU:CG | 2.46 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BD:11:GLY:HA3 | 1:CM:11:GLY:N | 2.25 | 0.52 |
| 1:A1:96:ALA:O | 1:A1:100:ALA:HB2 | 2.06 | 0.52 |
| 1:BG:120:ILE:HD11 | 1:BQ:130:LYS:HG3 | 1.91 | 0.52 |
| 1:CE:37:LEU:HD12 | 1:CE:47:ILE:HD11 | 1.91 | 0.52 |
| 1:AR:6:HIS:HB3 | 1:AR:147:HIS:CG | 2.45 | 0.52 |
| 1:C2:6:HIS:HB3 | 1:C2:147:HIS:CG | 2.45 | 0.52 |
| 1:CW:6:HIS:HB3 | 1:CW:147:HIS:CG | 2.45 | 0.52 |
| 1:B1:6:HIS:CE1 | 1:B1:8:VAL:HB | 2.44 | 0.52 |
| 1:AF:6:HIS:HB2 | 1:AF:147:HIS:ND1 | 2.24 | 0.52 |
| 1:CK:143:ILE:O | 1:CK:147:HIS:HB2 | 2.09 | 0.52 |
| 1:BP:6:HIS:HB2 | 1:BP:147:HIS:ND1 | 2.24 | 0.52 |
| 1:AP:6:HIS:HB2 | 1:AP:147:HIS:ND1 | 2.24 | 0.52 |
| 1:CD:35:ASP:O | 1:CD:39:ARG:HG3 | 2.10 | 0.52 |
| 1:BV:82:ARG:HG3 | 1:BV:118:GLU:OE2 | 2.10 | 0.52 |
| 1:BO:52:VAL:HB | 1:BO:53:PRO:CD | 2.35 | 0.52 |
| 1:CE:52:VAL:CB | 1:CE:53:PRO:HD2 | 2.34 | 0.52 |
| 1:BY:52:VAL:CB | 1:BY:53:PRO:HD2 | 2.34 | 0.52 |
| 1:AM:97:LYS:HE3 | 1:AN:97:LYS:HZ1 | 1.75 | 0.52 |
| 1:AD:97:LYS:HG3 | 1:AE:97:LYS:NZ | 2.25 | 0.52 |
| 1:CN:97:LYS:HG3 | 1:CO:97:LYS:NZ | 2.25 | 0.52 |
| 1:CG:144:GLU:CD | 1:CU:39:ARG:NH2 | 2.63 | 0.52 |
| 1:CH:6:HIS:HB3 | 1:CH:147:HIS:CG | 2.45 | 0.52 |
| 1:AV:6:HIS:CE1 | 1:AV:8:VAL:HB | 2.45 | 0.52 |
| 1:AZ:3:PHE:HD2 | 1:AZ:150:LYS:HE2 | 1.74 | 0.52 |
| 1:B3:6:HIS:HE1 | 1:B3:8:VAL:HB | 1.75 | 0.52 |
| 1:AI:28:LYS:HG3 | 1:AK:24:PHE:CD1 | 2.44 | 0.52 |
| 1:BD:97:LYS:HG3 | 1:BE:97:LYS:NZ | 2.25 | 0.52 |
| 1:AX:97:LYS:HG3 | 1:AY:97:LYS:NZ | 2.25 | 0.52 |
| 1:CB:100:ALA:HA | 1:CC:56:PHE:CZ | 2.42 | 0.52 |
| 1:CC:97:LYS:HG3 | 1:CD:97:LYS:NZ | 2.24 | 0.52 |
| 1:CW:97:LYS:HG3 | 1:CX:97:LYS:NZ | 2.24 | 0.52 |
| 1:CC:38:LYS:HZ2 | 1:CC:44:GLU:HA | 1.75 | 0.52 |
| 1:BH:70:LYS:HB2 | 1:BH:71:TYR:CE1 | 2.43 | 0.52 |
| 1:AT:37:LEU:HD12 | 1:AT:47:ILE:HD11 | 1.91 | 0.52 |
| 1:B4:37:LEU:HD12 | 1:B4:47:ILE:HD11 | 1.91 | 0.52 |
| 1:BO:37:LEU:HD12 | 1:BO:47:ILE:HD11 | 1.91 | 0.52 |
| 1:AE:152:TRP:HE3 | 1:AE:153:ALA:N | 2.07 | 0.52 |
| 1:A4:152:TRP:HE3 | 1:A4:153:ALA:N | 2.07 | 0.52 |
| 1:AF:3:PHE:HD2 | 1:AF:150:LYS:HE2 | 1.74 | 0.52 |
| 1:CI:35:ASP:O | 1:CI:39:ARG:HG3 | 2.10 | 0.52 |
| 1:AF:109:PRO:HB3 | 1:AF:145:MET:HB3 | 1.91 | 0.52 |
| 1:AP:109:PRO:HB3 | 1:AP:145:MET:HB3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CL:129:THR:HG22 | 1:CL:130:LYS:H | 1.72 | 0.52 |
| 1:C1:82:ARG:HG3 | 1:C1:118:GLU:OE2 | 2.10 | 0.52 |
| 1:CL:82:ARG:HG3 | 1:CL:118:GLU:OE2 | 2.10 | 0.52 |
| 1:BO:52:VAL:CB | 1:BO:53:PRO:HD2 | 2.34 | 0.52 |
| 1:AQ:13:LYS:CE | 1:BU:43:GLU:HG2 | 2.40 | 0.52 |
| 1:AH:129:THR:O | 1:AH:132:GLY:N | 2.25 | 0.52 |
| 1:BC:97:LYS:HG3 | 1:BD:97:LYS:NZ | 2.24 | 0.52 |
| 1:AR:97:LYS:HG3 | 1:AS:97:LYS:HZ1 | 1.75 | 0.52 |
| 1:CY:18:VAL:HG12 | 1:CY:77:LEU:CB | 2.37 | 0.52 |
| 1:CV:121:GLU:O | 1:CV:125:GLU:HG3 | 2.09 | 0.52 |
| 1:C4:37:LEU:HD12 | 1:C4:47:ILE:HD11 | 1.91 | 0.52 |
| 1:CE:152:TRP:HE3 | 1:CE:153:ALA:N | 2.07 | 0.52 |
| 1:AO:152:TRP:HE3 | 1:AO:153:ALA:N | 2.07 | 0.52 |
| 1:A1:6:HIS:CE1 | 1:A1:8:VAL:HB | 2.45 | 0.52 |
| 1:AP:3:PHE:HD2 | 1:AP:150:LYS:HE2 | 1.74 | 0.52 |
| 1:BZ:143:ILE:O | 1:BZ:147:HIS:HB2 | 2.09 | 0.52 |
| 1:BL:82:ARG:HG3 | 1:BL:118:GLU:OE2 | 2.10 | 0.52 |
| 1:BI:104:LEU:HD13 | 1:BJ:102:LEU:HG | 1.91 | 0.52 |
| 1:BG:82:ARG:HG3 | 1:BG:118:GLU:OE2 | 2.10 | 0.52 |
| 1:AK:109:PRO:HB3 | 1:AK:145:MET:HB3 | 1.92 | 0.52 |
| 1:BS:104:LEU:HD13 | 1:BT:102:LEU:HG | 1.91 | 0.52 |
| 1:AN:35:ASP:O | 1:AN:39:ARG:HG3 | 2.10 | 0.52 |
| 1:CP:109:PRO:HB3 | 1:CP:145:MET:HB3 | 1.91 | 0.52 |
| 1:AN:6:HIS:HE1 | 1:AN:8:VAL:HB | 1.75 | 0.52 |
| 1:BX:104:LEU:HD13 | 1:BY:102:LEU:HG | 1.91 | 0.52 |
| 1:CC:129:THR:CG2 | 1:CS:120:ILE:CD1 | 2.78 | 0.52 |
| 1:AT:109:PRO:HB3 | 1:AT:145:MET:HB3 | 1.92 | 0.52 |
| 1:CD:97:LYS:HG3 | 1:CE:97:LYS:NZ | 2.25 | 0.52 |
| 1:AI:97:LYS:HG3 | 1:AJ:97:LYS:NZ | 2.25 | 0.52 |
| 1:AJ:37:LEU:HD12 | 1:AJ:47:ILE:HD11 | 1.91 | 0.52 |
| 1:BD:7:LEU:HB3 | 1:BJ:39:ARG:O | 2.10 | 0.52 |
| 1:CV:6:HIS:CE1 | 1:CV:8:VAL:HB | 2.44 | 0.52 |
| 1:BA:109:PRO:HB3 | 1:BA:145:MET:HB3 | 1.91 | 0.52 |
| 1:A3:35:ASP:O | 1:A3:39:ARG:HG3 | 2.10 | 0.52 |
| 1:BS:6:HIS:HE1 | 1:BS:8:VAL:HB | 1.75 | 0.52 |
| 1:CS:6:HIS:HE1 | 1:CS:8:VAL:HB | 1.75 | 0.52 |
| 1:CW:129:THR:HG21 | 1:C3:120:ILE:CD1 | 2.40 | 0.51 |
| 1:AJ:109:PRO:HB3 | 1:AJ:145:MET:HB3 | 1.92 | 0.51 |
| 1:BM:97:LYS:HG3 | 1:BN:97:LYS:NZ | 2.24 | 0.51 |
| 1:AN:97:LYS:HG3 | 1:AO:97:LYS:NZ | 2.25 | 0.51 |
| 1:C2:97:LYS:HE3 | 1:C3:97:LYS:HZ3 | 1.75 | 0.51 |
| 1:AS:97:LYS:HG3 | 1:AT:97:LYS:NZ | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BR:97:LYS:HE3 | 1:BS:97:LYS:HZ1 | 1.75 | 0.51 |
| 1:CX:18:VAL:HG12 | 1:CX:77:LEU:CB | 2.37 | 0.51 |
| 1:CG:75:ILE:HG22 | 1:CG:77:LEU:HD13 | 1.90 | 0.51 |
| 1:BT:37:LEU:HD12 | 1:BT:47:ILE:HD11 | 1.91 | 0.51 |
| 1:CO:37:LEU:HD12 | 1:CO:47:ILE:HD11 | 1.91 | 0.51 |
| 1:AI:35:ASP:O | 1:AI:39:ARG:HG3 | 2.10 | 0.51 |
| 1:BD:35:ASP:O | 1:BD:39:ARG:HG3 | 2.10 | 0.51 |
| 1:CL:6:HIS:CE1 | 1:CL:8:VAL:HB | 2.45 | 0.51 |
| 1:BN:104:LEU:HD13 | 1:BO:102:LEU:HG | 1.91 | 0.51 |
| 1:CV:82:ARG:HG3 | 1:CV:118:GLU:OE2 | 2.10 | 0.51 |
| 1:AL:82:ARG:HG3 | 1:AL:118:GLU:OE2 | 2.10 | 0.51 |
| 1:CE:53:PRO:CG | 1:CE:57:GLU:CG | 2.46 | 0.51 |
| 1:B2:97:LYS:HG3 | 1:B3:97:LYS:NZ | 2.24 | 0.51 |
| 1:BI:97:LYS:HG3 | 1:BJ:97:LYS:NZ | 2.25 | 0.51 |
| 1:AB:144:GLU:CD | 1:AU:39:ARG:HH22 | 2.13 | 0.51 |
| 1:BI:18:VAL:HG12 | 1:BI:77:LEU:CB | 2.37 | 0.51 |
| 1:AU:125:GLU:CA | 1:AU:129:THR:OG1 | 2.57 | 0.51 |
| 1:BU:125:GLU:CA | 1:BU:129:THR:OG1 | 2.57 | 0.51 |
| 1:CT:37:LEU:HD12 | 1:CT:47:ILE:HD11 | 1.91 | 0.51 |
| 1:CJ:37:LEU:HD12 | 1:CJ:47:ILE:HD11 | 1.91 | 0.51 |
| 1:AL:6:HIS:CE1 | 1:AL:8:VAL:HB | 2.44 | 0.51 |
| 1:BQ:82:ARG:HG3 | 1:BQ:118:GLU:OE2 | 2.10 | 0.51 |
| 1:BN:35:ASP:O | 1:BN:39:ARG:HG3 | 2.10 | 0.51 |
| 1:BK:109:PRO:HB3 | 1:BK:145:MET:HB3 | 1.91 | 0.51 |
| 1:B3:104:LEU:HD13 | 1:B4:102:LEU:HG | 1.91 | 0.51 |
| 1:BS:97:LYS:HG3 | 1:BT:97:LYS:NZ | 2.25 | 0.51 |
| 1:BH:97:LYS:HG3 | 1:BI:97:LYS:NZ | 2.24 | 0.51 |
| 1:A3:97:LYS:HG3 | 1:A4:97:LYS:NZ | 2.25 | 0.51 |
| 1:CF:39:ARG:NH2 | 1:CQ:144:GLU:CD | 2.63 | 0.51 |
| 1:A3:18:VAL:HG12 | 1:A3:77:LEU:CB | 2.37 | 0.51 |
| 1:BA:125:GLU:CA | 1:BA:129:THR:OG1 | 2.57 | 0.51 |
| 1:AE:37:LEU:HD12 | 1:AE:47:ILE:HD11 | 1.91 | 0.51 |
| 1:A2:6:HIS:HB3 | 1:A2:147:HIS:CG | 2.45 | 0.51 |
| 1:CP:28:LYS:HD2 | 1:CW:24:PHE:CE1 | 2.45 | 0.51 |
| 1:CB:6:HIS:CE1 | 1:CB:8:VAL:HB | 2.45 | 0.51 |
| 1:A1:82:ARG:HG3 | 1:A1:118:GLU:OE2 | 2.10 | 0.51 |
| 1:BX:6:HIS:HE1 | 1:BX:8:VAL:HB | 1.75 | 0.51 |
| 1:AT:53:PRO:CG | 1:AT:57:GLU:CG | 2.46 | 0.51 |
| 1:B4:109:PRO:HB3 | 1:B4:145:MET:HB3 | 1.92 | 0.51 |
| 1:C3:97:LYS:HG3 | 1:C4:97:LYS:NZ | 2.25 | 0.51 |
| 1:CR:97:LYS:HG3 | 1:CS:97:LYS:NZ | 2.24 | 0.51 |
| 1:CD:18:VAL:HG12 | 1:CD:77:LEU:CB | 2.37 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:CM:6:HIS:HB3 | 1:CM:147:HIS:CG | 2.45 | 0.51 |
| 1:AH:6:HIS:HB3 | 1:AH:147:HIS:CG | 2.45 | 0.51 |
| 1:BQ:6:HIS:CE1 | 1:BQ:8:VAL:HB | 2.45 | 0.51 |
| 1:BL:6:HIS:CE1 | 1:BL:8:VAL:HB | 2.44 | 0.51 |
| 1:AD:23:GLU:HA | 1:AD:26:THR:OG1 | 2.11 | 0.51 |
| 1:CS:23:GLU:HA | 1:CS:26:THR:OG1 | 2.11 | 0.51 |
| 1:BI:6:HIS:HE1 | 1:BI:8:VAL:HB | 1.75 | 0.51 |
| 1:A3:23:GLU:HA | 1:A3:26:THR:OG1 | 2.11 | 0.51 |
| 1:AD:35:ASP:O | 1:AD:39:ARG:HG3 | 2.10 | 0.51 |
| 1:AU:109:PRO:HB3 | 1:AU:145:MET:HB3 | 1.91 | 0.51 |
| 1:AZ:109:PRO:HB3 | 1:AZ:145:MET:HB3 | 1.92 | 0.51 |
| 1:A4:109:PRO:HB3 | 1:A4:145:MET:HB3 | 1.92 | 0.51 |
| 1:BJ:109:PRO:HB3 | 1:BJ:145:MET:HB3 | 1.92 | 0.51 |
| 1:BN:97:LYS:HG3 | 1:BO:97:LYS:NZ | 2.25 | 0.51 |
| 1:C2:82:ARG:CG | 1:C2:82:ARG:NH1 | 2.73 | 0.51 |
| 1:BR:82:ARG:CG | 1:BR:82:ARG:NH1 | 2.73 | 0.51 |
| 1:AM:82:ARG:CG | 1:AM:82:ARG:NH1 | 2.73 | 0.51 |
| 1:AR:82:ARG:CG | 1:AR:82:ARG:NH1 | 2.73 | 0.51 |
| 1:B2:82:ARG:NH1 | 1:B2:82:ARG:CG | 2.73 | 0.51 |
| 1:BB:6:HIS:CE1 | 1:BB:8:VAL:HB | 2.45 | 0.51 |
| 1:AA:109:PRO:HB3 | 1:AA:145:MET:HB3 | 1.91 | 0.51 |
| 1:CD:23:GLU:HA | 1:CD:26:THR:OG1 | 2.11 | 0.51 |
| 1:CQ:82:ARG:HG3 | 1:CQ:118:GLU:OE2 | 2.10 | 0.51 |
| 1:B3:35:ASP:O | 1:B3:39:ARG:HG3 | 2.10 | 0.51 |
| 1:BD:6:HIS:HE1 | 1:BD:8:VAL:HB | 1.75 | 0.51 |
| 1:CA:109:PRO:HB3 | 1:CA:145:MET:HB3 | 1.91 | 0.51 |
| 1:CN:6:HIS:HE1 | 1:CN:8:VAL:HB | 1.75 | 0.51 |
| 1:BP:109:PRO:HB3 | 1:BP:145:MET:HB3 | 1.91 | 0.51 |
| 1:B4:52:VAL:CB | 1:B4:53:PRO:HD2 | 2.34 | 0.51 |
| 1:BT:109:PRO:HB3 | 1:BT:145:MET:HB3 | 1.92 | 0.51 |
| 1:CS:97:LYS:HG3 | 1:CT:97:LYS:NZ | 2.25 | 0.51 |
| 1:CX:97:LYS:HG3 | 1:CX:97:LYS:NZ | 2.25 | 0.51 |
| 1:A2:97:LYS:HE3 | 1:A3:97:LYS:HZ1 | 1.75 | 0.51 |
| 1:BM:38:LYS:HZ2 | 1:BM:44:GLU:HA | 1.75 | 0.51 |
| 1:C3:35:ASP:O | 1:C3:39:ARG:HG3 | 2.10 | 0.51 |
| 1:BH:6:HIS:HB3 | 1:BH:147:HIS:CG | 2.45 | 0.51 |
| 1:AC:24:PHE:CD1 | 1:AU:28:LYS:HD2 | 2.46 | 0.51 |
| 1:AX:6:HIS:HE1 | 1:AX:8:VAL:HB | 1.75 | 0.51 |
| 1:BN:23:GLU:HA | 1:BN:26:THR:OG1 | 2.11 | 0.51 |
| 1:BX:23:GLU:HA | 1:BX:26:THR:OG1 | 2.11 | 0.51 |
| 1:CB:82:ARG:HG3 | 1:CB:118:GLU:OE2 | 2.10 | 0.51 |
| 1:C3:6:HIS:HE1 | 1:C3:8:VAL:HB | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BI:35:ASP:O | 1:BI:39:ARG:HG3 | 2.10 | 0.51 |
| 1:CI:23:GLU:HA | 1:CI:26:THR:OG1 | 2.11 | 0.51 |
| 1:BO:53:PRO:CG | 1:BO:57:GLU:CG | 2.46 | 0.51 |
| 1:CE:109:PRO:HB3 | 1:CE:145:MET:HB3 | 1.92 | 0.51 |
| 1:AY:109:PRO:HB3 | 1:AY:145:MET:HB3 | 1.92 | 0.51 |
| 1:AM:97:LYS:HG3 | 1:AN:97:LYS:HZ1 | 1.74 | 0.51 |
| 1:CR:6:HIS:HB3 | 1:CR:147:HIS:CG | 2.45 | 0.51 |
| 1:BB:82:ARG:HG3 | 1:BB:118:GLU:OE2 | 2.10 | 0.51 |
| 1:AD:6:HIS:HE1 | 1:AD:8:VAL:HB | 1.75 | 0.51 |
| 1:C3:23:GLU:HA | 1:C3:26:THR:OG1 | 2.11 | 0.51 |
| 1:B1:82:ARG:HG3 | 1:B1:118:GLU:OE2 | 2.10 | 0.51 |
| 1:AS:35:ASP:O | 1:AS:39:ARG:HG3 | 2.10 | 0.51 |
| 1:CX:6:HIS:HE1 | 1:CX:8:VAL:HB | 1.75 | 0.51 |
| 1:CY:53:PRO:HD2 | 1:CY:57:GLU:HB2 | 1.93 | 0.51 |
| 1:BC:129:THR:HG21 | 1:BS:120:ILE:HD13 | 1.89 | 0.51 |
| 1:C4:109:PRO:HB3 | 1:C4:145:MET:HB3 | 1.92 | 0.51 |
| 1:AQ:97:LYS:HE3 | 1:AR:97:LYS:HZ3 | 1.76 | 0.51 |
| 1:B3:97:LYS:HG3 | 1:B4:97:LYS:NZ | 2.25 | 0.51 |
| 1:AW:65:MET:HE2 | 1:AW:71:TYR:CE1 | 2.46 | 0.51 |
| 1:BG:24:PHE:CE2 | 1:BQ:124:ILE:HD11 | 2.46 | 0.51 |
| 1:CQ:6:HIS:CE1 | 1:CQ:8:VAL:HB | 2.44 | 0.51 |
| 1:BF:3:PHE:HD2 | 1:BF:150:LYS:HE2 | 1.74 | 0.51 |
| 1:AX:39:ARG:O | 1:A4:7:LEU:HB3 | 2.11 | 0.51 |
| 1:AB:82:ARG:HG3 | 1:AB:118:GLU:OE2 | 2.10 | 0.51 |
| 1:A3:6:HIS:HE1 | 1:A3:8:VAL:HB | 1.75 | 0.51 |
| 1:CE:7:LEU:HB3 | 1:CN:39:ARG:O | 2.10 | 0.51 |
| 1:CX:23:GLU:HA | 1:CX:26:THR:OG1 | 2.11 | 0.51 |
| 1:CJ:53:PRO:HD2 | 1:CJ:57:GLU:HB2 | 1.93 | 0.51 |
| 1:BY:52:VAL:HB | 1:BY:53:PRO:CD | 2.35 | 0.51 |
| 1:A4:71:TYR:C | 1:A4:150:LYS:HZ3 | 2.15 | 0.51 |
| 1:BO:109:PRO:HB3 | 1:BO:145:MET:HB3 | 1.92 | 0.51 |
| 1:B4:71:TYR:C | 1:B4:150:LYS:HZ3 | 2.15 | 0.51 |
| 1:AW:97:LYS:HG3 | 1:AX:97:LYS:NZ | 2.24 | 0.51 |
| 1:CM:97:LYS:HE3 | 1:CN:97:LYS:HZ1 | 1.76 | 0.51 |
| 1:C1:6:HIS:CE1 | 1:C1:8:VAL:HB | 2.45 | 0.51 |
| 1:AS:104:LEU:HD13 | 1:AT:102:LEU:HG | 1.91 | 0.51 |
| 1:AQ:82:ARG:HG3 | 1:AQ:118:GLU:OE2 | 2.10 | 0.51 |
| 1:CG:82:ARG:HG3 | 1:CG:118:GLU:OE2 | 2.10 | 0.51 |
| 1:AN:23:GLU:HA | 1:AN:26:THR:OG1 | 2.11 | 0.51 |
| 1:BF:109:PRO:HB3 | 1:BF:145:MET:HB3 | 1.91 | 0.51 |
| 1:B4:53:PRO:HD2 | 1:B4:57:GLU:HB2 | 1.93 | 0.51 |
| 1:A4:52:VAL:HB | 1:A4:53:PRO:CD | 2.35 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A4:53:PRO:HD2 | 1:A4:57:GLU:HB2 | 1.93 | 0.51 |
| 1:AO:53:PRO:HG2 | 1:AO:57:GLU:HG3 | 0.65 | 0.51 |
| 1:AY:53:PRO:HD2 | 1:AY:57:GLU:HB2 | 1.93 | 0.51 |
| 1:CI:97:LYS:HG3 | 1:CJ:97:LYS:NZ | 2.25 | 0.51 |
| 1:CV:97:LYS:HE3 | 1:CW:97:LYS:HZ3 | 1.74 | 0.51 |
| 1:CI:18:VAL:HG12 | 1:CI:77:LEU:CB | 2.37 | 0.51 |
| 1:BW:82:ARG:NH1 | 1:BW:82:ARG:CG | 2.73 | 0.51 |
| 1:AC:82:ARG:CG | 1:AC:82:ARG:NH1 | 2.73 | 0.51 |
| 1:C2:38:LYS:HZ2 | 1:C2:44:GLU:HA | 1.75 | 0.51 |
| 1:AE:107:ASP:C | 1:AE:107:ASP:OD1 | 2.50 | 0.51 |
| 1:BJ:152:TRP:HE3 | 1:BJ:153:ALA:N | 2.07 | 0.51 |
| 1:AB:6:HIS:CE1 | 1:AB:8:VAL:HB | 2.45 | 0.51 |
| 1:CN:35:ASP:O | 1:CN:39:ARG:HG3 | 2.10 | 0.51 |
| 1:CF:109:PRO:HB3 | 1:CF:145:MET:HB3 | 1.91 | 0.51 |
| 1:CX:35:ASP:O | 1:CX:39:ARG:HG3 | 2.10 | 0.51 |
| 1:AO:53:PRO:CG | 1:AO:57:GLU:CG | 2.46 | 0.50 |
| 1:BX:97:LYS:HG3 | 1:BY:97:LYS:NZ | 2.25 | 0.50 |
| 1:CC:52:VAL:CG1 | 1:CC:61:ILE:HD12 | 2.35 | 0.50 |
| 1:AW:52:VAL:CG1 | 1:AW:61:ILE:HD12 | 2.35 | 0.50 |
| 1:AC:39:ARG:O | 1:AR:7:LEU:HB3 | 2.11 | 0.50 |
| 1:BW:38:LYS:HZ2 | 1:BW:44:GLU:HA | 1.76 | 0.50 |
| 1:CA:58:ILE:O | 1:CA:58:ILE:HG22 | 2.11 | 0.50 |
| 1:CS:35:ASP:O | 1:CS:39:ARG:HG3 | 2.10 | 0.50 |
| 1:BD:23:GLU:HA | 1:BD:26:THR:OG1 | 2.11 | 0.50 |
| 1:AG:82:ARG:HG3 | 1:AG:118:GLU:OE2 | 2.10 | 0.50 |
| 1:C4:53:PRO:HD2 | 1:C4:57:GLU:HB2 | 1.93 | 0.50 |
| 1:CO:52:VAL:HB | 1:CO:53:PRO:CD | 2.35 | 0.50 |
| 1:AE:71:TYR:C | 1:AE:150:LYS:HZ3 | 2.15 | 0.50 |
| 1:CJ:109:PRO:HB3 | 1:CJ:145:MET:HB3 | 1.92 | 0.50 |
| 1:BE:109:PRO:HB3 | 1:BE:145:MET:HB3 | 1.92 | 0.50 |
| 1:BB:125:GLU:HG2 | 1:BV:120:ILE:CD1 | 2.41 | 0.50 |
| 1:AA:102:LEU:CD2 | 1:AE:104:LEU:HD13 | 2.42 | 0.50 |
| 1:AU:102:LEU:CD2 | 1:AY:104:LEU:HD13 | 2.42 | 0.50 |
| 1:AP:102:LEU:CD2 | 1:AT:104:LEU:HD13 | 2.42 | 0.50 |
| 1:AV:82:ARG:HG3 | 1:AV:118:GLU:OE2 | 2.10 | 0.50 |
| 1:CD:6:HIS:HE1 | 1:CD:8:VAL:HB | 1.75 | 0.50 |
| 1:BJ:53:PRO:HD2 | 1:BJ:57:GLU:HB2 | 1.93 | 0.50 |
| 1:AT:53:PRO:HD2 | 1:AT:57:GLU:HB2 | 1.93 | 0.50 |
| 1:BJ:71:TYR:C | 1:BJ:150:LYS:HZ3 | 2.15 | 0.50 |
| 1:AS:18:VAL:HG12 | 1:AS:77:LEU:CB | 2.37 | 0.50 |
| 1:C3:18:VAL:HG12 | 1:C3:77:LEU:CB | 2.37 | 0.50 |
| 1:CW:82:ARG:NH1 | 1:CW:82:ARG:CG | 2.73 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:CP:125:GLU:CA | 1:CP:129:THR:OG1 | 2.57 | 0.50 |
| 1:AY:107:ASP:OD1 | 1:AY:107:ASP:C | 2.50 | 0.50 |
| 1:CG:6:HIS:CE1 | 1:CG:8:VAL:HB | 2.44 | 0.50 |
| 1:BZ:102:LEU:CD2 | 1:B4:104:LEU:HD13 | 2.42 | 0.50 |
| 1:AZ:102:LEU:CD2 | 1:A4:104:LEU:HD13 | 2.42 | 0.50 |
| 1:AI:6:HIS:HE1 | 1:AI:8:VAL:HB | 1.75 | 0.50 |
| 1:BY:53:PRO:HD2 | 1:BY:57:GLU:HB2 | 1.93 | 0.50 |
| 1:CO:53:PRO:HD2 | 1:CO:57:GLU:HB2 | 1.93 | 0.50 |
| 1:CN:18:VAL:HG12 | 1:CN:77:LEU:CB | 2.37 | 0.50 |
| 1:BJ:107:ASP:OD1 | 1:BJ:107:ASP:C | 2.50 | 0.50 |
| 1:AJ:107:ASP:OD1 | 1:AJ:107:ASP:C | 2.50 | 0.50 |
| 1:CJ:107:ASP:OD1 | 1:CJ:107:ASP:C | 2.50 | 0.50 |
| 1:AJ:53:PRO:HD2 | 1:AJ:57:GLU:HB2 | 1.93 | 0.50 |
| 1:BB:152:TRP:C | 1:BB:152:TRP:CD1 | 2.85 | 0.50 |
| 1:B1:152:TRP:CD1 | 1:B1:152:TRP:C | 2.85 | 0.50 |
| 1:AE:109:PRO:HB3 | 1:AE:145:MET:HB3 | 1.92 | 0.50 |
| 1:AO:109:PRO:HB3 | 1:AO:145:MET:HB3 | 1.92 | 0.50 |
| 1:CO:109:PRO:HB3 | 1:CO:145:MET:HB3 | 1.92 | 0.50 |
| 1:CY:109:PRO:HB3 | 1:CY:145:MET:HB3 | 1.92 | 0.50 |
| 1:C1:97:LYS:HE3 | 1:C2:97:LYS:HZ3 | 1.75 | 0.50 |
| 1:CX:20:ARG:NH1 | 1:C2:39:ARG:CZ | 2.74 | 0.50 |
| 1:AA:58:ILE:HG22 | 1:AA:58:ILE:O | 2.11 | 0.50 |
| 1:CP:58:ILE:HG22 | 1:CP:58:ILE:O | 2.11 | 0.50 |
| 1:BE:107:ASP:OD1 | 1:BE:107:ASP:C | 2.50 | 0.50 |
| 1:CP:102:LEU:CD2 | 1:CT:104:LEU:HD13 | 2.42 | 0.50 |
| 1:BU:109:PRO:HB3 | 1:BU:145:MET:HB3 | 1.91 | 0.50 |
| 1:AT:71:TYR:C | 1:AT:150:LYS:HZ3 | 2.15 | 0.50 |
| 1:AG:96:ALA:O | 1:AG:100:ALA:HB2 | 2.06 | 0.50 |
| 1:BO:16:VAL:HG22 | 1:BO:49:VAL:HG22 | 1.94 | 0.50 |
| 1:CE:16:VAL:HG22 | 1:CE:49:VAL:HG22 | 1.94 | 0.50 |
| 1:A4:107:ASP:C | 1:A4:107:ASP:OD1 | 2.50 | 0.50 |
| 1:AO:107:ASP:OD1 | 1:AO:107:ASP:C | 2.50 | 0.50 |
| 1:CZ:102:LEU:CD2 | 1:C4:104:LEU:HD13 | 2.42 | 0.50 |
| 1:BK:18:VAL:HG21 | 1:BK:30:LEU:HD13 | 1.94 | 0.50 |
| 1:AI:23:GLU:HA | 1:AI:26:THR:OG1 | 2.11 | 0.50 |
| 1:AS:23:GLU:HA | 1:AS:26:THR:OG1 | 2.11 | 0.50 |
| 1:CS:116:THR:O | 1:CT:85:THR:HB | 2.12 | 0.50 |
| 1:BT:53:PRO:HD2 | 1:BT:57:GLU:HB2 | 1.93 | 0.50 |
| 1:BE:52:VAL:CB | 1:BE:53:PRO:HD2 | 2.34 | 0.50 |
| 1:CB:152:TRP:C | 1:CB:152:TRP:CD1 | 2.85 | 0.50 |
| 1:BY:109:PRO:HB3 | 1:BY:145:MET:HB3 | 1.92 | 0.50 |
| 1:CH:97:LYS:HG3 | 1:CI:97:LYS:HZ3 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:BF:125:GLU:CA | 1:BF:129:THR:OG1 | 2.57 | 0.50 |
| 1:AZ:125:GLU:CA | 1:AZ:129:THR:OG1 | 2.57 | 0.50 |
| 1:CC:8:VAL:HG22 | 1:CR:8:VAL:HG22 | 1.93 | 0.50 |
| 1:A1:152:TRP:CD1 | 1:A1:152:TRP:C | 2.85 | 0.50 |
| 1:CO:82:ARG:HG3 | 1:CO:118:GLU:OE2 | 2.12 | 0.50 |
| 1:AX:23:GLU:HA | 1:AX:26:THR:OG1 | 2.11 | 0.50 |
| 1:BN:6:HIS:HE1 | 1:BN:8:VAL:HB | 1.75 | 0.50 |
| 1:AE:82:ARG:HG3 | 1:AE:118:GLU:OE2 | 2.12 | 0.50 |
| 1:BI:23:GLU:HA | 1:BI:26:THR:OG1 | 2.11 | 0.50 |
| 1:BS:23:GLU:HA | 1:BS:26:THR:OG1 | 2.11 | 0.50 |
| 1:CG:152:TRP:CD1 | 1:CG:152:TRP:C | 2.85 | 0.50 |
| 1:BG:96:ALA:O | 1:BG:100:ALA:HB2 | 2.06 | 0.50 |
| 1:AH:82:ARG:CG | 1:AH:82:ARG:NH1 | 2.73 | 0.50 |
| 1:AO:16:VAL:HG22 | 1:AO:49:VAL:HG22 | 1.94 | 0.50 |
| 1:AF:125:GLU:CA | 1:AF:129:THR:OG1 | 2.57 | 0.50 |
| 1:BA:58:ILE:O | 1:BA:58:ILE:HG22 | 2.11 | 0.50 |
| 1:B4:107:ASP:C | 1:B4:107:ASP:OD1 | 2.50 | 0.50 |
| 1:AF:102:LEU:CD2 | 1:AJ:104:LEU:HD13 | 2.42 | 0.50 |
| 1:AZ:18:VAL:HG21 | 1:AZ:30:LEU:HD13 | 1.94 | 0.50 |
| 1:CA:18:VAL:HG21 | 1:CA:30:LEU:HD13 | 1.94 | 0.50 |
| 1:BU:18:VAL:HG21 | 1:BU:30:LEU:HD13 | 1.94 | 0.50 |
| 1:AI:28:LYS:NZ | 1:AK:28:LYS:NZ | 2.59 | 0.50 |
| 1:BC:28:LYS:HZ3 | 1:BU:28:LYS:CE | 2.25 | 0.50 |
| 1:BT:82:ARG:HG3 | 1:BT:118:GLU:OE2 | 2.12 | 0.50 |
| 1:CN:23:GLU:HA | 1:CN:26:THR:OG1 | 2.11 | 0.50 |
| 1:BX:116:THR:O | 1:BY:85:THR:HB | 2.12 | 0.50 |
| 1:BD:116:THR:O | 1:BE:85:THR:HB | 2.12 | 0.50 |
| 1:BT:53:PRO:CG | 1:BT:57:GLU:CG | 2.46 | 0.50 |
| 1:BE:53:PRO:HD2 | 1:BE:57:GLU:HB2 | 1.93 | 0.50 |
| 1:BV:152:TRP:CD1 | 1:BV:152:TRP:C | 2.85 | 0.50 |
| 1:CW:52:VAL:CG1 | 1:CW:61:ILE:HD12 | 2.35 | 0.50 |
| 1:CR:82:ARG:CG | 1:CR:82:ARG:NH1 | 2.73 | 0.50 |
| 1:AE:16:VAL:HG22 | 1:AE:49:VAL:HG22 | 1.94 | 0.50 |
| 1:AT:16:VAL:HG22 | 1:AT:49:VAL:HG22 | 1.94 | 0.50 |
| 1:CA:125:GLU:CA | 1:CA:129:THR:OG1 | 2.57 | 0.50 |
| 1:CY:107:ASP:C | 1:CY:107:ASP:OD1 | 2.50 | 0.50 |
| 1:AV:152:TRP:CD1 | 1:AV:152:TRP:C | 2.85 | 0.50 |
| 1:CP:18:VAL:HG21 | 1:CP:30:LEU:HD13 | 1.94 | 0.50 |
| 1:AD:6:HIS:CE1 | 1:AD:8:VAL:HB | 2.47 | 0.50 |
| 1:AX:116:THR:O | 1:AY:85:THR:HB | 2.12 | 0.50 |
| 1:CX:116:THR:O | 1:CY:85:THR:HB | 2.12 | 0.50 |
| 1:C4:82:ARG:HG3 | 1:C4:118:GLU:OE2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:AJ:82:ARG:HG3 | 1:AJ:118:GLU:OE2 | 2.12 | 0.50 |
| 1:AE:53:PRO:HD2 | 1:AE:57:GLU:HB2 | 1.93 | 0.49 |
| 1:B4:53:PRO:CG | 1:B4:57:GLU:CG | 2.46 | 0.49 |
| 1:AO:53:PRO:HD2 | 1:AO:57:GLU:HB2 | 1.93 | 0.49 |
| 1:CQ:152:TRP:CD1 | 1:CQ:152:TRP:C | 2.85 | 0.49 |
| 1:BG:152:TRP:C | 1:BG:152:TRP:CD1 | 2.85 | 0.49 |
| 1:CL:152:TRP:CD1 | 1:CL:152:TRP:C | 2.85 | 0.49 |
| 1:AJ:71:TYR:C | 1:AJ:150:LYS:HZ3 | 2.15 | 0.49 |
| 1:BY:16:VAL:HG22 | 1:BY:49:VAL:HG22 | 1.94 | 0.49 |
| 1:BJ:16:VAL:HG22 | 1:BJ:49:VAL:HG22 | 1.94 | 0.49 |
| 1:CE:107:ASP:OD1 | 1:CE:107:ASP:C | 2.50 | 0.49 |
| 1:AL:152:TRP:C | 1:AL:152:TRP:CD1 | 2.85 | 0.49 |
| 1:BA:102:LEU:CD2 | 1:BE:104:LEU:HD13 | 2.42 | 0.49 |
| 1:BU:102:LEU:CD2 | 1:BY:104:LEU:HD13 | 2.42 | 0.49 |
| 1:CZ:18:VAL:HG21 | 1:CZ:30:LEU:HD13 | 1.94 | 0.49 |
| 1:C3:6:HIS:CE1 | 1:C3:8:VAL:HB | 2.47 | 0.49 |
| 1:CJ:24:PHE:CD1 | 1:CO:28:LYS:HG3 | 2.46 | 0.49 |
| 1:CI:6:HIS:HE1 | 1:CI:8:VAL:HB | 1.75 | 0.49 |
| 1:AO:82:ARG:HG3 | 1:AO:118:GLU:OE2 | 2.12 | 0.49 |
| 1:AN:116:THR:O | 1:AO:85:THR:HB | 2.12 | 0.49 |
| 1:CT:109:PRO:HB3 | 1:CT:145:MET:HB3 | 1.92 | 0.49 |
| 1:BK:58:ILE:HG22 | 1:BK:58:ILE:O | 2.11 | 0.49 |
| 1:AA:18:VAL:HG21 | 1:AA:30:LEU:HD13 | 1.94 | 0.49 |
| 1:AF:18:VAL:HG21 | 1:AF:30:LEU:HD13 | 1.94 | 0.49 |
| 1:AI:6:HIS:CE1 | 1:AI:8:VAL:HB | 2.47 | 0.49 |
| 1:C2:17:VAL:HG21 | 1:C2:62:ALA:HA | 1.94 | 0.49 |
| 1:B3:23:GLU:HA | 1:B3:26:THR:OG1 | 2.11 | 0.49 |
| 1:CT:82:ARG:HG3 | 1:CT:118:GLU:OE2 | 2.12 | 0.49 |
| 1:BE:7:LEU:HD23 | 1:BN:40:HIS:CE1 | 2.46 | 0.49 |
| 1:C3:116:THR:O | 1:C4:85:THR:HB | 2.12 | 0.49 |
| 1:AJ:52:VAL:HB | 1:AJ:53:PRO:CD | 2.35 | 0.49 |
| 1:C1:152:TRP:C | 1:C1:152:TRP:CD1 | 2.85 | 0.49 |
| 1:B2:52:VAL:CG1 | 1:B2:61:ILE:HD12 | 2.35 | 0.49 |
| 1:B4:16:VAL:HG22 | 1:B4:49:VAL:HG22 | 1.94 | 0.49 |
| 1:BY:107:ASP:C | 1:BY:107:ASP:OD1 | 2.50 | 0.49 |
| 1:C4:107:ASP:C | 1:C4:107:ASP:OD1 | 2.50 | 0.49 |
| 1:C2:18:VAL:HG22 | 1:C2:77:LEU:HB2 | 1.94 | 0.49 |
| 1:BF:18:VAL:HG21 | 1:BF:30:LEU:HD13 | 1.94 | 0.49 |
| 1:BI:6:HIS:CE1 | 1:BI:8:VAL:HB | 2.47 | 0.49 |
| 1:CX:6:HIS:CE1 | 1:CX:8:VAL:HB | 2.47 | 0.49 |
| 1:B2:17:VAL:HG21 | 1:B2:62:ALA:HA | 1.94 | 0.49 |
| 1:BO:71:TYR:C | 1:BO:150:LYS:HZ3 | 2.15 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:BQ:97:LYS:HE3 | 1:BR:97:LYS:HZ3 | 1.77 | 0.49 |
| 1:BG:58:ILE:HG22 | 1:BG:58:ILE:O | 2.13 | 0.49 |
| 1:BJ:18:VAL:HG23 | 1:BJ:51:TRP:CE3 | 2.48 | 0.49 |
| 1:CT:16:VAL:HG22 | 1:CT:49:VAL:HG22 | 1.94 | 0.49 |
| 1:BT:107:ASP:C | 1:BT:107:ASP:OD1 | 2.50 | 0.49 |
| 1:BO:107:ASP:OD1 | 1:BO:107:ASP:C | 2.50 | 0.49 |
| 1:AP:18:VAL:HG21 | 1:AP:30:LEU:HD13 | 1.94 | 0.49 |
| 1:AM:18:VAL:HG22 | 1:AM:77:LEU:HB2 | 1.94 | 0.49 |
| 1:CH:18:VAL:HG22 | 1:CH:77:LEU:HB2 | 1.94 | 0.49 |
| 1:AK:18:VAL:HG21 | 1:AK:30:LEU:HD13 | 1.94 | 0.49 |
| 1:AN:6:HIS:CE1 | 1:AN:8:VAL:HB | 2.47 | 0.49 |
| 1:AY:82:ARG:HG3 | 1:AY:118:GLU:OE2 | 2.12 | 0.49 |
| 1:AD:116:THR:O | 1:AE:85:THR:HB | 2.12 | 0.49 |
| 1:B3:116:THR:O | 1:B4:85:THR:HB | 2.12 | 0.49 |
| 1:CW:17:VAL:HG21 | 1:CW:62:ALA:HA | 1.95 | 0.49 |
| 1:BB:96:ALA:O | 1:BB:100:ALA:HB2 | 2.06 | 0.49 |
| 1:AB:58:ILE:HG22 | 1:AB:58:ILE:O | 2.13 | 0.49 |
| 1:AY:16:VAL:HG22 | 1:AY:49:VAL:HG22 | 1.94 | 0.49 |
| 1:CY:16:VAL:HG22 | 1:CY:49:VAL:HG22 | 1.94 | 0.49 |
| 1:BT:16:VAL:HG22 | 1:BT:49:VAL:HG22 | 1.94 | 0.49 |
| 1:CE:18:VAL:HG23 | 1:CE:51:TRP:CE3 | 2.48 | 0.49 |
| 1:BE:18:VAL:HG23 | 1:BE:51:TRP:CE3 | 2.48 | 0.49 |
| 1:AQ:152:TRP:C | 1:AQ:152:TRP:CD1 | 2.85 | 0.49 |
| 1:BF:102:LEU:CD2 | 1:BJ:104:LEU:HD13 | 2.42 | 0.49 |
| 1:CB:12:LEU:HD11 | 1:CB:143:ILE:HG23 | 1.95 | 0.49 |
| 1:BI:116:THR:O | 1:BJ:85:THR:HB | 2.12 | 0.49 |
| 1:BE:82:ARG:HG3 | 1:BE:118:GLU:OE2 | 2.12 | 0.49 |
| 1:CR:17:VAL:HG21 | 1:CR:62:ALA:HA | 1.95 | 0.49 |
| 1:AY:71:TYR:C | 1:AY:150:LYS:HZ3 | 2.15 | 0.49 |
| 1:AI:106:THR:O | 1:AI:107:ASP:HB3 | 2.13 | 0.49 |
| 1:BL:96:ALA:O | 1:BL:100:ALA:HB2 | 2.06 | 0.49 |
| 1:BL:58:ILE:O | 1:BL:58:ILE:HG22 | 2.13 | 0.49 |
| 1:BO:18:VAL:HG23 | 1:BO:51:TRP:CE3 | 2.48 | 0.49 |
| 1:AE:18:VAL:HG23 | 1:AE:51:TRP:CE3 | 2.48 | 0.49 |
| 1:A4:16:VAL:HG22 | 1:A4:49:VAL:HG22 | 1.94 | 0.49 |
| 1:A4:18:VAL:HG23 | 1:A4:51:TRP:CE3 | 2.48 | 0.49 |
| 1:CK:125:GLU:CA | 1:CK:129:THR:OG1 | 2.57 | 0.49 |
| 1:AB:152:TRP:C | 1:AB:152:TRP:CD1 | 2.85 | 0.49 |
| 1:CA:102:LEU:CD2 | 1:CE:104:LEU:HD13 | 2.42 | 0.49 |
| 1:AK:102:LEU:CD2 | 1:AO:104:LEU:HD13 | 2.42 | 0.49 |
| 1:BZ:18:VAL:HG21 | 1:BZ:30:LEU:HD13 | 1.94 | 0.49 |
| 1:AH:18:VAL:HG22 | 1:AH:77:LEU:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:BX:6:HIS:CE1 | 1:BX:8:VAL:HB | 2.47 | 0.49 |
| 1:AI:116:THR:O | 1:AJ:85:THR:HB | 2.12 | 0.49 |
| 1:CV:12:LEU:HD11 | 1:CV:143:ILE:HG23 | 1.95 | 0.49 |
| 1:BQ:12:LEU:HD11 | 1:BQ:143:ILE:HG23 | 1.95 | 0.49 |
| 1:A4:82:ARG:HG3 | 1:A4:118:GLU:OE2 | 2.12 | 0.49 |
| 1:CT:53:PRO:HD2 | 1:CT:57:GLU:HB2 | 1.93 | 0.49 |
| 1:CE:53:PRO:HD2 | 1:CE:57:GLU:HB2 | 1.93 | 0.49 |
| 1:CC:129:THR:CG2 | 1:CS:120:ILE:HD11 | 2.40 | 0.49 |
| 1:BT:18:VAL:HG23 | 1:BT:51:TRP:CE3 | 2.48 | 0.49 |
| 1:CM:82:ARG:CG | 1:CM:82:ARG:NH1 | 2.73 | 0.49 |
| 1:AP:58:ILE:HG22 | 1:AP:58:ILE:O | 2.11 | 0.49 |
| 1:CF:102:LEU:CD2 | 1:CJ:104:LEU:HD13 | 2.42 | 0.49 |
| 1:BK:102:LEU:CD2 | 1:BO:104:LEU:HD13 | 2.42 | 0.49 |
| 1:CK:18:VAL:HG21 | 1:CK:30:LEU:HD13 | 1.94 | 0.49 |
| 1:CU:18:VAL:HG21 | 1:CU:30:LEU:HD13 | 1.94 | 0.49 |
| 1:A2:17:VAL:HG21 | 1:A2:62:ALA:HA | 1.95 | 0.49 |
| 1:CC:17:VAL:HG21 | 1:CC:62:ALA:HA | 1.95 | 0.49 |
| 1:A1:12:LEU:HD11 | 1:A1:143:ILE:HG23 | 1.95 | 0.49 |
| 1:A3:116:THR:O | 1:A4:85:THR:HB | 2.12 | 0.49 |
| 1:AV:12:LEU:HD11 | 1:AV:143:ILE:HG23 | 1.95 | 0.49 |
| 1:CN:106:THR:O | 1:CN:107:ASP:HB3 | 2.13 | 0.49 |
| 1:CD:106:THR:O | 1:CD:107:ASP:HB3 | 2.13 | 0.49 |
| 1:BQ:152:TRP:CD1 | 1:BQ:152:TRP:C | 2.85 | 0.49 |
| 1:AG:58:ILE:O | 1:AG:58:ILE:HG22 | 2.13 | 0.49 |
| 1:CD:28:LYS:HZ1 | 1:CF:28:LYS:HZ2 | 1.57 | 0.49 |
| 1:AY:18:VAL:HG23 | 1:AY:51:TRP:CE3 | 2.48 | 0.49 |
| 1:CJ:16:VAL:HG22 | 1:CJ:49:VAL:HG22 | 1.94 | 0.49 |
| 1:C4:16:VAL:HG22 | 1:C4:49:VAL:HG22 | 1.94 | 0.49 |
| 1:CT:107:ASP:C | 1:CT:107:ASP:OD1 | 2.50 | 0.49 |
| 1:AT:107:ASP:C | 1:AT:107:ASP:OD1 | 2.50 | 0.49 |
| 1:CK:102:LEU:CD2 | 1:CO:104:LEU:HD13 | 2.42 | 0.49 |
| 1:BP:102:LEU:CD2 | 1:BT:104:LEU:HD13 | 2.42 | 0.49 |
| 1:CM:18:VAL:HG22 | 1:CM:77:LEU:HB2 | 1.94 | 0.49 |
| 1:CW:18:VAL:HG22 | 1:CW:77:LEU:HB2 | 1.94 | 0.49 |
| 1:CD:6:HIS:CE1 | 1:CD:8:VAL:HB | 2.47 | 0.49 |
| 1:BN:6:HIS:CE1 | 1:BN:8:VAL:HB | 2.47 | 0.49 |
| 1:BT:24:PHE:CD1 | 1:BY:28:LYS:HG3 | 2.48 | 0.49 |
| 1:CE:82:ARG:HG3 | 1:CE:118:GLU:OE2 | 2.12 | 0.49 |
| 1:AL:65:MET:O | 1:AL:68:SER:HB3 | 2.13 | 0.49 |
| 1:BB:12:LEU:HD11 | 1:BB:143:ILE:HG23 | 1.95 | 0.49 |
| 1:BO:53:PRO:HG2 | 1:BO:57:GLU:HG3 | 0.65 | 0.49 |
| 1:AY:52:VAL:CB | 1:AY:53:PRO:HD2 | 2.33 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:CV:152:TRP:CD1 | 1:CV:152:TRP:C | 2.85 | 0.49 |
| 1:BE:71:TYR:C | 1:BE:150:LYS:HZ3 | 2.16 | 0.49 |
| 1:C4:71:TYR:C | 1:C4:150:LYS:HZ3 | 2.16 | 0.49 |
| 1:CY:18:VAL:HG23 | 1:CY:51:TRP:CE3 | 2.48 | 0.49 |
| 1:CO:18:VAL:HG23 | 1:CO:51:TRP:CE3 | 2.48 | 0.49 |
| 1:BP:58:ILE:HG22 | 1:BP:58:ILE:O | 2.12 | 0.49 |
| 1:CO:107:ASP:OD1 | 1:CO:107:ASP:C | 2.50 | 0.49 |
| 1:BC:18:VAL:HG22 | 1:BC:77:LEU:HB2 | 1.95 | 0.49 |
| 1:AC:18:VAL:HG22 | 1:AC:77:LEU:HB2 | 1.94 | 0.49 |
| 1:AU:18:VAL:HG21 | 1:AU:30:LEU:HD13 | 1.94 | 0.49 |
| 1:AS:6:HIS:CE1 | 1:AS:8:VAL:HB | 2.47 | 0.49 |
| 1:CS:6:HIS:CE1 | 1:CS:8:VAL:HB | 2.47 | 0.49 |
| 1:BY:82:ARG:HG3 | 1:BY:118:GLU:OE2 | 2.12 | 0.49 |
| 1:CN:98:GLY:O | 1:CN:102:LEU:HB2 | 2.13 | 0.49 |
| 1:CH:17:VAL:HG21 | 1:CH:62:ALA:HA | 1.95 | 0.49 |
| 1:CY:82:ARG:HG3 | 1:CY:118:GLU:OE2 | 2.12 | 0.49 |
| 1:B1:65:MET:O | 1:B1:68:SER:HB3 | 2.13 | 0.49 |
| 1:AL:12:LEU:HD11 | 1:AL:143:ILE:HG23 | 1.95 | 0.49 |
| 1:A4:53:PRO:CG | 1:A4:57:GLU:CG | 2.46 | 0.49 |
| 1:BT:52:VAL:CB | 1:BT:53:PRO:HD2 | 2.33 | 0.49 |
| 1:CJ:71:TYR:C | 1:CJ:150:LYS:HZ3 | 2.15 | 0.49 |
| 1:BI:106:THR:O | 1:BI:107:ASP:HB3 | 2.13 | 0.49 |
| 1:AX:106:THR:O | 1:AX:107:ASP:HB3 | 2.13 | 0.49 |
| 1:B3:106:THR:O | 1:B3:107:ASP:HB3 | 2.13 | 0.49 |
| 1:B2:38:LYS:HZ2 | 1:B2:44:GLU:HA | 1.78 | 0.49 |
| 1:AR:38:LYS:HZ2 | 1:AR:44:GLU:HA | 1.78 | 0.49 |
| 1:C4:18:VAL:HG23 | 1:C4:51:TRP:CE3 | 2.48 | 0.49 |
| 1:CT:18:VAL:HG23 | 1:CT:51:TRP:CE3 | 2.48 | 0.49 |
| 1:AW:18:VAL:HG22 | 1:AW:77:LEU:HB2 | 1.94 | 0.49 |
| 1:BS:6:HIS:CE1 | 1:BS:8:VAL:HB | 2.47 | 0.49 |
| 1:AR:17:VAL:HG21 | 1:AR:62:ALA:HA | 1.95 | 0.49 |
| 1:BR:17:VAL:HG21 | 1:BR:62:ALA:HA | 1.95 | 0.49 |
| 1:CI:116:THR:O | 1:CJ:85:THR:HB | 2.12 | 0.49 |
| 1:AS:98:GLY:O | 1:AS:102:LEU:HB2 | 2.13 | 0.49 |
| 1:AT:82:ARG:HG3 | 1:AT:118:GLU:OE2 | 2.12 | 0.49 |
| 1:BK:65:MET:HE3 | 1:BK:71:TYR:CE2 | 2.48 | 0.49 |
| 1:CD:116:THR:O | 1:CE:85:THR:HB | 2.12 | 0.49 |
| 1:BG:12:LEU:HD11 | 1:BG:143:ILE:HG23 | 1.95 | 0.49 |
| 1:AQ:65:MET:O | 1:AQ:68:SER:HB3 | 2.13 | 0.49 |
| 1:BV:12:LEU:HD11 | 1:BV:143:ILE:HG23 | 1.95 | 0.49 |
| 1:BY:71:TYR:C | 1:BY:150:LYS:HZ3 | 2.16 | 0.48 |
| 1:BL:152:TRP:C | 1:BL:152:TRP:CD1 | 2.85 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:BN:106:THR:O | 1:BN:107:ASP:HB3 | 2.13 | 0.48 |
| 1:AN:106:THR:O | 1:AN:107:ASP:HB3 | 2.13 | 0.48 |
| 1:CI:106:THR:O | 1:CI:107:ASP:HB3 | 2.13 | 0.48 |
| 1:BH:38:LYS:HZ2 | 1:BH:44:GLU:HA | 1.78 | 0.48 |
| 1:BH:82:ARG:CG | 1:BH:82:ARG:NH1 | 2.73 | 0.48 |
| 1:AT:18:VAL:HG23 | 1:AT:51:TRP:CE3 | 2.48 | 0.48 |
| 1:CT:39:ARG:O | 1:C3:7:LEU:HB3 | 2.13 | 0.48 |
| 1:CU:102:LEU:CD2 | 1:CY:104:LEU:HD13 | 2.42 | 0.48 |
| 1:BM:18:VAL:HG22 | 1:BM:77:LEU:HB2 | 1.94 | 0.48 |
| 1:B3:6:HIS:CE1 | 1:B3:8:VAL:HB | 2.47 | 0.48 |
| 1:CN:6:HIS:CE1 | 1:CN:8:VAL:HB | 2.47 | 0.48 |
| 1:CI:6:HIS:CE1 | 1:CI:8:VAL:HB | 2.47 | 0.48 |
| 1:AG:12:LEU:HD11 | 1:AG:143:ILE:HG23 | 1.95 | 0.48 |
| 1:A1:65:MET:O | 1:A1:68:SER:HB3 | 2.13 | 0.48 |
| 1:CN:116:THR:O | 1:CO:85:THR:HB | 2.12 | 0.48 |
| 1:BS:106:THR:O | 1:BS:107:ASP:HB3 | 2.13 | 0.48 |
| 1:BB:58:ILE:O | 1:BB:58:ILE:HG22 | 2.13 | 0.48 |
| 1:CB:58:ILE:HG22 | 1:CB:58:ILE:O | 2.13 | 0.48 |
| 1:AX:18:VAL:HG12 | 1:AX:77:LEU:CB | 2.37 | 0.48 |
| 1:AJ:16:VAL:HG22 | 1:AJ:49:VAL:HG22 | 1.94 | 0.48 |
| 1:CO:16:VAL:HG22 | 1:CO:49:VAL:HG22 | 1.94 | 0.48 |
| 1:AP:125:GLU:CA | 1:AP:129:THR:OG1 | 2.57 | 0.48 |
| 1:A3:6:HIS:CE1 | 1:A3:8:VAL:HB | 2.47 | 0.48 |
| 1:C1:12:LEU:HD11 | 1:C1:143:ILE:HG23 | 1.95 | 0.48 |
| 1:CQ:65:MET:O | 1:CQ:68:SER:HB3 | 2.13 | 0.48 |
| 1:AD:98:GLY:O | 1:AD:102:LEU:HB2 | 2.13 | 0.48 |
| 1:AX:98:GLY:O | 1:AX:102:LEU:HB2 | 2.13 | 0.48 |
| 1:BN:98:GLY:O | 1:BN:102:LEU:HB2 | 2.13 | 0.48 |
| 1:CE:71:TYR:C | 1:CE:150:LYS:HZ3 | 2.15 | 0.48 |
| 1:AJ:71:TYR:O | 1:AJ:150:LYS:NZ | 2.44 | 0.48 |
| 1:AD:106:THR:O | 1:AD:107:ASP:HB3 | 2.13 | 0.48 |
| 1:CS:106:THR:O | 1:CS:107:ASP:HB3 | 2.13 | 0.48 |
| 1:CW:97:LYS:HG3 | 1:CX:97:LYS:HZ1 | 1.76 | 0.48 |
| 1:BD:18:VAL:HG12 | 1:BD:77:LEU:CB | 2.37 | 0.48 |
| 1:A2:82:ARG:CG | 1:A2:82:ARG:NH1 | 2.73 | 0.48 |
| 1:AG:152:TRP:C | 1:AG:152:TRP:CD1 | 2.85 | 0.48 |
| 1:AX:6:HIS:CE1 | 1:AX:8:VAL:HB | 2.47 | 0.48 |
| 1:BN:116:THR:O | 1:BO:85:THR:HB | 2.12 | 0.48 |
| 1:AC:17:VAL:HG21 | 1:AC:62:ALA:HA | 1.95 | 0.48 |
| 1:AH:17:VAL:HG21 | 1:AH:62:ALA:HA | 1.95 | 0.48 |
| 1:CJ:82:ARG:HG3 | 1:CJ:118:GLU:OE2 | 2.12 | 0.48 |
| 1:CD:98:GLY:O | 1:CD:102:LEU:HB2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:CV:65:MET:O | 1:CV:68:SER:HB3 | 2.13 | 0.48 |
| 1:BO:53:PRO:HD2 | 1:BO:57:GLU:HB2 | 1.93 | 0.48 |
| 1:CE:52:VAL:HB | 1:CE:53:PRO:CD | 2.35 | 0.48 |
| 1:AO:71:TYR:C | 1:AO:150:LYS:HZ3 | 2.15 | 0.48 |
| 1:AS:106:THR:O | 1:AS:107:ASP:HB3 | 2.13 | 0.48 |
| 1:AB:97:LYS:HE3 | 1:AC:97:LYS:HZ3 | 1.75 | 0.48 |
| 1:BI:52:VAL:CG1 | 1:BI:61:ILE:HD12 | 2.35 | 0.48 |
| 1:BE:16:VAL:HG22 | 1:BE:49:VAL:HG22 | 1.94 | 0.48 |
| 1:BZ:58:ILE:HG22 | 1:BZ:58:ILE:O | 2.11 | 0.48 |
| 1:B2:18:VAL:HG22 | 1:B2:77:LEU:HB2 | 1.95 | 0.48 |
| 1:A2:18:VAL:HG22 | 1:A2:77:LEU:HB2 | 1.94 | 0.48 |
| 1:AD:39:ARG:O | 1:AJ:7:LEU:HB3 | 2.13 | 0.48 |
| 1:CS:66:ALA:HB2 | 1:CS:74:VAL:HG21 | 1.96 | 0.48 |
| 1:AB:12:LEU:HD11 | 1:AB:143:ILE:HG23 | 1.95 | 0.48 |
| 1:CG:65:MET:O | 1:CG:68:SER:HB3 | 2.13 | 0.48 |
| 1:C1:65:MET:O | 1:C1:68:SER:HB3 | 2.13 | 0.48 |
| 1:AN:66:ALA:HB2 | 1:AN:74:VAL:HG21 | 1.96 | 0.48 |
| 1:BD:66:ALA:HB2 | 1:BD:74:VAL:HG21 | 1.96 | 0.48 |
| 1:AX:66:ALA:HB2 | 1:AX:74:VAL:HG21 | 1.96 | 0.48 |
| 1:AG:65:MET:O | 1:AG:68:SER:HB3 | 2.13 | 0.48 |
| 1:BG:65:MET:O | 1:BG:68:SER:HB3 | 2.13 | 0.48 |
| 1:AI:98:GLY:O | 1:AI:102:LEU:HB2 | 2.13 | 0.48 |
| 1:CO:71:TYR:O | 1:CO:150:LYS:NZ | 2.44 | 0.48 |
| 1:BT:71:TYR:C | 1:BT:150:LYS:HZ3 | 2.15 | 0.48 |
| 1:CN:30:LEU:HA | 1:CN:77:LEU:HD23 | 1.96 | 0.48 |
| 1:BY:18:VAL:HG23 | 1:BY:51:TRP:CE3 | 2.48 | 0.48 |
| 1:CJ:18:VAL:HG23 | 1:CJ:51:TRP:CE3 | 2.48 | 0.48 |
| 1:B4:18:VAL:HG23 | 1:B4:51:TRP:CE3 | 2.48 | 0.48 |
| 1:CO:121:GLU:O | 1:CO:125:GLU:HB2 | 2.14 | 0.48 |
| 1:BT:121:GLU:O | 1:BT:125:GLU:HB2 | 2.14 | 0.48 |
| 1:BF:58:ILE:O | 1:BF:58:ILE:HG22 | 2.11 | 0.48 |
| 1:AS:149:SER:HB3 | 1:AS:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:CR:18:VAL:HG22 | 1:CR:77:LEU:HB2 | 1.95 | 0.48 |
| 1:BA:18:VAL:HG21 | 1:BA:30:LEU:HD13 | 1.94 | 0.48 |
| 1:BV:12:LEU:HB2 | 1:BV:42:VAL:HG13 | 1.96 | 0.48 |
| 1:BS:98:GLY:O | 1:BS:102:LEU:HB2 | 2.13 | 0.48 |
| 1:BJ:82:ARG:HG3 | 1:BJ:118:GLU:OE2 | 2.12 | 0.48 |
| 1:BC:17:VAL:HG21 | 1:BC:62:ALA:HA | 1.95 | 0.48 |
| 1:C3:66:ALA:HB2 | 1:C3:74:VAL:HG21 | 1.96 | 0.48 |
| 1:AE:52:VAL:CB | 1:AE:53:PRO:HD2 | 2.34 | 0.48 |
| 1:CC:97:LYS:HE3 | 1:CD:97:LYS:HZ3 | 1.78 | 0.48 |
| 1:AC:97:LYS:HG3 | 1:AD:97:LYS:HZ3 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B1:58:ILE:HG22 | 1:B1:58:ILE:O | 2.13 | 0.48 |
| 1:CS:52:VAL:CG1 | 1:CS:61:ILE:HD12 | 2.35 | 0.48 |
| 1:BM:52:VAL:CG1 | 1:BM:61:ILE:HD12 | 2.35 | 0.48 |
| 1:CF:58:ILE:HG22 | 1:CF:58:ILE:O | 2.11 | 0.48 |
| 1:AF:58:ILE:HG22 | 1:AF:58:ILE:O | 2.12 | 0.48 |
| 1:B4:121:GLU:O | 1:B4:125:GLU:HB2 | 2.14 | 0.48 |
| 1:BE:121:GLU:O | 1:BE:125:GLU:HB2 | 2.14 | 0.48 |
| 1:BN:149:SER:HB3 | 1:BN:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:CX:149:SER:HB3 | 1:CX:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:BR:106:THR:HG23 | 1:BR:108:ILE:H | 1.79 | 0.48 |
| 1:CF:18:VAL:HG21 | 1:CF:30:LEU:HD13 | 1.94 | 0.48 |
| 1:BF:28:LYS:CE | 1:BR:28:LYS:NZ | 2.76 | 0.48 |
| 1:BD:6:HIS:CE1 | 1:BD:8:VAL:HB | 2.47 | 0.48 |
| 1:CL:12:LEU:HD11 | 1:CL:143:ILE:HG23 | 1.95 | 0.48 |
| 1:BQ:65:MET:O | 1:BQ:68:SER:HB3 | 2.13 | 0.48 |
| 1:BO:82:ARG:HG3 | 1:BO:118:GLU:OE2 | 2.12 | 0.48 |
| 1:AS:66:ALA:HB2 | 1:AS:74:VAL:HG21 | 1.96 | 0.48 |
| 1:B3:66:ALA:HB2 | 1:B3:74:VAL:HG21 | 1.96 | 0.48 |
| 1:AQ:12:LEU:HB2 | 1:AQ:42:VAL:HG13 | 1.96 | 0.48 |
| 1:A3:149:SER:HB3 | 1:A3:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:CI:149:SER:HB3 | 1:CI:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:BI:39:ARG:O | 1:BO:7:LEU:HB3 | 2.14 | 0.48 |
| 1:CM:17:VAL:HG21 | 1:CM:62:ALA:HA | 1.95 | 0.48 |
| 1:AV:65:MET:O | 1:AV:68:SER:HB3 | 2.13 | 0.48 |
| 1:BI:98:GLY:O | 1:BI:102:LEU:HB2 | 2.13 | 0.48 |
| 1:AV:116:THR:O | 1:AW:85:THR:HB | 2.14 | 0.48 |
| 1:BL:65:MET:O | 1:BL:68:SER:HB3 | 2.13 | 0.48 |
| 1:AN:98:GLY:O | 1:AN:102:LEU:HB2 | 2.13 | 0.48 |
| 1:AL:116:THR:O | 1:AM:85:THR:HB | 2.14 | 0.48 |
| 1:CV:116:THR:O | 1:CW:85:THR:HB | 2.14 | 0.48 |
| 1:BX:66:ALA:HB2 | 1:BX:74:VAL:HG21 | 1.96 | 0.48 |
| 1:BD:106:THR:O | 1:BD:107:ASP:HB3 | 2.13 | 0.48 |
| 1:CB:97:LYS:HE3 | 1:CC:97:LYS:HZ3 | 1.79 | 0.48 |
| 1:A1:58:ILE:O | 1:A1:58:ILE:HG22 | 2.13 | 0.48 |
| 1:BO:121:GLU:O | 1:BO:125:GLU:HB2 | 2.14 | 0.48 |
| 1:A4:121:GLU:O | 1:A4:125:GLU:HB2 | 2.14 | 0.48 |
| 1:AJ:121:GLU:O | 1:AJ:125:GLU:HB2 | 2.14 | 0.48 |
| 1:BX:149:SER:HB3 | 1:BX:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:BS:149:SER:HB3 | 1:BS:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:AN:149:SER:HB3 | 1:AN:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:BR:18:VAL:HG22 | 1:BR:77:LEU:HB2 | 1.94 | 0.48 |
| 1:BH:18:VAL:HG22 | 1:BH:77:LEU:HB2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BW:18:VAL:HG22 | 1:BW:77:LEU:HB2 | 1.94 | 0.48 |
| 1:CB:12:LEU:HB2 | 1:CB:42:VAL:HG13 | 1.96 | 0.48 |
| 1:BX:98:GLY:O | 1:BX:102:LEU:HB2 | 2.13 | 0.48 |
| 1:BW:17:VAL:HG21 | 1:BW:62:ALA:HA | 1.95 | 0.48 |
| 1:AW:17:VAL:HG21 | 1:AW:62:ALA:HA | 1.95 | 0.48 |
| 1:BS:66:ALA:HB2 | 1:BS:74:VAL:HG21 | 1.96 | 0.48 |
| 1:AB:65:MET:O | 1:AB:68:SER:HB3 | 2.13 | 0.48 |
| 1:BS:116:THR:O | 1:BT:85:THR:HB | 2.12 | 0.48 |
| 1:CB:65:MET:O | 1:CB:68:SER:HB3 | 2.13 | 0.48 |
| 1:CH:24:PHE:CE1 | 1:CU:28:LYS:HD2 | 2.49 | 0.48 |
| 1:BX:106:THR:O | 1:BX:107:ASP:HB3 | 2.13 | 0.48 |
| 1:AB:144:GLU:OE2 | 1:AC:20:ARG:HD2 | 2.14 | 0.48 |
| 1:A1:144:GLU:OE2 | 1:A2:20:ARG:HD2 | 2.14 | 0.48 |
| 1:AO:18:VAL:HG23 | 1:AO:51:TRP:CE3 | 2.48 | 0.48 |
| 1:AJ:18:VAL:HG23 | 1:AJ:51:TRP:CE3 | 2.48 | 0.48 |
| 1:C4:121:GLU:O | 1:C4:125:GLU:HB2 | 2.14 | 0.48 |
| 1:B3:149:SER:HB3 | 1:B3:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:BI:149:SER:HB3 | 1:BI:152:TRP:CZ2 | 2.49 | 0.48 |
| 1:AM:106:THR:HG23 | 1:AM:108:ILE:H | 1.79 | 0.48 |
| 1:BS:137:GLU:O | 1:BS:140:VAL:HG12 | 2.14 | 0.48 |
| 1:CR:152:TRP:HE1 | 1:CS:64:LYS:C | 2.18 | 0.48 |
| 1:BP:18:VAL:HG21 | 1:BP:30:LEU:HD13 | 1.94 | 0.48 |
| 1:AR:152:TRP:HE1 | 1:AS:64:LYS:C | 2.17 | 0.48 |
| 1:CN:66:ALA:HB2 | 1:CN:74:VAL:HG21 | 1.96 | 0.48 |
| 1:B1:12:LEU:HB2 | 1:B1:42:VAL:HG13 | 1.96 | 0.48 |
| 1:AB:116:THR:O | 1:AC:85:THR:HB | 2.14 | 0.48 |
| 1:AM:17:VAL:HG21 | 1:AM:62:ALA:HA | 1.95 | 0.48 |
| 1:BM:45:ASN:HA | 1:BM:45:ASN:HD22 | 1.64 | 0.48 |
| 1:BV:65:MET:O | 1:BV:68:SER:HB3 | 2.13 | 0.48 |
| 1:BB:116:THR:O | 1:BC:85:THR:HB | 2.14 | 0.48 |
| 1:C4:52:VAL:HB | 1:C4:53:PRO:CD | 2.35 | 0.48 |
| 1:CO:52:VAL:CB | 1:CO:53:PRO:HD2 | 2.34 | 0.48 |
| 1:C3:106:THR:O | 1:C3:107:ASP:HB3 | 2.13 | 0.48 |
| 1:BM:97:LYS:HE3 | 1:BN:97:LYS:HZ3 | 1.78 | 0.48 |
| 1:AL:58:ILE:HG22 | 1:AL:58:ILE:O | 2.13 | 0.48 |
| 1:CC:39:ARG:O | 1:CR:7:LEU:HB3 | 2.14 | 0.48 |
| 1:CR:106:THR:HG23 | 1:CR:108:ILE:H | 1.79 | 0.48 |
| 1:B2:106:THR:HG23 | 1:B2:108:ILE:H | 1.79 | 0.48 |
| 1:BH:106:THR:HG23 | 1:BH:108:ILE:H | 1.79 | 0.48 |
| 1:A3:137:GLU:O | 1:A3:140:VAL:HG12 | 2.14 | 0.48 |
| 1:AX:137:GLU:O | 1:AX:140:VAL:HG12 | 2.14 | 0.48 |
| 1:CW:152:TRP:HE1 | 1:CX:64:LYS:C | 2.18 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BC:152:TRP:HE1 | 1:BD:64:LYS:C | 2.18 | 0.48 |
| 1:AR:18:VAL:HG22 | 1:AR:77:LEU:HB2 | 1.94 | 0.48 |
| 1:BG:12:LEU:HB2 | 1:BG:42:VAL:HG13 | 1.96 | 0.48 |
| 1:AQ:12:LEU:HD11 | 1:AQ:143:ILE:HG23 | 1.95 | 0.48 |
| 1:BG:116:THR:O | 1:BH:85:THR:HB | 2.14 | 0.48 |
| 1:B4:82:ARG:HG3 | 1:B4:118:GLU:OE2 | 2.12 | 0.48 |
| 1:BL:116:THR:O | 1:BM:85:THR:HB | 2.14 | 0.48 |
| 1:CP:65:MET:HE3 | 1:CP:71:TYR:CE2 | 2.48 | 0.48 |
| 1:CV:13:LYS:HD2 | 1:CV:46:ASP:OD2 | 2.14 | 0.48 |
| 1:BL:13:LYS:HD2 | 1:BL:46:ASP:OD2 | 2.14 | 0.48 |
| 1:BM:17:VAL:HG21 | 1:BM:62:ALA:HA | 1.95 | 0.48 |
| 1:CG:12:LEU:HD11 | 1:CG:143:ILE:HG23 | 1.95 | 0.48 |
| 1:A3:66:ALA:HB2 | 1:A3:74:VAL:HG21 | 1.96 | 0.48 |
| 1:B3:98:GLY:O | 1:B3:102:LEU:HB2 | 2.13 | 0.48 |
| 1:CQ:90:TYR:O | 1:CQ:94:GLU:HG2 | 2.14 | 0.48 |
| 1:CO:71:TYR:C | 1:CO:150:LYS:HZ3 | 2.15 | 0.47 |
| 1:CL:58:ILE:O | 1:CL:58:ILE:HG22 | 2.13 | 0.47 |
| 1:BV:144:GLU:OE2 | 1:BW:20:ARG:HD2 | 2.14 | 0.47 |
| 1:BX:30:LEU:HA | 1:BX:77:LEU:HD23 | 1.96 | 0.47 |
| 1:AN:30:LEU:HA | 1:AN:77:LEU:HD23 | 1.96 | 0.47 |
| 1:CA:121:GLU:O | 1:CA:125:GLU:HG3 | 2.14 | 0.47 |
| 1:BW:106:THR:HG23 | 1:BW:108:ILE:H | 1.79 | 0.47 |
| 1:AH:106:THR:HG23 | 1:AH:108:ILE:H | 1.79 | 0.47 |
| 1:AI:137:GLU:O | 1:AI:140:VAL:HG12 | 2.14 | 0.47 |
| 1:CD:137:GLU:O | 1:CD:140:VAL:HG12 | 2.14 | 0.47 |
| 1:AW:152:TRP:HE1 | 1:AX:64:LYS:C | 2.18 | 0.47 |
| 1:BX:137:GLU:O | 1:BX:140:VAL:HG12 | 2.14 | 0.47 |
| 1:CC:152:TRP:HE1 | 1:CD:64:LYS:C | 2.18 | 0.47 |
| 1:AG:12:LEU:HB2 | 1:AG:42:VAL:HG13 | 1.96 | 0.47 |
| 1:B1:12:LEU:HD11 | 1:B1:143:ILE:HG23 | 1.95 | 0.47 |
| 1:BD:98:GLY:O | 1:BD:102:LEU:HB2 | 2.13 | 0.47 |
| 1:AS:116:THR:O | 1:AT:85:THR:HB | 2.12 | 0.47 |
| 1:BI:66:ALA:HB2 | 1:BI:74:VAL:HG21 | 1.96 | 0.47 |
| 1:BB:65:MET:O | 1:BB:68:SER:HB3 | 2.13 | 0.47 |
| 1:AD:82:ARG:HG3 | 1:AD:118:GLU:OE2 | 2.14 | 0.47 |
| 1:AB:13:LYS:HD2 | 1:AB:46:ASP:OD2 | 2.14 | 0.47 |
| 1:AD:66:ALA:HB2 | 1:AD:74:VAL:HG21 | 1.96 | 0.47 |
| 1:BB:152:TRP:O | 1:BB:152:TRP:CD1 | 2.67 | 0.47 |
| 1:A3:106:THR:O | 1:A3:107:ASP:HB3 | 2.13 | 0.47 |
| 1:CX:106:THR:O | 1:CX:107:ASP:HB3 | 2.13 | 0.47 |
| 1:AG:97:LYS:HE3 | 1:AH:97:LYS:HZ3 | 1.79 | 0.47 |
| 1:AX:52:VAL:CG1 | 1:AX:61:ILE:HD12 | 2.35 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BG:144:GLU:OE2 | 1:BH:20:ARG:HD2 | 2.14 | 0.47 |
| 1:CS:30:LEU:HA | 1:CS:77:LEU:HD23 | 1.96 | 0.47 |
| 1:AI:30:LEU:HA | 1:AI:77:LEU:HD23 | 1.96 | 0.47 |
| 1:BP:121:GLU:O | 1:BP:125:GLU:HG3 | 2.14 | 0.47 |
| 1:CH:82:ARG:CG | 1:CH:82:ARG:NH1 | 2.73 | 0.47 |
| 1:AY:121:GLU:O | 1:AY:125:GLU:HB2 | 2.14 | 0.47 |
| 1:C2:106:THR:HG23 | 1:C2:108:ILE:H | 1.79 | 0.47 |
| 1:CM:152:TRP:HE1 | 1:CN:64:LYS:C | 2.17 | 0.47 |
| 1:BM:152:TRP:HE1 | 1:BN:64:LYS:C | 2.17 | 0.47 |
| 1:CC:18:VAL:HG22 | 1:CC:77:LEU:HB2 | 1.94 | 0.47 |
| 1:AE:7:LEU:HB3 | 1:AN:39:ARG:O | 2.13 | 0.47 |
| 1:AV:12:LEU:HB2 | 1:AV:42:VAL:HG13 | 1.96 | 0.47 |
| 1:CL:13:LYS:HD2 | 1:CL:46:ASP:OD2 | 2.14 | 0.47 |
| 1:BB:13:LYS:HD2 | 1:BB:46:ASP:OD2 | 2.15 | 0.47 |
| 1:CB:13:LYS:HD2 | 1:CB:46:ASP:OD2 | 2.14 | 0.47 |
| 1:BV:116:THR:O | 1:BW:85:THR:HB | 2.14 | 0.47 |
| 1:C3:98:GLY:O | 1:C3:102:LEU:HB2 | 2.13 | 0.47 |
| 1:CQ:12:LEU:HB2 | 1:CQ:42:VAL:HG13 | 1.96 | 0.47 |
| 1:BG:13:LYS:HD2 | 1:BG:46:ASP:OD2 | 2.14 | 0.47 |
| 1:BL:152:TRP:O | 1:BL:152:TRP:CD1 | 2.67 | 0.47 |
| 1:CG:152:TRP:CD1 | 1:CG:152:TRP:O | 2.67 | 0.47 |
| 1:CB:55:ALA:HB1 | 1:CB:95:VAL:CG2 | 2.40 | 0.47 |
| 1:AI:52:VAL:CG1 | 1:AI:61:ILE:HD12 | 2.35 | 0.47 |
| 1:CV:144:GLU:OE2 | 1:CW:20:ARG:HD2 | 2.14 | 0.47 |
| 1:AS:30:LEU:HA | 1:AS:77:LEU:HD23 | 1.96 | 0.47 |
| 1:AN:18:VAL:HG12 | 1:AN:77:LEU:CB | 2.37 | 0.47 |
| 1:C3:30:LEU:HA | 1:C3:77:LEU:HD23 | 1.96 | 0.47 |
| 1:AH:70:LYS:HB2 | 1:AH:71:TYR:CD1 | 2.50 | 0.47 |
| 1:BK:121:GLU:O | 1:BK:125:GLU:HG3 | 2.14 | 0.47 |
| 1:BZ:125:GLU:CA | 1:BZ:129:THR:OG1 | 2.57 | 0.47 |
| 1:CY:121:GLU:O | 1:CY:125:GLU:HB2 | 2.14 | 0.47 |
| 1:AE:121:GLU:O | 1:AE:125:GLU:HB2 | 2.14 | 0.47 |
| 1:AX:149:SER:HB3 | 1:AX:152:TRP:CZ2 | 2.49 | 0.47 |
| 1:BM:106:THR:HG23 | 1:BM:108:ILE:H | 1.79 | 0.47 |
| 1:AL:152:TRP:O | 1:AL:152:TRP:CD1 | 2.68 | 0.47 |
| 1:CO:83:GLY:HA3 | 2:CO:4201:PO4:O2 | 2.15 | 0.47 |
| 1:AJ:83:GLY:HA3 | 2:AJ:1001:PO4:O2 | 2.14 | 0.47 |
| 1:C2:152:TRP:HE1 | 1:C3:64:LYS:C | 2.18 | 0.47 |
| 1:B2:152:TRP:HE1 | 1:B3:64:LYS:C | 2.17 | 0.47 |
| 1:AL:12:LEU:HB2 | 1:AL:42:VAL:HG13 | 1.96 | 0.47 |
| 1:CQ:12:LEU:HD11 | 1:CQ:143:ILE:HG23 | 1.95 | 0.47 |
| 1:BH:17:VAL:HG21 | 1:BH:62:ALA:HA | 1.94 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CS:98:GLY:O | 1:CS:102:LEU:HB2 | 2.13 | 0.47 |
| 1:AG:13:LYS:HD2 | 1:AG:46:ASP:OD2 | 2.15 | 0.47 |
| 1:CQ:13:LYS:HD2 | 1:CQ:46:ASP:OD2 | 2.15 | 0.47 |
| 1:AI:128:GLY:O | 1:AK:22:ASN:HA | 2.14 | 0.47 |
| 1:CX:120:ILE:HG12 | 1:C2:129:THR:HG21 | 1.97 | 0.47 |
| 1:C1:152:TRP:CD1 | 1:C1:152:TRP:O | 2.67 | 0.47 |
| 1:CB:152:TRP:O | 1:CB:152:TRP:CD1 | 2.68 | 0.47 |
| 1:BG:152:TRP:O | 1:BG:152:TRP:CD1 | 2.68 | 0.47 |
| 1:AQ:58:ILE:HG22 | 1:AQ:58:ILE:O | 2.13 | 0.47 |
| 1:BW:97:LYS:HE3 | 1:BX:97:LYS:HZ1 | 1.79 | 0.47 |
| 1:AQ:144:GLU:OE2 | 1:AR:20:ARG:HD2 | 2.14 | 0.47 |
| 1:CW:70:LYS:HB2 | 1:CW:71:TYR:CD1 | 2.50 | 0.47 |
| 1:AT:121:GLU:O | 1:AT:125:GLU:HB2 | 2.14 | 0.47 |
| 1:AD:149:SER:HB3 | 1:AD:152:TRP:CZ2 | 2.49 | 0.47 |
| 1:CC:106:THR:HG23 | 1:CC:108:ILE:H | 1.79 | 0.47 |
| 1:AW:106:THR:HG23 | 1:AW:108:ILE:H | 1.79 | 0.47 |
| 1:AB:152:TRP:O | 1:AB:152:TRP:CD1 | 2.68 | 0.47 |
| 1:AQ:152:TRP:O | 1:AQ:152:TRP:CD1 | 2.68 | 0.47 |
| 1:AO:83:GLY:HA3 | 2:AO:1001:PO4:O2 | 2.15 | 0.47 |
| 1:CJ:83:GLY:HA3 | 2:CJ:4201:PO4:O2 | 2.15 | 0.47 |
| 1:A4:83:GLY:HA3 | 2:A4:1001:PO4:O2 | 2.15 | 0.47 |
| 1:BR:152:TRP:HE1 | 1:BS:64:LYS:C | 2.18 | 0.47 |
| 1:CV:12:LEU:HB2 | 1:CV:42:VAL:HG13 | 1.96 | 0.47 |
| 1:C1:12:LEU:HB2 | 1:C1:42:VAL:HG13 | 1.96 | 0.47 |
| 1:BL:12:LEU:HD11 | 1:BL:143:ILE:HG23 | 1.95 | 0.47 |
| 1:AL:13:LYS:HD2 | 1:AL:46:ASP:OD2 | 2.14 | 0.47 |
| 1:CI:98:GLY:O | 1:CI:102:LEU:HB2 | 2.13 | 0.47 |
| 1:AQ:90:TYR:O | 1:AQ:94:GLU:HG2 | 2.14 | 0.47 |
| 1:AK:65:MET:HE3 | 1:AK:71:TYR:CE2 | 2.50 | 0.47 |
| 1:BI:82:ARG:HG3 | 1:BI:118:GLU:OE2 | 2.14 | 0.47 |
| 1:BA:65:MET:HE3 | 1:BA:71:TYR:CE2 | 2.49 | 0.47 |
| 1:A3:98:GLY:O | 1:A3:102:LEU:HB2 | 2.13 | 0.47 |
| 1:A3:82:ARG:HG3 | 1:A3:118:GLU:OE2 | 2.15 | 0.47 |
| 1:BL:90:TYR:O | 1:BL:94:GLU:HG2 | 2.14 | 0.47 |
| 1:CL:90:TYR:O | 1:CL:94:GLU:HG2 | 2.14 | 0.47 |
| 1:C1:106:THR:O | 1:C1:107:ASP:HB3 | 2.15 | 0.47 |
| 1:CV:152:TRP:CD1 | 1:CV:152:TRP:O | 2.68 | 0.47 |
| 1:CV:58:ILE:O | 1:CV:58:ILE:HG22 | 2.13 | 0.47 |
| 1:CL:144:GLU:OE2 | 1:CM:20:ARG:HD2 | 2.14 | 0.47 |
| 1:CQ:144:GLU:OE2 | 1:CR:20:ARG:HD2 | 2.14 | 0.47 |
| 1:CF:121:GLU:O | 1:CF:125:GLU:HG3 | 2.14 | 0.47 |
| 1:CF:125:GLU:CA | 1:CF:129:THR:OG1 | 2.57 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B2:70:LYS:HB2 | 1:B2:71:TYR:CD1 | 2.50 | 0.47 |
| 1:AU:121:GLU:O | 1:AU:125:GLU:HG3 | 2.14 | 0.47 |
| 1:BM:70:LYS:HB2 | 1:BM:71:TYR:CD1 | 2.50 | 0.47 |
| 1:BC:70:LYS:HB2 | 1:BC:71:TYR:CD1 | 2.50 | 0.47 |
| 1:CU:121:GLU:O | 1:CU:125:GLU:HG3 | 2.14 | 0.47 |
| 1:AM:70:LYS:HB2 | 1:AM:71:TYR:CD1 | 2.50 | 0.47 |
| 1:BR:70:LYS:HB2 | 1:BR:71:TYR:CD1 | 2.50 | 0.47 |
| 1:CW:106:THR:HG23 | 1:CW:108:ILE:H | 1.79 | 0.47 |
| 1:AG:152:TRP:O | 1:AG:152:TRP:CD1 | 2.68 | 0.47 |
| 1:AE:83:GLY:HA3 | 2:AE:1001:PO4:O2 | 2.15 | 0.47 |
| 1:CI:137:GLU:O | 1:CI:140:VAL:HG12 | 2.14 | 0.47 |
| 1:BR:30:LEU:HA | 1:BR:77:LEU:HD23 | 1.97 | 0.47 |
| 1:CG:130:LYS:HG3 | 1:CV:120:ILE:HD11 | 1.95 | 0.47 |
| 1:CB:37:LEU:O | 1:CB:42:VAL:HG23 | 2.15 | 0.47 |
| 1:AL:37:LEU:O | 1:AL:42:VAL:HG23 | 2.15 | 0.47 |
| 1:CV:90:TYR:O | 1:CV:94:GLU:HG2 | 2.14 | 0.47 |
| 1:CN:82:ARG:HG3 | 1:CN:118:GLU:OE2 | 2.14 | 0.47 |
| 1:BG:90:TYR:O | 1:BG:94:GLU:HG2 | 2.14 | 0.47 |
| 1:C1:13:LYS:HD2 | 1:C1:46:ASP:OD2 | 2.14 | 0.47 |
| 1:BS:82:ARG:HG3 | 1:BS:118:GLU:OE2 | 2.14 | 0.47 |
| 1:CL:65:MET:O | 1:CL:68:SER:HB3 | 2.13 | 0.47 |
| 1:B3:82:ARG:HG3 | 1:B3:118:GLU:OE2 | 2.14 | 0.47 |
| 1:BP:65:MET:HE3 | 1:BP:71:TYR:CE2 | 2.49 | 0.47 |
| 1:CL:116:THR:O | 1:CM:85:THR:HB | 2.14 | 0.47 |
| 1:AQ:13:LYS:HD2 | 1:AQ:46:ASP:OD2 | 2.14 | 0.47 |
| 1:BL:106:THR:O | 1:BL:107:ASP:HB3 | 2.15 | 0.47 |
| 1:BQ:58:ILE:O | 1:BQ:58:ILE:HG22 | 2.13 | 0.47 |
| 1:CG:58:ILE:HG22 | 1:CG:58:ILE:O | 2.13 | 0.47 |
| 1:CX:52:VAL:CG1 | 1:CX:61:ILE:HD12 | 2.35 | 0.47 |
| 1:B3:30:LEU:HA | 1:B3:77:LEU:HD23 | 1.96 | 0.47 |
| 1:AD:30:LEU:HA | 1:AD:77:LEU:HD23 | 1.96 | 0.47 |
| 1:BD:30:LEU:HA | 1:BD:77:LEU:HD23 | 1.96 | 0.47 |
| 1:CI:30:LEU:HA | 1:CI:77:LEU:HD23 | 1.96 | 0.47 |
| 1:AH:63:LYS:C | 1:AH:65:MET:H | 2.18 | 0.47 |
| 1:CR:70:LYS:HB2 | 1:CR:71:TYR:CD1 | 2.50 | 0.47 |
| 1:BW:70:LYS:HB2 | 1:BW:71:TYR:CD1 | 2.50 | 0.47 |
| 1:AK:58:ILE:O | 1:AK:58:ILE:HG22 | 2.11 | 0.47 |
| 1:BY:121:GLU:O | 1:BY:125:GLU:HB2 | 2.14 | 0.47 |
| 1:CD:149:SER:HB3 | 1:CD:152:TRP:CZ2 | 2.49 | 0.47 |
| 1:BW:63:LYS:C | 1:BW:65:MET:H | 2.18 | 0.47 |
| 1:CV:129:THR:CG2 | 1:CV:130:LYS:H | 2.28 | 0.47 |
| 1:B3:137:GLU:O | 1:B3:140:VAL:HG12 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BT:83:GLY:HA3 | 2:BT:1001:PO4:O2 | 2.15 | 0.47 |
| 1:CM:75:ILE:HG22 | 1:CM:77:LEU:HD13 | 1.97 | 0.47 |
| 1:AW:30:LEU:HA | 1:AW:77:LEU:HD23 | 1.97 | 0.47 |
| 1:AM:152:TRP:HE1 | 1:AN:64:LYS:C | 2.18 | 0.47 |
| 1:BW:152:TRP:HE1 | 1:BX:64:LYS:C | 2.18 | 0.47 |
| 1:B1:129:THR:CG2 | 1:B1:130:LYS:H | 2.28 | 0.47 |
| 1:CL:12:LEU:HB2 | 1:CL:42:VAL:HG13 | 1.96 | 0.47 |
| 1:AQ:37:LEU:O | 1:AQ:42:VAL:HG23 | 2.15 | 0.47 |
| 1:AI:66:ALA:HB2 | 1:AI:74:VAL:HG21 | 1.96 | 0.47 |
| 1:A1:116:THR:O | 1:A2:85:THR:HB | 2.14 | 0.47 |
| 1:AL:90:TYR:O | 1:AL:94:GLU:HG2 | 2.14 | 0.47 |
| 1:BB:90:TYR:O | 1:BB:94:GLU:HG2 | 2.14 | 0.47 |
| 1:AV:90:TYR:O | 1:AV:94:GLU:HG2 | 2.14 | 0.47 |
| 1:B1:116:THR:O | 1:B2:85:THR:HB | 2.14 | 0.47 |
| 1:AP:65:MET:HE3 | 1:AP:71:TYR:CE2 | 2.50 | 0.47 |
| 1:AG:116:THR:O | 1:AH:85:THR:HB | 2.14 | 0.47 |
| 1:CB:106:THR:O | 1:CB:107:ASP:HB3 | 2.15 | 0.47 |
| 1:CL:106:THR:O | 1:CL:107:ASP:HB3 | 2.15 | 0.47 |
| 1:CY:71:TYR:C | 1:CY:150:LYS:HZ3 | 2.18 | 0.47 |
| 1:BB:144:GLU:OE2 | 1:BC:20:ARG:HD2 | 2.14 | 0.47 |
| 1:BQ:144:GLU:OE2 | 1:BR:20:ARG:HD2 | 2.14 | 0.47 |
| 1:AW:82:ARG:CG | 1:AW:82:ARG:NH1 | 2.73 | 0.47 |
| 1:CR:38:LYS:HZ2 | 1:CR:44:GLU:HA | 1.80 | 0.47 |
| 1:AR:70:LYS:HB2 | 1:AR:71:TYR:CD1 | 2.50 | 0.47 |
| 1:AW:70:LYS:HB2 | 1:AW:71:TYR:CD1 | 2.50 | 0.47 |
| 1:CC:70:LYS:HB2 | 1:CC:71:TYR:CD1 | 2.50 | 0.47 |
| 1:BU:121:GLU:O | 1:BU:125:GLU:HG3 | 2.14 | 0.47 |
| 1:AZ:58:ILE:O | 1:AZ:58:ILE:HG22 | 2.12 | 0.47 |
| 1:BR:63:LYS:C | 1:BR:65:MET:H | 2.18 | 0.47 |
| 1:CH:63:LYS:C | 1:CH:65:MET:H | 2.18 | 0.47 |
| 1:C2:70:LYS:HB2 | 1:C2:71:TYR:CD1 | 2.50 | 0.47 |
| 1:BJ:121:GLU:O | 1:BJ:125:GLU:HB2 | 2.14 | 0.47 |
| 1:AZ:121:GLU:O | 1:AZ:125:GLU:HG3 | 2.14 | 0.47 |
| 1:CE:121:GLU:O | 1:CE:125:GLU:HB2 | 2.14 | 0.47 |
| 1:CJ:121:GLU:O | 1:CJ:125:GLU:HB2 | 2.14 | 0.47 |
| 1:BD:149:SER:HB3 | 1:BD:152:TRP:CZ2 | 2.49 | 0.47 |
| 1:A2:106:THR:HG23 | 1:A2:108:ILE:H | 1.79 | 0.47 |
| 1:CH:106:THR:HG23 | 1:CH:108:ILE:H | 1.79 | 0.47 |
| 1:CT:7:LEU:CB | 1:C3:39:ARG:O | 2.63 | 0.47 |
| 1:CR:63:LYS:C | 1:CR:65:MET:H | 2.18 | 0.47 |
| 1:AN:137:GLU:O | 1:AN:140:VAL:HG12 | 2.14 | 0.47 |
| 1:BE:83:GLY:HA3 | 2:BE:1001:PO4:O2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BN:137:GLU:O | 1:BN:140:VAL:HG12 | 2.14 | 0.47 |
| 1:CY:83:GLY:HA3 | 2:CY:4201:PO4:O2 | 2.15 | 0.47 |
| 1:BI:137:GLU:O | 1:BI:140:VAL:HG12 | 2.14 | 0.47 |
| 1:AC:152:TRP:HE1 | 1:AD:64:LYS:C | 2.17 | 0.47 |
| 1:AT:83:GLY:HA3 | 2:AT:1001:PO4:O2 | 2.15 | 0.47 |
| 1:B4:83:GLY:HA3 | 2:B4:1001:PO4:O2 | 2.15 | 0.47 |
| 1:BC:30:LEU:HA | 1:BC:77:LEU:HD23 | 1.97 | 0.47 |
| 1:BH:30:LEU:HA | 1:BH:77:LEU:HD23 | 1.97 | 0.47 |
| 1:AR:75:ILE:HG22 | 1:AR:77:LEU:HD13 | 1.97 | 0.47 |
| 1:CR:75:ILE:HG22 | 1:CR:77:LEU:HD13 | 1.97 | 0.47 |
| 1:CC:30:LEU:HA | 1:CC:77:LEU:HD23 | 1.97 | 0.47 |
| 1:AV:37:LEU:O | 1:AV:42:VAL:HG23 | 2.15 | 0.47 |
| 1:BV:37:LEU:O | 1:BV:42:VAL:HG23 | 2.15 | 0.47 |
| 1:C1:37:LEU:O | 1:C1:42:VAL:HG23 | 2.15 | 0.47 |
| 1:BL:12:LEU:HB2 | 1:BL:42:VAL:HG13 | 1.96 | 0.47 |
| 1:BX:82:ARG:HG3 | 1:BX:118:GLU:OE2 | 2.15 | 0.47 |
| 1:BV:13:LYS:HD2 | 1:BV:46:ASP:OD2 | 2.14 | 0.47 |
| 1:CX:82:ARG:HG3 | 1:CX:118:GLU:OE2 | 2.14 | 0.47 |
| 1:CB:116:THR:O | 1:CC:85:THR:HB | 2.14 | 0.47 |
| 1:CX:98:GLY:O | 1:CX:102:LEU:HB2 | 2.13 | 0.47 |
| 1:C1:116:THR:O | 1:C2:85:THR:HB | 2.14 | 0.47 |
| 1:CI:66:ALA:HB2 | 1:CI:74:VAL:HG21 | 1.96 | 0.47 |
| 1:CG:116:THR:O | 1:CH:85:THR:HB | 2.14 | 0.47 |
| 1:AB:90:TYR:O | 1:AB:94:GLU:HG2 | 2.14 | 0.47 |
| 1:BN:66:ALA:HB2 | 1:BN:74:VAL:HG21 | 1.96 | 0.47 |
| 1:CG:106:THR:O | 1:CG:107:ASP:HB3 | 2.15 | 0.47 |
| 1:BQ:106:THR:O | 1:BQ:107:ASP:HB3 | 2.15 | 0.47 |
| 1:AV:58:ILE:O | 1:AV:58:ILE:HG22 | 2.13 | 0.47 |
| 1:AG:144:GLU:OE2 | 1:AH:20:ARG:HD2 | 2.14 | 0.47 |
| 1:CB:144:GLU:OE2 | 1:CC:20:ARG:HD2 | 2.14 | 0.47 |
| 1:BL:144:GLU:OE2 | 1:BM:20:ARG:HD2 | 2.14 | 0.47 |
| 1:BN:30:LEU:HA | 1:BN:77:LEU:HD23 | 1.96 | 0.47 |
| 1:CH:38:LYS:HZ2 | 1:CH:44:GLU:HA | 1.79 | 0.47 |
| 1:CP:121:GLU:O | 1:CP:125:GLU:HG3 | 2.14 | 0.47 |
| 1:AR:106:THR:HG23 | 1:AR:108:ILE:H | 1.79 | 0.47 |
| 1:AC:106:THR:HG23 | 1:AC:108:ILE:H | 1.79 | 0.47 |
| 1:AV:152:TRP:CD1 | 1:AV:152:TRP:O | 2.67 | 0.47 |
| 1:A1:152:TRP:CD1 | 1:A1:152:TRP:O | 2.67 | 0.47 |
| 1:AY:83:GLY:HA3 | 2:AY:1001:PO4:O2 | 2.15 | 0.47 |
| 1:BO:83:GLY:HA3 | 2:BO:1001:PO4:O2 | 2.15 | 0.47 |
| 1:CT:83:GLY:HA3 | 2:CT:4201:PO4:O2 | 2.15 | 0.47 |
| 1:BR:75:ILE:HG22 | 1:BR:77:LEU:HD13 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AC:75:ILE:HG22 | 1:AC:77:LEU:HD13 | 1.97 | 0.47 |
| 1:CI:40:HIS:CE1 | 1:CO:7:LEU:HD23 | 2.50 | 0.47 |
| 1:BD:117:THR:HG22 | 1:BE:85:THR:HG21 | 1.97 | 0.47 |
| 1:C3:117:THR:HG22 | 1:C4:85:THR:HG21 | 1.97 | 0.47 |
| 1:BB:12:LEU:HB2 | 1:BB:42:VAL:HG13 | 1.96 | 0.47 |
| 1:BB:37:LEU:O | 1:BB:42:VAL:HG23 | 2.15 | 0.47 |
| 1:CG:37:LEU:O | 1:CG:42:VAL:HG23 | 2.15 | 0.47 |
| 1:AG:90:TYR:O | 1:AG:94:GLU:HG2 | 2.14 | 0.47 |
| 1:AH:45:ASN:HA | 1:AH:45:ASN:HD22 | 1.64 | 0.47 |
| 1:AR:148:LEU:HD23 | 1:AR:148:LEU:HA | 1.79 | 0.47 |
| 1:AN:82:ARG:HG3 | 1:AN:118:GLU:OE2 | 2.14 | 0.47 |
| 1:CK:65:MET:HE3 | 1:CK:71:TYR:CE2 | 2.49 | 0.47 |
| 1:CD:82:ARG:HG3 | 1:CD:118:GLU:OE2 | 2.14 | 0.47 |
| 1:B1:152:TRP:CD1 | 1:B1:152:TRP:O | 2.68 | 0.47 |
| 1:CQ:152:TRP:O | 1:CQ:152:TRP:CD1 | 2.68 | 0.47 |
| 1:AE:71:TYR:O | 1:AE:150:LYS:NZ | 2.44 | 0.47 |
| 1:CJ:71:TYR:O | 1:CJ:150:LYS:NZ | 2.44 | 0.47 |
| 1:CL:152:TRP:CD1 | 1:CL:152:TRP:O | 2.67 | 0.47 |
| 1:AL:100:ALA:CA | 1:AM:56:PHE:HZ | 2.28 | 0.47 |
| 1:C1:58:ILE:HG22 | 1:C1:58:ILE:O | 2.13 | 0.47 |
| 1:AX:30:LEU:HA | 1:AX:77:LEU:HD23 | 1.96 | 0.47 |
| 1:A3:30:LEU:HA | 1:A3:77:LEU:HD23 | 1.96 | 0.47 |
| 1:BM:82:ARG:NH1 | 1:BM:82:ARG:CG | 2.73 | 0.47 |
| 1:AR:63:LYS:C | 1:AR:65:MET:H | 2.18 | 0.47 |
| 1:BM:63:LYS:C | 1:BM:65:MET:H | 2.18 | 0.47 |
| 1:AA:121:GLU:O | 1:AA:125:GLU:HG3 | 2.14 | 0.47 |
| 1:BF:121:GLU:O | 1:BF:125:GLU:HG3 | 2.14 | 0.47 |
| 1:CP:58:ILE:H | 1:CP:59:PRO:HD2 | 1.80 | 0.47 |
| 1:AI:149:SER:HB3 | 1:AI:152:TRP:CZ2 | 2.49 | 0.47 |
| 1:CX:137:GLU:O | 1:CX:140:VAL:HG12 | 2.14 | 0.47 |
| 1:BH:152:TRP:HE1 | 1:BI:64:LYS:C | 2.17 | 0.47 |
| 1:A2:75:ILE:HG22 | 1:A2:77:LEU:HD13 | 1.97 | 0.47 |
| 1:AX:117:THR:HG22 | 1:AY:85:THR:HG21 | 1.97 | 0.47 |
| 1:AN:117:THR:HG22 | 1:AO:85:THR:HG21 | 1.97 | 0.47 |
| 1:CI:117:THR:HG22 | 1:CJ:85:THR:HG21 | 1.97 | 0.47 |
| 1:BG:37:LEU:O | 1:BG:42:VAL:HG23 | 2.15 | 0.47 |
| 1:BQ:13:LYS:HD2 | 1:BQ:46:ASP:OD2 | 2.14 | 0.47 |
| 1:BQ:116:THR:O | 1:BR:85:THR:HB | 2.14 | 0.47 |
| 1:CG:90:TYR:O | 1:CG:94:GLU:HG2 | 2.14 | 0.47 |
| 1:AY:29:LEU:HD11 | 1:AY:134:LYS:HB3 | 1.97 | 0.47 |
| 1:AE:29:LEU:HD11 | 1:AE:134:LYS:HB3 | 1.97 | 0.47 |
| 1:A1:13:LYS:HD2 | 1:A1:46:ASP:OD2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BE:29:LEU:HD11 | 1:BE:134:LYS:HB3 | 1.97 | 0.47 |
| 1:BB:106:THR:O | 1:BB:107:ASP:HB3 | 2.15 | 0.47 |
| 1:BG:106:THR:O | 1:BG:107:ASP:HB3 | 2.15 | 0.47 |
| 1:BJ:71:TYR:O | 1:BJ:150:LYS:NZ | 2.44 | 0.47 |
| 1:B1:97:LYS:HE3 | 1:B2:97:LYS:HZ3 | 1.78 | 0.47 |
| 1:CQ:100:ALA:CA | 1:CR:56:PHE:HZ | 2.28 | 0.47 |
| 1:BV:58:ILE:HG22 | 1:BV:58:ILE:O | 2.13 | 0.47 |
| 1:AW:63:LYS:C | 1:AW:65:MET:H | 2.18 | 0.47 |
| 1:A2:63:LYS:C | 1:A2:65:MET:H | 2.18 | 0.47 |
| 1:CT:121:GLU:O | 1:CT:125:GLU:HB2 | 2.14 | 0.47 |
| 1:AM:63:LYS:C | 1:AM:65:MET:H | 2.18 | 0.47 |
| 1:CK:121:GLU:O | 1:CK:125:GLU:HG3 | 2.14 | 0.47 |
| 1:AC:63:LYS:C | 1:AC:65:MET:H | 2.18 | 0.47 |
| 1:AF:121:GLU:O | 1:AF:125:GLU:HG3 | 2.14 | 0.47 |
| 1:C3:137:GLU:O | 1:C3:140:VAL:HG12 | 2.14 | 0.47 |
| 1:AO:121:GLU:O | 1:AO:125:GLU:HB2 | 2.14 | 0.47 |
| 1:CS:149:SER:HB3 | 1:CS:152:TRP:CZ2 | 2.49 | 0.47 |
| 1:BD:137:GLU:O | 1:BD:140:VAL:HG12 | 2.14 | 0.47 |
| 1:BS:48:ASP:HB2 | 1:BS:71:TYR:CE1 | 2.50 | 0.47 |
| 1:CX:48:ASP:HB2 | 1:CX:71:TYR:CE1 | 2.50 | 0.47 |
| 1:AS:137:GLU:O | 1:AS:140:VAL:HG12 | 2.14 | 0.47 |
| 1:AW:75:ILE:HG22 | 1:AW:77:LEU:HD13 | 1.97 | 0.47 |
| 1:AM:30:LEU:HA | 1:AM:77:LEU:HD23 | 1.97 | 0.47 |
| 1:A2:152:TRP:HE1 | 1:A3:64:LYS:C | 2.18 | 0.47 |
| 1:BX:117:THR:HG22 | 1:BY:85:THR:HG21 | 1.97 | 0.47 |
| 1:AS:117:THR:HG22 | 1:AT:85:THR:HG21 | 1.97 | 0.47 |
| 1:AV:13:LYS:HD2 | 1:AV:46:ASP:OD2 | 2.14 | 0.47 |
| 1:CX:66:ALA:HB2 | 1:CX:74:VAL:HG21 | 1.96 | 0.47 |
| 1:CO:29:LEU:HD11 | 1:CO:134:LYS:HB3 | 1.97 | 0.47 |
| 1:B1:13:LYS:HD2 | 1:B1:46:ASP:OD2 | 2.14 | 0.47 |
| 1:CZ:65:MET:HE3 | 1:CZ:71:TYR:CE2 | 2.50 | 0.47 |
| 1:BO:29:LEU:HD11 | 1:BO:134:LYS:HB3 | 1.97 | 0.47 |
| 1:CS:82:ARG:HG3 | 1:CS:118:GLU:OE2 | 2.14 | 0.47 |
| 1:CI:82:ARG:HG3 | 1:CI:118:GLU:OE2 | 2.14 | 0.47 |
| 1:CD:66:ALA:HB2 | 1:CD:74:VAL:HG21 | 1.96 | 0.47 |
| 1:CW:9:GLY:HA3 | 1:CW:12:LEU:HD12 | 1.97 | 0.47 |
| 1:C1:90:TYR:O | 1:C1:94:GLU:HG2 | 2.14 | 0.47 |
| 1:CV:106:THR:O | 1:CV:107:ASP:HB3 | 2.15 | 0.46 |
| 1:BV:106:THR:O | 1:BV:107:ASP:HB3 | 2.15 | 0.46 |
| 1:BT:71:TYR:O | 1:BT:150:LYS:NZ | 2.44 | 0.46 |
| 1:BQ:152:TRP:O | 1:BQ:152:TRP:CD1 | 2.68 | 0.46 |
| 1:AM:52:VAL:CG1 | 1:AM:61:ILE:HD12 | 2.35 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CM:38:LYS:HZ2 | 1:CM:44:GLU:HA | 1.80 | 0.46 |
| 1:BZ:121:GLU:O | 1:BZ:125:GLU:HG3 | 2.14 | 0.46 |
| 1:C3:149:SER:HB3 | 1:C3:152:TRP:CZ2 | 2.49 | 0.46 |
| 1:CM:106:THR:HG23 | 1:CM:108:ILE:H | 1.79 | 0.46 |
| 1:B2:63:LYS:C | 1:B2:65:MET:H | 2.18 | 0.46 |
| 1:CS:137:GLU:O | 1:CS:140:VAL:HG12 | 2.14 | 0.46 |
| 1:BJ:83:GLY:HA3 | 2:BJ:1001:PO4:O2 | 2.15 | 0.46 |
| 1:BY:83:GLY:HA3 | 2:BY:1001:PO4:O2 | 2.15 | 0.46 |
| 1:C2:30:LEU:HA | 1:C2:77:LEU:HD23 | 1.97 | 0.46 |
| 1:BV:129:THR:CG2 | 1:BV:130:LYS:H | 2.28 | 0.46 |
| 1:AH:30:LEU:HA | 1:AH:77:LEU:HD23 | 1.97 | 0.46 |
| 1:CS:117:THR:HG22 | 1:CT:85:THR:HG21 | 1.97 | 0.46 |
| 1:CV:37:LEU:O | 1:CV:42:VAL:HG23 | 2.15 | 0.46 |
| 1:BQ:12:LEU:HB2 | 1:BQ:42:VAL:HG13 | 1.96 | 0.46 |
| 1:AG:37:LEU:O | 1:AG:42:VAL:HG23 | 2.15 | 0.46 |
| 1:CN:117:THR:HG22 | 1:CO:85:THR:HG21 | 1.97 | 0.46 |
| 1:AB:12:LEU:HB2 | 1:AB:42:VAL:HG13 | 1.96 | 0.46 |
| 1:AB:65:MET:HE3 | 1:AB:71:TYR:CZ | 2.51 | 0.46 |
| 1:CH:104:LEU:HD13 | 1:CI:102:LEU:HG | 1.98 | 0.46 |
| 1:BY:29:LEU:HD11 | 1:BY:134:LYS:HB3 | 1.97 | 0.46 |
| 1:AQ:116:THR:O | 1:AR:85:THR:HB | 2.14 | 0.46 |
| 1:B1:90:TYR:O | 1:B1:94:GLU:HG2 | 2.14 | 0.46 |
| 1:C1:100:ALA:CA | 1:C2:56:PHE:HZ | 2.28 | 0.46 |
| 1:AB:100:ALA:CA | 1:AC:56:PHE:HZ | 2.28 | 0.46 |
| 1:CQ:58:ILE:O | 1:CQ:58:ILE:HG22 | 2.13 | 0.46 |
| 1:AV:144:GLU:OE2 | 1:AW:20:ARG:HD2 | 2.14 | 0.46 |
| 1:CZ:125:GLU:CA | 1:CZ:129:THR:OG1 | 2.57 | 0.46 |
| 1:CW:63:LYS:C | 1:CW:65:MET:H | 2.18 | 0.46 |
| 1:CN:149:SER:HB3 | 1:CN:152:TRP:CZ2 | 2.49 | 0.46 |
| 1:BC:106:THR:HG23 | 1:BC:108:ILE:H | 1.79 | 0.46 |
| 1:C4:83:GLY:HA3 | 2:C4:4201:PO4:O2 | 2.15 | 0.46 |
| 1:CH:152:TRP:HE1 | 1:CI:64:LYS:C | 2.18 | 0.46 |
| 1:CN:137:GLU:O | 1:CN:140:VAL:HG12 | 2.14 | 0.46 |
| 1:AG:129:THR:CG2 | 1:AG:130:LYS:H | 2.28 | 0.46 |
| 1:CH:75:ILE:HG22 | 1:CH:77:LEU:HD13 | 1.97 | 0.46 |
| 1:A1:12:LEU:HB2 | 1:A1:42:VAL:HG13 | 1.96 | 0.46 |
| 1:BN:117:THR:HG22 | 1:BO:85:THR:HG21 | 1.97 | 0.46 |
| 1:B2:104:LEU:HD13 | 1:B3:102:LEU:HG | 1.98 | 0.46 |
| 1:CC:9:GLY:HA3 | 1:CC:12:LEU:HD12 | 1.97 | 0.46 |
| 1:AS:82:ARG:HG3 | 1:AS:118:GLU:OE2 | 2.14 | 0.46 |
| 1:CW:45:ASN:HD22 | 1:CW:45:ASN:HA | 1.64 | 0.46 |
| 1:BT:29:LEU:HD11 | 1:BT:134:LYS:HB3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BV:90:TYR:O | 1:BV:94:GLU:HG2 | 2.14 | 0.46 |
| 1:B1:96:ALA:O | 1:B1:100:ALA:HB2 | 2.06 | 0.46 |
| 1:A1:100:ALA:CA | 1:A2:56:PHE:HZ | 2.28 | 0.46 |
| 1:BH:52:VAL:CG1 | 1:BH:61:ILE:HD12 | 2.35 | 0.46 |
| 1:B1:144:GLU:OE2 | 1:B2:20:ARG:HD2 | 2.14 | 0.46 |
| 1:BH:70:LYS:HB2 | 1:BH:71:TYR:CD1 | 2.50 | 0.46 |
| 1:CC:63:LYS:C | 1:CC:65:MET:H | 2.18 | 0.46 |
| 1:A2:70:LYS:HB2 | 1:A2:71:TYR:CD1 | 2.50 | 0.46 |
| 1:CM:63:LYS:C | 1:CM:65:MET:H | 2.18 | 0.46 |
| 1:CH:70:LYS:HB2 | 1:CH:71:TYR:CD1 | 2.50 | 0.46 |
| 1:CF:58:ILE:H | 1:CF:59:PRO:HD2 | 1.80 | 0.46 |
| 1:BC:63:LYS:C | 1:BC:65:MET:H | 2.18 | 0.46 |
| 1:BC:65:MET:HE2 | 1:BC:65:MET:HB3 | 1.51 | 0.46 |
| 1:B2:75:ILE:HG22 | 1:B2:77:LEU:HD13 | 1.97 | 0.46 |
| 1:CW:75:ILE:HG22 | 1:CW:77:LEU:HD13 | 1.97 | 0.46 |
| 1:AQ:129:THR:CG2 | 1:AQ:130:LYS:H | 2.28 | 0.46 |
| 1:AL:129:THR:CG2 | 1:AL:130:LYS:H | 2.28 | 0.46 |
| 1:CH:30:LEU:HA | 1:CH:77:LEU:HD23 | 1.97 | 0.46 |
| 1:B3:117:THR:HG22 | 1:B4:85:THR:HG21 | 1.97 | 0.46 |
| 1:BI:117:THR:HG22 | 1:BJ:85:THR:HG21 | 1.97 | 0.46 |
| 1:A3:117:THR:HG22 | 1:A4:85:THR:HG21 | 1.97 | 0.46 |
| 1:C2:104:LEU:HD13 | 1:C3:102:LEU:HG | 1.98 | 0.46 |
| 1:CQ:37:LEU:O | 1:CQ:42:VAL:HG23 | 2.15 | 0.46 |
| 1:BL:37:LEU:O | 1:BL:42:VAL:HG23 | 2.15 | 0.46 |
| 1:CQ:116:THR:O | 1:CR:85:THR:HB | 2.14 | 0.46 |
| 1:BQ:90:TYR:O | 1:BQ:94:GLU:HG2 | 2.14 | 0.46 |
| 1:AT:29:LEU:HD11 | 1:AT:134:LYS:HB3 | 1.97 | 0.46 |
| 1:BV:152:TRP:O | 1:BV:152:TRP:CD1 | 2.67 | 0.46 |
| 1:CQ:106:THR:O | 1:CQ:107:ASP:HB3 | 2.15 | 0.46 |
| 1:AL:144:GLU:OE2 | 1:AM:20:ARG:HD2 | 2.14 | 0.46 |
| 1:CG:144:GLU:OE2 | 1:CH:20:ARG:HD2 | 2.14 | 0.46 |
| 1:C1:144:GLU:OE2 | 1:C2:20:ARG:HD2 | 2.14 | 0.46 |
| 1:CP:39:ARG:NH2 | 1:CV:144:GLU:CD | 2.68 | 0.46 |
| 1:BX:18:VAL:HG12 | 1:BX:77:LEU:CB | 2.37 | 0.46 |
| 1:CD:30:LEU:HA | 1:CD:77:LEU:HD23 | 1.96 | 0.46 |
| 1:CM:70:LYS:HB2 | 1:CM:71:TYR:CD1 | 2.50 | 0.46 |
| 1:AC:70:LYS:HB2 | 1:AC:71:TYR:CD1 | 2.50 | 0.46 |
| 1:AP:121:GLU:O | 1:AP:125:GLU:HG3 | 2.14 | 0.46 |
| 1:AK:121:GLU:O | 1:AK:125:GLU:HG3 | 2.14 | 0.46 |
| 1:BM:30:LEU:HA | 1:BM:77:LEU:HD23 | 1.97 | 0.46 |
| 1:AC:104:LEU:HD13 | 1:AD:102:LEU:HG | 1.98 | 0.46 |
| 1:AG:65:MET:HE3 | 1:AG:71:TYR:CZ | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CG:13:LYS:HD2 | 1:CG:46:ASP:OD2 | 2.14 | 0.46 |
| 1:BJ:29:LEU:HD11 | 1:BJ:134:LYS:HB3 | 1.97 | 0.46 |
| 1:CX:120:ILE:HD11 | 1:C2:129:THR:HG21 | 1.97 | 0.46 |
| 1:CH:52:VAL:CG1 | 1:CH:61:ILE:HD12 | 2.35 | 0.46 |
| 1:AX:75:ILE:HG22 | 1:AX:77:LEU:HD13 | 1.98 | 0.46 |
| 1:BI:30:LEU:HA | 1:BI:77:LEU:HD23 | 1.96 | 0.46 |
| 1:CX:75:ILE:HG22 | 1:CX:77:LEU:HD13 | 1.98 | 0.46 |
| 1:A3:18:VAL:HG11 | 1:A3:30:LEU:HD13 | 1.98 | 0.46 |
| 1:AN:75:ILE:HG22 | 1:AN:77:LEU:HD13 | 1.98 | 0.46 |
| 1:C3:75:ILE:HG22 | 1:C3:77:LEU:HD13 | 1.98 | 0.46 |
| 1:CK:58:ILE:H | 1:CK:59:PRO:HD2 | 1.80 | 0.46 |
| 1:CZ:121:GLU:O | 1:CZ:125:GLU:HG3 | 2.14 | 0.46 |
| 1:CE:83:GLY:HA3 | 2:CE:1001:PO4:O2 | 2.15 | 0.46 |
| 1:AD:137:GLU:O | 1:AD:140:VAL:HG12 | 2.14 | 0.46 |
| 1:BC:75:ILE:HG22 | 1:BC:77:LEU:HD13 | 1.97 | 0.46 |
| 1:CM:30:LEU:HA | 1:CM:77:LEU:HD23 | 1.97 | 0.46 |
| 1:AC:30:LEU:HA | 1:AC:77:LEU:HD23 | 1.97 | 0.46 |
| 1:BM:75:ILE:HG22 | 1:BM:77:LEU:HD13 | 1.97 | 0.46 |
| 1:A1:37:LEU:O | 1:A1:42:VAL:HG23 | 2.15 | 0.46 |
| 1:A1:65:MET:HE3 | 1:A1:71:TYR:CZ | 2.50 | 0.46 |
| 1:B1:37:LEU:O | 1:B1:42:VAL:HG23 | 2.15 | 0.46 |
| 1:AI:82:ARG:HG3 | 1:AI:118:GLU:OE2 | 2.14 | 0.46 |
| 1:BD:13:LYS:NZ | 1:CM:13:LYS:HD3 | 2.30 | 0.46 |
| 1:CT:29:LEU:HD11 | 1:CT:134:LYS:HB3 | 1.97 | 0.46 |
| 1:C2:45:ASN:HA | 1:C2:45:ASN:HD22 | 1.63 | 0.46 |
| 1:BF:65:MET:HE3 | 1:BF:71:TYR:CE2 | 2.50 | 0.46 |
| 1:AX:82:ARG:HG3 | 1:AX:118:GLU:OE2 | 2.15 | 0.46 |
| 1:AO:29:LEU:HD11 | 1:AO:134:LYS:HB3 | 1.97 | 0.46 |
| 1:BN:82:ARG:HG3 | 1:BN:118:GLU:OE2 | 2.14 | 0.46 |
| 1:BX:18:VAL:HG11 | 1:BX:30:LEU:HD13 | 1.98 | 0.46 |
| 1:BS:30:LEU:HA | 1:BS:77:LEU:HD23 | 1.96 | 0.46 |
| 1:AA:58:ILE:O | 1:AA:62:ALA:CB | 2.64 | 0.46 |
| 1:BA:121:GLU:O | 1:BA:125:GLU:HG3 | 2.14 | 0.46 |
| 1:AZ:58:ILE:H | 1:AZ:59:PRO:HD2 | 1.80 | 0.46 |
| 1:CP:7:LEU:HD23 | 1:CV:40:HIS:CE1 | 2.51 | 0.46 |
| 1:BE:39:ARG:O | 1:BN:7:LEU:HB3 | 2.16 | 0.46 |
| 1:BB:129:THR:CG2 | 1:BB:130:LYS:H | 2.28 | 0.46 |
| 1:B2:30:LEU:HA | 1:B2:77:LEU:HD23 | 1.97 | 0.46 |
| 1:AM:75:ILE:HG22 | 1:AM:77:LEU:HD13 | 1.97 | 0.46 |
| 1:BD:9:GLY:HA2 | 1:BD:147:HIS:HE1 | 1.81 | 0.46 |
| 1:CD:117:THR:HG22 | 1:CE:85:THR:HG21 | 1.97 | 0.46 |
| 1:CQ:65:MET:HE3 | 1:CQ:71:TYR:CZ | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BS:117:THR:HG22 | 1:BT:85:THR:HG21 | 1.97 | 0.46 |
| 1:CG:12:LEU:HB2 | 1:CG:42:VAL:HG13 | 1.96 | 0.46 |
| 1:A2:104:LEU:HD13 | 1:A3:102:LEU:HG | 1.98 | 0.46 |
| 1:C3:82:ARG:HG3 | 1:C3:118:GLU:OE2 | 2.15 | 0.46 |
| 1:BW:9:GLY:HA3 | 1:BW:12:LEU:HD12 | 1.98 | 0.46 |
| 1:CM:9:GLY:HA3 | 1:CM:12:LEU:HD12 | 1.97 | 0.46 |
| 1:A1:90:TYR:O | 1:A1:94:GLU:HG2 | 2.14 | 0.46 |
| 1:BD:82:ARG:HG3 | 1:BD:118:GLU:OE2 | 2.14 | 0.46 |
| 1:A4:71:TYR:O | 1:A4:150:LYS:NZ | 2.44 | 0.46 |
| 1:B3:18:VAL:HG11 | 1:B3:30:LEU:HD13 | 1.98 | 0.46 |
| 1:BX:75:ILE:HG22 | 1:BX:77:LEU:HD13 | 1.98 | 0.46 |
| 1:BI:18:VAL:HG11 | 1:BI:30:LEU:HD13 | 1.98 | 0.46 |
| 1:BI:75:ILE:HG22 | 1:BI:77:LEU:HD13 | 1.98 | 0.46 |
| 1:BS:75:ILE:HG22 | 1:BS:77:LEU:HD13 | 1.98 | 0.46 |
| 1:CD:75:ILE:HG22 | 1:CD:77:LEU:HD13 | 1.98 | 0.46 |
| 1:CK:58:ILE:O | 1:CK:62:ALA:CB | 2.64 | 0.46 |
| 1:BZ:58:ILE:O | 1:BZ:62:ALA:CB | 2.64 | 0.46 |
| 1:AK:58:ILE:O | 1:AK:62:ALA:CB | 2.64 | 0.46 |
| 1:BW:75:ILE:HG22 | 1:BW:77:LEU:HD13 | 1.97 | 0.46 |
| 1:AH:152:TRP:HE1 | 1:AI:64:LYS:C | 2.17 | 0.46 |
| 1:CR:30:LEU:HA | 1:CR:77:LEU:HD23 | 1.97 | 0.46 |
| 1:CC:75:ILE:HG22 | 1:CC:77:LEU:HD13 | 1.97 | 0.46 |
| 1:CN:9:GLY:HA2 | 1:CN:147:HIS:HE1 | 1.81 | 0.46 |
| 1:AX:9:GLY:HA2 | 1:AX:147:HIS:HE1 | 1.81 | 0.46 |
| 1:CX:9:GLY:HA2 | 1:CX:147:HIS:HE1 | 1.81 | 0.46 |
| 1:CF:65:MET:HE3 | 1:CF:71:TYR:CE2 | 2.51 | 0.46 |
| 1:AJ:29:LEU:HD11 | 1:AJ:134:LYS:HB3 | 1.97 | 0.46 |
| 1:CJ:29:LEU:HD11 | 1:CJ:134:LYS:HB3 | 1.97 | 0.46 |
| 1:A4:29:LEU:HD11 | 1:A4:134:LYS:HB3 | 1.97 | 0.46 |
| 1:AR:9:GLY:HA3 | 1:AR:12:LEU:HD12 | 1.98 | 0.46 |
| 1:AM:9:GLY:HA3 | 1:AM:12:LEU:HD12 | 1.97 | 0.46 |
| 1:BD:120:ILE:HD13 | 1:BR:129:THR:HG21 | 1.96 | 0.46 |
| 1:B4:71:TYR:O | 1:B4:150:LYS:NZ | 2.44 | 0.46 |
| 1:BB:97:LYS:HE3 | 1:BC:97:LYS:HZ3 | 1.78 | 0.46 |
| 1:CM:52:VAL:CG1 | 1:CM:61:ILE:HD12 | 2.35 | 0.46 |
| 1:CX:30:LEU:HA | 1:CX:77:LEU:HD23 | 1.96 | 0.46 |
| 1:C3:18:VAL:HG11 | 1:C3:30:LEU:HD13 | 1.98 | 0.46 |
| 1:CZ:58:ILE:O | 1:CZ:58:ILE:HG22 | 2.11 | 0.46 |
| 1:CZ:58:ILE:O | 1:CZ:62:ALA:CB | 2.64 | 0.46 |
| 1:C2:63:LYS:C | 1:C2:65:MET:H | 2.18 | 0.46 |
| 1:AF:58:ILE:H | 1:AF:59:PRO:HD2 | 1.80 | 0.46 |
| 1:AI:40:HIS:CE1 | 1:AO:7:LEU:HD23 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BD:48:ASP:HB2 | 1:BD:71:TYR:CE1 | 2.50 | 0.46 |
| 1:B3:48:ASP:HB2 | 1:B3:71:TYR:CE1 | 2.50 | 0.46 |
| 1:CQ:129:THR:CG2 | 1:CQ:130:LYS:H | 2.28 | 0.46 |
| 1:AH:75:ILE:HG22 | 1:AH:77:LEU:HD13 | 1.97 | 0.46 |
| 1:BX:9:GLY:HA2 | 1:BX:147:HIS:HE1 | 1.81 | 0.46 |
| 1:AD:9:GLY:HA2 | 1:AD:147:HIS:HE1 | 1.81 | 0.46 |
| 1:AR:104:LEU:HD13 | 1:AS:102:LEU:HG | 1.98 | 0.46 |
| 1:AB:37:LEU:O | 1:AB:42:VAL:HG23 | 2.15 | 0.46 |
| 1:AV:65:MET:HE3 | 1:AV:71:TYR:CZ | 2.51 | 0.46 |
| 1:BW:104:LEU:HD13 | 1:BX:102:LEU:HG | 1.97 | 0.46 |
| 1:B4:29:LEU:HD11 | 1:B4:134:LYS:HB3 | 1.97 | 0.46 |
| 1:A2:45:ASN:HD22 | 1:A2:45:ASN:HA | 1.64 | 0.46 |
| 1:C4:29:LEU:HD11 | 1:C4:134:LYS:HB3 | 1.97 | 0.46 |
| 1:CH:9:GLY:HA3 | 1:CH:12:LEU:HD12 | 1.98 | 0.46 |
| 1:BQ:100:ALA:CA | 1:BR:56:PHE:HZ | 2.28 | 0.46 |
| 1:BD:75:ILE:HG22 | 1:BD:77:LEU:HD13 | 1.98 | 0.46 |
| 1:CS:75:ILE:HG22 | 1:CS:77:LEU:HD13 | 1.98 | 0.46 |
| 1:A3:75:ILE:HG22 | 1:A3:77:LEU:HD13 | 1.98 | 0.46 |
| 1:CK:58:ILE:HG22 | 1:CK:58:ILE:O | 2.11 | 0.46 |
| 1:AZ:58:ILE:O | 1:AZ:62:ALA:CB | 2.64 | 0.46 |
| 1:BR:67:ASN:HA | 1:BR:67:ASN:HD22 | 1.59 | 0.46 |
| 1:BX:48:ASP:HB2 | 1:BX:71:TYR:CE1 | 2.50 | 0.46 |
| 1:AX:7:LEU:HB3 | 1:A4:39:ARG:O | 2.16 | 0.46 |
| 1:B3:9:GLY:HA2 | 1:B3:147:HIS:HE1 | 1.81 | 0.46 |
| 1:AI:117:THR:HG22 | 1:AJ:85:THR:HG21 | 1.97 | 0.46 |
| 1:CV:65:MET:HE3 | 1:CV:71:TYR:CZ | 2.51 | 0.46 |
| 1:CW:104:LEU:HD13 | 1:CX:102:LEU:HG | 1.98 | 0.46 |
| 1:CY:29:LEU:HD11 | 1:CY:134:LYS:HB3 | 1.97 | 0.46 |
| 1:BD:148:LEU:HA | 1:BD:148:LEU:HD23 | 1.82 | 0.46 |
| 1:CB:90:TYR:O | 1:CB:94:GLU:HG2 | 2.14 | 0.46 |
| 1:BO:109:PRO:HG3 | 1:BO:149:SER:CB | 2.46 | 0.46 |
| 1:BO:71:TYR:O | 1:BO:150:LYS:NZ | 2.44 | 0.46 |
| 1:BV:100:ALA:CA | 1:BW:56:PHE:HZ | 2.28 | 0.46 |
| 1:A1:97:LYS:N | 1:A1:100:ALA:HB2 | 2.31 | 0.46 |
| 1:AF:39:ARG:NH2 | 1:AQ:144:GLU:CD | 2.68 | 0.46 |
| 1:CI:75:ILE:HG22 | 1:CI:77:LEU:HD13 | 1.98 | 0.46 |
| 1:CN:18:VAL:HG11 | 1:CN:30:LEU:HD13 | 1.98 | 0.46 |
| 1:CN:75:ILE:HG22 | 1:CN:77:LEU:HD13 | 1.98 | 0.46 |
| 1:AI:75:ILE:HG22 | 1:AI:77:LEU:HD13 | 1.98 | 0.46 |
| 1:BH:63:LYS:C | 1:BH:65:MET:H | 2.18 | 0.46 |
| 1:CU:58:ILE:O | 1:CU:58:ILE:HG22 | 2.11 | 0.46 |
| 1:CU:58:ILE:O | 1:CU:62:ALA:CB | 2.64 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BA:58:ILE:O | 1:BA:62:ALA:CB | 2.64 | 0.46 |
| 1:BP:58:ILE:H | 1:BP:59:PRO:HD2 | 1.80 | 0.46 |
| 1:CF:58:ILE:O | 1:CF:62:ALA:CB | 2.64 | 0.46 |
| 1:CD:20:ARG:CZ | 1:CR:39:ARG:NE | 2.78 | 0.46 |
| 1:AB:129:THR:CG2 | 1:AB:130:LYS:H | 2.28 | 0.46 |
| 1:BQ:37:LEU:O | 1:BQ:42:VAL:HG23 | 2.15 | 0.46 |
| 1:AQ:65:MET:HE3 | 1:AQ:71:TYR:CZ | 2.51 | 0.46 |
| 1:AC:83:GLY:HA3 | 2:AC:1001:PO4:O4 | 2.16 | 0.46 |
| 1:AH:9:GLY:HA3 | 1:AH:12:LEU:HD12 | 1.97 | 0.46 |
| 1:CR:83:GLY:HA3 | 2:CR:2201:PO4:O4 | 2.16 | 0.46 |
| 1:BJ:109:PRO:HG3 | 1:BJ:149:SER:CB | 2.46 | 0.45 |
| 1:CB:100:ALA:CA | 1:CC:56:PHE:HZ | 2.28 | 0.45 |
| 1:BL:100:ALA:CA | 1:BM:56:PHE:HZ | 2.28 | 0.45 |
| 1:BN:75:ILE:HG22 | 1:BN:77:LEU:HD13 | 1.98 | 0.45 |
| 1:AD:48:ASP:HB2 | 1:AD:71:TYR:CE1 | 2.50 | 0.45 |
| 1:BH:75:ILE:HG22 | 1:BH:77:LEU:HD13 | 1.97 | 0.45 |
| 1:BW:30:LEU:HA | 1:BW:77:LEU:HD23 | 1.97 | 0.45 |
| 1:A2:30:LEU:HA | 1:A2:77:LEU:HD23 | 1.97 | 0.45 |
| 1:AL:65:MET:HE3 | 1:AL:71:TYR:CZ | 2.52 | 0.45 |
| 1:CL:37:LEU:O | 1:CL:42:VAL:HG23 | 2.15 | 0.45 |
| 1:CQ:70:LYS:O | 1:CQ:70:LYS:HG2 | 2.17 | 0.45 |
| 1:CM:83:GLY:HA3 | 2:CM:2201:PO4:O4 | 2.16 | 0.45 |
| 1:C2:9:GLY:HA3 | 1:C2:12:LEU:HD12 | 1.98 | 0.45 |
| 1:AT:109:PRO:HG3 | 1:AT:149:SER:CB | 2.46 | 0.45 |
| 1:BQ:97:LYS:N | 1:BQ:100:ALA:HB2 | 2.31 | 0.45 |
| 1:BD:18:VAL:HG11 | 1:BD:30:LEU:HD13 | 1.98 | 0.45 |
| 1:BU:58:ILE:O | 1:BU:58:ILE:HG22 | 2.11 | 0.45 |
| 1:BF:58:ILE:H | 1:BF:59:PRO:HD2 | 1.80 | 0.45 |
| 1:CP:58:ILE:O | 1:CP:62:ALA:CB | 2.64 | 0.45 |
| 1:AM:108:ILE:O | 1:AM:110:VAL:HG23 | 2.17 | 0.45 |
| 1:BC:108:ILE:O | 1:BC:110:VAL:HG23 | 2.17 | 0.45 |
| 1:B1:4:GLU:CG | 1:B2:51:TRP:HD1 | 2.29 | 0.45 |
| 1:AZ:7:LEU:HD12 | 1:AZ:7:LEU:HA | 1.84 | 0.45 |
| 1:BW:65:MET:HB3 | 1:BW:65:MET:HE2 | 1.51 | 0.45 |
| 1:CS:48:ASP:HB2 | 1:CS:71:TYR:CE1 | 2.50 | 0.45 |
| 1:CN:48:ASP:HB2 | 1:CN:71:TYR:CE1 | 2.50 | 0.45 |
| 1:BG:65:MET:HE3 | 1:BG:71:TYR:CZ | 2.51 | 0.45 |
| 1:AH:104:LEU:HD13 | 1:AI:102:LEU:HG | 1.98 | 0.45 |
| 1:AD:24:PHE:CD1 | 1:AR:28:LYS:HG3 | 2.52 | 0.45 |
| 1:CH:148:LEU:HA | 1:CH:148:LEU:HD23 | 1.80 | 0.45 |
| 1:BR:45:ASN:HD22 | 1:BR:45:ASN:HA | 1.63 | 0.45 |
| 1:C2:83:GLY:HA3 | 2:C2:2201:PO4:O4 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AO:109:PRO:HG3 | 1:AO:149:SER:CB | 2.46 | 0.45 |
| 1:CE:109:PRO:HG3 | 1:CE:149:SER:CB | 2.46 | 0.45 |
| 1:A4:109:PRO:HG3 | 1:A4:149:SER:CB | 2.46 | 0.45 |
| 1:BC:52:VAL:CG1 | 1:BC:61:ILE:HD12 | 2.35 | 0.45 |
| 1:CD:52:VAL:CG1 | 1:CD:61:ILE:HD12 | 2.35 | 0.45 |
| 1:CX:18:VAL:HG11 | 1:CX:30:LEU:HD13 | 1.98 | 0.45 |
| 1:BS:18:VAL:HG23 | 1:BS:51:TRP:CE3 | 2.52 | 0.45 |
| 1:CD:18:VAL:HG11 | 1:CD:30:LEU:HD13 | 1.98 | 0.45 |
| 1:AN:18:VAL:HG11 | 1:AN:30:LEU:HD13 | 1.98 | 0.45 |
| 1:AI:18:VAL:HG11 | 1:AI:30:LEU:HD13 | 1.98 | 0.45 |
| 1:BU:58:ILE:O | 1:BU:62:ALA:CB | 2.64 | 0.45 |
| 1:CU:58:ILE:H | 1:CU:59:PRO:HD2 | 1.80 | 0.45 |
| 1:BF:58:ILE:O | 1:BF:62:ALA:CB | 2.64 | 0.45 |
| 1:CA:58:ILE:O | 1:CA:62:ALA:CB | 2.64 | 0.45 |
| 1:BK:58:ILE:O | 1:BK:62:ALA:CB | 2.64 | 0.45 |
| 1:CR:108:ILE:O | 1:CR:110:VAL:HG23 | 2.17 | 0.45 |
| 1:BR:108:ILE:O | 1:BR:110:VAL:HG23 | 2.17 | 0.45 |
| 1:BV:4:GLU:CG | 1:BW:51:TRP:HD1 | 2.29 | 0.45 |
| 1:CW:30:LEU:HA | 1:CW:77:LEU:HD23 | 1.97 | 0.45 |
| 1:AN:9:GLY:HA2 | 1:AN:147:HIS:HE1 | 1.81 | 0.45 |
| 1:CG:65:MET:HE3 | 1:CG:71:TYR:CZ | 2.51 | 0.45 |
| 1:BQ:65:MET:HE3 | 1:BQ:71:TYR:CZ | 2.50 | 0.45 |
| 1:BB:65:MET:HE3 | 1:BB:71:TYR:CE2 | 2.51 | 0.45 |
| 1:CL:70:LYS:O | 1:CL:70:LYS:HG2 | 2.16 | 0.45 |
| 1:CR:104:LEU:HD13 | 1:CS:102:LEU:HG | 1.98 | 0.45 |
| 1:CC:83:GLY:HA3 | 2:CC:1001:PO4:O4 | 2.16 | 0.45 |
| 1:CR:9:GLY:HA3 | 1:CR:12:LEU:HD12 | 1.98 | 0.45 |
| 1:CY:109:PRO:HG3 | 1:CY:149:SER:CB | 2.46 | 0.45 |
| 1:AQ:100:ALA:CA | 1:AR:56:PHE:HZ | 2.28 | 0.45 |
| 1:CL:58:ILE:O | 1:CL:58:ILE:CG2 | 2.65 | 0.45 |
| 1:AD:18:VAL:HG11 | 1:AD:30:LEU:HD13 | 1.98 | 0.45 |
| 1:BX:18:VAL:HG23 | 1:BX:51:TRP:CE3 | 2.52 | 0.45 |
| 1:BH:67:ASN:HD22 | 1:BH:67:ASN:HA | 1.60 | 0.45 |
| 1:AR:30:LEU:HA | 1:AR:77:LEU:HD23 | 1.97 | 0.45 |
| 1:A3:9:GLY:HA2 | 1:A3:147:HIS:HE1 | 1.81 | 0.45 |
| 1:CI:9:GLY:HA2 | 1:CI:147:HIS:HE1 | 1.81 | 0.45 |
| 1:CB:65:MET:HE3 | 1:CB:71:TYR:CZ | 2.51 | 0.45 |
| 1:BC:104:LEU:HD13 | 1:BD:102:LEU:HG | 1.98 | 0.45 |
| 1:B2:9:GLY:HA3 | 1:B2:12:LEU:HD12 | 1.97 | 0.45 |
| 1:CA:28:LYS:NZ | 1:CN:28:LYS:NZ | 2.65 | 0.45 |
| 1:AR:83:GLY:HA3 | 2:AR:1001:PO4:O4 | 2.16 | 0.45 |
| 1:AQ:70:LYS:O | 1:AQ:70:LYS:HG2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BT:109:PRO:HG3 | 1:BT:149:SER:CB | 2.46 | 0.45 |
| 1:CG:55:ALA:CB | 1:CG:95:VAL:HG21 | 2.40 | 0.45 |
| 1:BN:18:VAL:HG23 | 1:BN:51:TRP:CE3 | 2.52 | 0.45 |
| 1:AF:58:ILE:O | 1:AF:62:ALA:CB | 2.64 | 0.45 |
| 1:CN:149:SER:HB3 | 1:CN:152:TRP:CH2 | 2.52 | 0.45 |
| 1:BS:149:SER:HB3 | 1:BS:152:TRP:CH2 | 2.52 | 0.45 |
| 1:BW:108:ILE:O | 1:BW:110:VAL:HG23 | 2.17 | 0.45 |
| 1:AH:108:ILE:O | 1:AH:110:VAL:HG23 | 2.17 | 0.45 |
| 1:CR:65:MET:HE2 | 1:CR:65:MET:HB3 | 1.52 | 0.45 |
| 1:BQ:6:HIS:HB3 | 1:BQ:147:HIS:CG | 2.52 | 0.45 |
| 1:CD:48:ASP:HB2 | 1:CD:71:TYR:CE1 | 2.50 | 0.45 |
| 1:C2:75:ILE:HG22 | 1:C2:77:LEU:HD13 | 1.97 | 0.45 |
| 1:CD:9:GLY:HA2 | 1:CD:147:HIS:HE1 | 1.81 | 0.45 |
| 1:BN:9:GLY:HA2 | 1:BN:147:HIS:HE1 | 1.81 | 0.45 |
| 1:CM:104:LEU:HD13 | 1:CN:102:LEU:HG | 1.98 | 0.45 |
| 1:AR:45:ASN:HA | 1:AR:45:ASN:HD22 | 1.63 | 0.45 |
| 1:A3:148:LEU:HD23 | 1:A3:148:LEU:HA | 1.82 | 0.45 |
| 1:B2:83:GLY:HA3 | 2:B2:1001:PO4:O4 | 2.16 | 0.45 |
| 1:B1:106:THR:O | 1:B1:107:ASP:HB3 | 2.15 | 0.45 |
| 1:BY:109:PRO:HG3 | 1:BY:149:SER:CB | 2.46 | 0.45 |
| 1:AV:100:ALA:CA | 1:AW:56:PHE:HZ | 2.28 | 0.45 |
| 1:BG:97:LYS:N | 1:BG:100:ALA:HB2 | 2.31 | 0.45 |
| 1:CI:52:VAL:CG1 | 1:CI:61:ILE:HD12 | 2.35 | 0.45 |
| 1:BD:18:VAL:HG23 | 1:BD:51:TRP:CE3 | 2.52 | 0.45 |
| 1:AH:67:ASN:HA | 1:AH:67:ASN:HD22 | 1.59 | 0.45 |
| 1:CK:58:ILE:HG21 | 1:CK:76:THR:OG1 | 2.17 | 0.45 |
| 1:BA:58:ILE:HG21 | 1:BA:76:THR:OG1 | 2.17 | 0.45 |
| 1:BP:58:ILE:HG21 | 1:BP:76:THR:OG1 | 2.17 | 0.45 |
| 1:B3:149:SER:HB3 | 1:B3:152:TRP:CH2 | 2.52 | 0.45 |
| 1:BI:149:SER:HB3 | 1:BI:152:TRP:CH2 | 2.52 | 0.45 |
| 1:B2:108:ILE:O | 1:B2:110:VAL:HG23 | 2.17 | 0.45 |
| 1:AR:108:ILE:O | 1:AR:110:VAL:HG23 | 2.17 | 0.45 |
| 1:BB:4:GLU:CG | 1:BC:51:TRP:HD1 | 2.29 | 0.45 |
| 1:CQ:4:GLU:CG | 1:CR:51:TRP:HD1 | 2.29 | 0.45 |
| 1:CL:6:HIS:HB3 | 1:CL:147:HIS:CG | 2.52 | 0.45 |
| 1:BG:6:HIS:HB3 | 1:BG:147:HIS:CG | 2.52 | 0.45 |
| 1:AX:48:ASP:HB2 | 1:AX:71:TYR:CE1 | 2.50 | 0.45 |
| 1:CX:117:THR:HG22 | 1:CY:85:THR:HG21 | 1.97 | 0.45 |
| 1:AV:9:GLY:HA3 | 1:AV:12:LEU:HD12 | 1.99 | 0.45 |
| 1:CL:65:MET:HE3 | 1:CL:71:TYR:CZ | 2.51 | 0.45 |
| 1:BQ:70:LYS:O | 1:BQ:70:LYS:HG2 | 2.17 | 0.45 |
| 1:CA:22:ASN:HA | 1:CN:128:GLY:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AW:9:GLY:HA3 | 1:AW:12:LEU:HD12 | 1.97 | 0.45 |
| 1:BH:9:GLY:HA3 | 1:BH:12:LEU:HD12 | 1.98 | 0.45 |
| 1:AJ:109:PRO:HG3 | 1:AJ:149:SER:CB | 2.46 | 0.45 |
| 1:AL:97:LYS:N | 1:AL:100:ALA:HB2 | 2.31 | 0.45 |
| 1:BV:55:ALA:CB | 1:BV:95:VAL:HG21 | 2.40 | 0.45 |
| 1:B3:75:ILE:HG22 | 1:B3:77:LEU:HD13 | 1.98 | 0.45 |
| 1:AN:18:VAL:HG23 | 1:AN:51:TRP:CE3 | 2.52 | 0.45 |
| 1:AI:18:VAL:HG23 | 1:AI:51:TRP:CE3 | 2.52 | 0.45 |
| 1:AU:58:ILE:HG21 | 1:AU:76:THR:OG1 | 2.17 | 0.45 |
| 1:BZ:58:ILE:HG21 | 1:BZ:76:THR:OG1 | 2.17 | 0.45 |
| 1:AI:149:SER:HB3 | 1:AI:152:TRP:CH2 | 2.52 | 0.45 |
| 1:C3:149:SER:HB3 | 1:C3:152:TRP:CH2 | 2.52 | 0.45 |
| 1:CD:149:SER:HB3 | 1:CD:152:TRP:CH2 | 2.52 | 0.45 |
| 1:BH:108:ILE:O | 1:BH:110:VAL:HG23 | 2.16 | 0.45 |
| 1:BB:6:HIS:HB3 | 1:BB:147:HIS:CG | 2.52 | 0.45 |
| 1:AG:6:HIS:HB3 | 1:AG:147:HIS:CG | 2.52 | 0.45 |
| 1:A3:48:ASP:HB2 | 1:A3:71:TYR:CE1 | 2.50 | 0.45 |
| 1:C3:9:GLY:HA2 | 1:C3:147:HIS:HE1 | 1.81 | 0.45 |
| 1:CC:104:LEU:HD13 | 1:CD:102:LEU:HG | 1.98 | 0.45 |
| 1:BL:70:LYS:O | 1:BL:70:LYS:HG2 | 2.17 | 0.45 |
| 1:AH:83:GLY:HA3 | 2:AH:1001:PO4:O4 | 2.17 | 0.45 |
| 1:CE:29:LEU:HD11 | 1:CE:134:LYS:HB3 | 1.97 | 0.45 |
| 1:AZ:65:MET:HE3 | 1:AZ:71:TYR:CE2 | 2.51 | 0.45 |
| 1:A2:9:GLY:HA3 | 1:A2:12:LEU:HD12 | 1.98 | 0.45 |
| 1:CO:109:PRO:HG3 | 1:CO:149:SER:CB | 2.47 | 0.45 |
| 1:C1:97:LYS:N | 1:C1:100:ALA:HB2 | 2.31 | 0.45 |
| 1:AC:97:LYS:HE3 | 1:AD:97:LYS:NZ | 2.32 | 0.45 |
| 1:CL:97:LYS:N | 1:CL:100:ALA:HB2 | 2.31 | 0.45 |
| 1:AC:52:VAL:CG1 | 1:AC:61:ILE:HD12 | 2.35 | 0.45 |
| 1:AX:18:VAL:HG23 | 1:AX:51:TRP:CE3 | 2.52 | 0.45 |
| 1:BX:75:ILE:HD13 | 1:BX:139:ALA:HA | 1.99 | 0.45 |
| 1:C3:18:VAL:HG23 | 1:C3:51:TRP:CE3 | 2.52 | 0.45 |
| 1:AU:58:ILE:O | 1:AU:62:ALA:CB | 2.64 | 0.45 |
| 1:AN:149:SER:HB3 | 1:AN:152:TRP:CH2 | 2.52 | 0.45 |
| 1:C2:108:ILE:O | 1:C2:110:VAL:HG23 | 2.17 | 0.45 |
| 1:A2:108:ILE:O | 1:A2:110:VAL:HG23 | 2.17 | 0.45 |
| 1:CG:4:GLU:CG | 1:CH:51:TRP:HD1 | 2.29 | 0.45 |
| 1:AL:6:HIS:HB3 | 1:AL:147:HIS:CG | 2.52 | 0.45 |
| 1:AV:6:HIS:HB3 | 1:AV:147:HIS:CG | 2.52 | 0.45 |
| 1:AD:117:THR:HG22 | 1:AE:85:THR:HG21 | 1.97 | 0.45 |
| 1:CV:9:GLY:HA3 | 1:CV:12:LEU:HD12 | 1.99 | 0.45 |
| 1:BH:83:GLY:HA3 | 2:BH:1001:PO4:O4 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:AN:34:LEU:O | 1:AN:38:LYS:HG3 | 2.17 | 0.45 |
| 1:BC:83:GLY:HA3 | 2:BC:1001:PO4:O4 | 2.16 | 0.45 |
| 1:BS:148:LEU:HD23 | 1:BS:148:LEU:HA | 1.82 | 0.45 |
| 1:CW:83:GLY:HA3 | 2:CW:2201:PO4:O4 | 2.16 | 0.45 |
| 1:CO:53:PRO:CG | 1:CO:57:GLU:CG | 2.46 | 0.45 |
| 1:AE:109:PRO:HG3 | 1:AE:149:SER:CB | 2.46 | 0.45 |
| 1:AO:71:TYR:O | 1:AO:150:LYS:NZ | 2.44 | 0.45 |
| 1:AG:97:LYS:N | 1:AG:100:ALA:HB2 | 2.31 | 0.45 |
| 1:AG:55:ALA:HB1 | 1:AG:95:VAL:CG2 | 2.40 | 0.45 |
| 1:BR:52:VAL:CG1 | 1:BR:61:ILE:HD12 | 2.35 | 0.45 |
| 1:AD:18:VAL:HG23 | 1:AD:51:TRP:CE3 | 2.52 | 0.45 |
| 1:CC:7:LEU:CD2 | 1:CR:40:HIS:CE1 | 2.97 | 0.45 |
| 1:BD:75:ILE:HD13 | 1:BD:139:ALA:HA | 1.99 | 0.45 |
| 1:CI:18:VAL:HG11 | 1:CI:30:LEU:HD13 | 1.98 | 0.45 |
| 1:CX:18:VAL:HG23 | 1:CX:51:TRP:CE3 | 2.52 | 0.45 |
| 1:CC:82:ARG:NH1 | 1:CC:82:ARG:CG | 2.73 | 0.45 |
| 1:AA:58:ILE:HG21 | 1:AA:76:THR:OG1 | 2.17 | 0.45 |
| 1:CZ:58:ILE:HG21 | 1:CZ:76:THR:OG1 | 2.17 | 0.45 |
| 1:BP:58:ILE:O | 1:BP:62:ALA:CB | 2.64 | 0.45 |
| 1:AP:58:ILE:O | 1:AP:62:ALA:CB | 2.64 | 0.45 |
| 1:CX:149:SER:HB3 | 1:CX:152:TRP:CH2 | 2.52 | 0.45 |
| 1:CL:4:GLU:CG | 1:CM:51:TRP:HD1 | 2.29 | 0.45 |
| 1:CA:7:LEU:HD12 | 1:CA:7:LEU:HA | 1.84 | 0.45 |
| 1:AS:48:ASP:HB2 | 1:AS:71:TYR:CE1 | 2.50 | 0.45 |
| 1:CI:7:LEU:HD23 | 1:CO:40:HIS:CE1 | 2.52 | 0.45 |
| 1:B1:65:MET:HE3 | 1:B1:71:TYR:CZ | 2.52 | 0.45 |
| 1:C1:65:MET:HE3 | 1:C1:71:TYR:CZ | 2.51 | 0.45 |
| 1:BL:65:MET:HE3 | 1:BL:71:TYR:CE2 | 2.52 | 0.45 |
| 1:CG:70:LYS:O | 1:CG:70:LYS:HG2 | 2.17 | 0.45 |
| 1:AD:22:ASN:HA | 1:AR:128:GLY:O | 2.17 | 0.45 |
| 1:BD:34:LEU:O | 1:BD:38:LYS:HG3 | 2.17 | 0.45 |
| 1:AX:34:LEU:O | 1:AX:38:LYS:HG3 | 2.17 | 0.45 |
| 1:BW:83:GLY:HA3 | 2:BW:1001:PO4:O4 | 2.16 | 0.45 |
| 1:CN:34:LEU:O | 1:CN:38:LYS:HG3 | 2.17 | 0.45 |
| 1:BR:9:GLY:HA3 | 1:BR:12:LEU:HD12 | 1.97 | 0.45 |
| 1:AI:34:LEU:O | 1:AI:38:LYS:HG3 | 2.17 | 0.45 |
| 1:AF:65:MET:HE3 | 1:AF:71:TYR:CE2 | 2.52 | 0.45 |
| 1:CB:58:ILE:O | 1:CB:58:ILE:CG2 | 2.65 | 0.45 |
| 1:AQ:97:LYS:N | 1:AQ:100:ALA:HB2 | 2.31 | 0.45 |
| 1:CQ:97:LYS:N | 1:CQ:100:ALA:HB2 | 2.31 | 0.45 |
| 1:BG:58:ILE:CG2 | 1:BG:58:ILE:O | 2.65 | 0.45 |
| 1:BH:97:LYS:HE3 | 1:BI:97:LYS:NZ | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AS:75:ILE:HG22 | 1:AS:77:LEU:HD13 | 1.98 | 0.45 |
| 1:CN:18:VAL:HG23 | 1:CN:51:TRP:CE3 | 2.52 | 0.45 |
| 1:A3:18:VAL:HG23 | 1:A3:51:TRP:CE3 | 2.52 | 0.45 |
| 1:CD:18:VAL:HG23 | 1:CD:51:TRP:CE3 | 2.52 | 0.45 |
| 1:CC:34:LEU:HD22 | 1:CC:38:LYS:CE | 2.43 | 0.45 |
| 1:CU:58:ILE:HG21 | 1:CU:76:THR:OG1 | 2.17 | 0.45 |
| 1:AK:58:ILE:H | 1:AK:59:PRO:HD2 | 1.80 | 0.45 |
| 1:BU:7:LEU:HA | 1:BU:7:LEU:HD12 | 1.85 | 0.45 |
| 1:AX:149:SER:HB3 | 1:AX:152:TRP:CH2 | 2.52 | 0.45 |
| 1:AD:149:SER:HB3 | 1:AD:152:TRP:CH2 | 2.52 | 0.45 |
| 1:CW:108:ILE:O | 1:CW:110:VAL:HG23 | 2.17 | 0.45 |
| 1:AA:7:LEU:HD12 | 1:AA:7:LEU:HA | 1.84 | 0.45 |
| 1:CR:67:ASN:HD22 | 1:CR:67:ASN:HA | 1.60 | 0.45 |
| 1:BV:6:HIS:HB3 | 1:BV:147:HIS:CG | 2.52 | 0.45 |
| 1:BL:6:HIS:HB3 | 1:BL:147:HIS:CG | 2.52 | 0.45 |
| 1:C3:48:ASP:HB2 | 1:C3:71:TYR:CE1 | 2.50 | 0.45 |
| 1:BL:129:THR:CG2 | 1:BL:130:LYS:H | 2.28 | 0.45 |
| 1:BX:39:ARG:O | 1:B4:7:LEU:HB3 | 2.17 | 0.45 |
| 1:AS:9:GLY:HA2 | 1:AS:147:HIS:HE1 | 1.81 | 0.45 |
| 1:AI:9:GLY:HA2 | 1:AI:147:HIS:HE1 | 1.81 | 0.45 |
| 1:BM:104:LEU:HD13 | 1:BN:102:LEU:HG | 1.98 | 0.45 |
| 1:BH:104:LEU:HD13 | 1:BI:102:LEU:HG | 1.98 | 0.45 |
| 1:AM:104:LEU:HD13 | 1:AN:102:LEU:HG | 1.97 | 0.45 |
| 1:BG:70:LYS:O | 1:BG:70:LYS:HG2 | 2.17 | 0.45 |
| 1:AM:66:ALA:HB2 | 1:AM:74:VAL:HG21 | 1.99 | 0.45 |
| 1:A2:83:GLY:HA3 | 2:A2:1001:PO4:O4 | 2.16 | 0.45 |
| 1:CH:83:GLY:HA3 | 2:CH:2201:PO4:O4 | 2.16 | 0.45 |
| 1:BW:45:ASN:HA | 1:BW:45:ASN:HD22 | 1.64 | 0.45 |
| 1:CM:66:ALA:HB2 | 1:CM:74:VAL:HG21 | 1.99 | 0.45 |
| 1:AT:71:TYR:O | 1:AT:150:LYS:NZ | 2.44 | 0.44 |
| 1:AW:97:LYS:HE3 | 1:AX:97:LYS:NZ | 2.32 | 0.44 |
| 1:CC:97:LYS:HE3 | 1:CD:97:LYS:NZ | 2.32 | 0.44 |
| 1:AQ:55:ALA:HB1 | 1:AQ:95:VAL:CG2 | 2.40 | 0.44 |
| 1:B1:97:LYS:N | 1:B1:100:ALA:HB2 | 2.31 | 0.44 |
| 1:B1:100:ALA:CA | 1:B2:56:PHE:HZ | 2.28 | 0.44 |
| 1:A2:97:LYS:HE3 | 1:A3:97:LYS:NZ | 2.32 | 0.44 |
| 1:BN:18:VAL:HG11 | 1:BN:30:LEU:HD13 | 1.98 | 0.44 |
| 1:AD:75:ILE:HG22 | 1:AD:77:LEU:HD13 | 1.98 | 0.44 |
| 1:AS:18:VAL:HG11 | 1:AS:30:LEU:HD13 | 1.98 | 0.44 |
| 1:AS:18:VAL:HG23 | 1:AS:51:TRP:CE3 | 2.52 | 0.44 |
| 1:CW:38:LYS:HZ2 | 1:CW:44:GLU:HA | 1.81 | 0.44 |
| 1:BS:18:VAL:HG11 | 1:BS:30:LEU:HD13 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:AH:34:LEU:HD22 | 1:AH:38:LYS:CE | 2.43 | 0.44 |
| 1:AR:67:ASN:HD22 | 1:AR:67:ASN:HA | 1.59 | 0.44 |
| 1:BU:58:ILE:HG21 | 1:BU:76:THR:OG1 | 2.17 | 0.44 |
| 1:AK:58:ILE:HG21 | 1:AK:76:THR:OG1 | 2.17 | 0.44 |
| 1:CF:58:ILE:HG21 | 1:CF:76:THR:OG1 | 2.17 | 0.44 |
| 1:AW:108:ILE:O | 1:AW:110:VAL:HG23 | 2.17 | 0.44 |
| 1:CM:108:ILE:O | 1:CM:110:VAL:HG23 | 2.17 | 0.44 |
| 1:CN:121:GLU:O | 1:CN:125:GLU:HG3 | 2.18 | 0.44 |
| 1:AQ:6:HIS:HB3 | 1:AQ:147:HIS:CG | 2.52 | 0.44 |
| 1:CU:144:GLU:O | 1:CU:148:LEU:HB2 | 2.18 | 0.44 |
| 1:BB:9:GLY:HA3 | 1:BB:12:LEU:HD12 | 1.99 | 0.44 |
| 1:CL:9:GLY:HA3 | 1:CL:12:LEU:HD12 | 1.99 | 0.44 |
| 1:CV:70:LYS:O | 1:CV:70:LYS:HG2 | 2.17 | 0.44 |
| 1:BL:9:GLY:HA3 | 1:BL:12:LEU:HD12 | 1.99 | 0.44 |
| 1:BC:9:GLY:HA3 | 1:BC:12:LEU:HD12 | 1.98 | 0.44 |
| 1:BM:9:GLY:HA3 | 1:BM:12:LEU:HD12 | 1.97 | 0.44 |
| 1:BH:66:ALA:HB2 | 1:BH:74:VAL:HG21 | 1.99 | 0.44 |
| 1:AW:66:ALA:HB2 | 1:AW:74:VAL:HG21 | 1.99 | 0.44 |
| 1:B3:34:LEU:O | 1:B3:38:LYS:HG3 | 2.17 | 0.44 |
| 1:AU:65:MET:HE3 | 1:AU:71:TYR:CE2 | 2.52 | 0.44 |
| 1:C3:34:LEU:O | 1:C3:38:LYS:HG3 | 2.17 | 0.44 |
| 1:BM:83:GLY:HA3 | 2:BM:1001:PO4:O4 | 2.16 | 0.44 |
| 1:AC:9:GLY:HA3 | 1:AC:12:LEU:HD12 | 1.98 | 0.44 |
| 1:CJ:109:PRO:HG3 | 1:CJ:149:SER:CB | 2.46 | 0.44 |
| 1:B4:109:PRO:HG3 | 1:B4:149:SER:CB | 2.46 | 0.44 |
| 1:BC:97:LYS:HE3 | 1:BD:97:LYS:HZ3 | 1.82 | 0.44 |
| 1:AV:58:ILE:O | 1:AV:58:ILE:CG2 | 2.65 | 0.44 |
| 1:BL:97:LYS:N | 1:BL:100:ALA:HB2 | 2.31 | 0.44 |
| 1:AL:58:ILE:O | 1:AL:58:ILE:CG2 | 2.65 | 0.44 |
| 1:B2:97:LYS:HE3 | 1:B3:97:LYS:NZ | 2.32 | 0.44 |
| 1:BN:75:ILE:HD13 | 1:BN:139:ALA:HA | 1.99 | 0.44 |
| 1:AX:18:VAL:HG11 | 1:AX:30:LEU:HD13 | 1.98 | 0.44 |
| 1:BC:82:ARG:HG3 | 1:BC:118:GLU:OE2 | 2.18 | 0.44 |
| 1:CW:82:ARG:HG3 | 1:CW:118:GLU:OE2 | 2.17 | 0.44 |
| 1:CC:82:ARG:HG3 | 1:CC:118:GLU:OE2 | 2.17 | 0.44 |
| 1:AM:82:ARG:HG3 | 1:AM:118:GLU:OE2 | 2.17 | 0.44 |
| 1:AU:58:ILE:H | 1:AU:59:PRO:HD2 | 1.80 | 0.44 |
| 1:AU:58:ILE:O | 1:AU:62:ALA:HB2 | 2.17 | 0.44 |
| 1:AZ:58:ILE:O | 1:AZ:62:ALA:HB2 | 2.18 | 0.44 |
| 1:CU:58:ILE:O | 1:CU:62:ALA:HB2 | 2.18 | 0.44 |
| 1:CA:58:ILE:HG21 | 1:CA:76:THR:OG1 | 2.17 | 0.44 |
| 1:CF:58:ILE:O | 1:CF:62:ALA:HB2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BK:58:ILE:O | 1:BK:62:ALA:HB2 | 2.18 | 0.44 |
| 1:CH:108:ILE:O | 1:CH:110:VAL:HG23 | 2.17 | 0.44 |
| 1:B1:6:HIS:HB3 | 1:B1:147:HIS:CG | 2.52 | 0.44 |
| 1:BK:144:GLU:O | 1:BK:148:LEU:HB2 | 2.18 | 0.44 |
| 1:AP:144:GLU:O | 1:AP:148:LEU:HB2 | 2.18 | 0.44 |
| 1:CB:6:HIS:HB3 | 1:CB:147:HIS:CG | 2.52 | 0.44 |
| 1:CF:144:GLU:O | 1:CF:148:LEU:HB2 | 2.17 | 0.44 |
| 1:CV:6:HIS:HB3 | 1:CV:147:HIS:CG | 2.52 | 0.44 |
| 1:A1:6:HIS:HB3 | 1:A1:147:HIS:CG | 2.52 | 0.44 |
| 1:AI:28:LYS:NZ | 1:AK:28:LYS:HZ2 | 2.15 | 0.44 |
| 1:BI:9:GLY:HA2 | 1:BI:147:HIS:HE1 | 1.81 | 0.44 |
| 1:CH:24:PHE:CD1 | 1:CU:28:LYS:HD2 | 2.52 | 0.44 |
| 1:AG:70:LYS:O | 1:AG:70:LYS:HG2 | 2.17 | 0.44 |
| 1:AV:70:LYS:HG2 | 1:AV:70:LYS:O | 2.17 | 0.44 |
| 1:BN:34:LEU:O | 1:BN:38:LYS:HG3 | 2.17 | 0.44 |
| 1:AW:83:GLY:HA3 | 2:AW:201:PO4:O4 | 2.16 | 0.44 |
| 1:AM:83:GLY:HA3 | 2:AM:1001:PO4:O4 | 2.16 | 0.44 |
| 1:AR:97:LYS:HE3 | 1:AS:97:LYS:NZ | 2.32 | 0.44 |
| 1:AB:55:ALA:CB | 1:AB:95:VAL:HG21 | 2.40 | 0.44 |
| 1:CM:97:LYS:HE3 | 1:CN:97:LYS:NZ | 2.32 | 0.44 |
| 1:AX:75:ILE:HD13 | 1:AX:139:ALA:HA | 1.99 | 0.44 |
| 1:CI:18:VAL:HG23 | 1:CI:51:TRP:CE3 | 2.52 | 0.44 |
| 1:AH:82:ARG:HG3 | 1:AH:118:GLU:OE2 | 2.17 | 0.44 |
| 1:A3:75:ILE:HD13 | 1:A3:139:ALA:HA | 1.99 | 0.44 |
| 1:CM:82:ARG:HG3 | 1:CM:118:GLU:OE2 | 2.18 | 0.44 |
| 1:AS:149:SER:HB3 | 1:AS:152:TRP:CH2 | 2.52 | 0.44 |
| 1:C1:4:GLU:CG | 1:C2:51:TRP:HD1 | 2.29 | 0.44 |
| 1:BI:121:GLU:O | 1:BI:125:GLU:HG3 | 2.18 | 0.44 |
| 1:A3:121:GLU:O | 1:A3:125:GLU:HG3 | 2.18 | 0.44 |
| 1:AN:121:GLU:O | 1:AN:125:GLU:HG3 | 2.17 | 0.44 |
| 1:B3:121:GLU:O | 1:B3:125:GLU:HG3 | 2.18 | 0.44 |
| 1:AD:121:GLU:O | 1:AD:125:GLU:HG3 | 2.18 | 0.44 |
| 1:BC:67:ASN:HA | 1:BC:67:ASN:HD22 | 1.59 | 0.44 |
| 1:AZ:144:GLU:O | 1:AZ:148:LEU:HB2 | 2.18 | 0.44 |
| 1:CQ:6:HIS:HB3 | 1:CQ:147:HIS:CG | 2.52 | 0.44 |
| 1:CU:98:GLY:O | 1:CU:102:LEU:HB2 | 2.18 | 0.44 |
| 1:BS:9:GLY:HA2 | 1:BS:147:HIS:HE1 | 1.81 | 0.44 |
| 1:BQ:9:GLY:HA3 | 1:BQ:12:LEU:HD12 | 1.99 | 0.44 |
| 1:AW:104:LEU:HD13 | 1:AX:102:LEU:HG | 1.98 | 0.44 |
| 1:BR:104:LEU:HD13 | 1:BS:102:LEU:HG | 1.98 | 0.44 |
| 1:BV:65:MET:HE3 | 1:BV:71:TYR:CZ | 2.52 | 0.44 |
| 1:CH:104:LEU:CD2 | 1:CI:60:LEU:HA | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A1:70:LYS:HG2 | 1:A1:70:LYS:O | 2.17 | 0.44 |
| 1:BR:66:ALA:HB2 | 1:BR:74:VAL:HG21 | 1.99 | 0.44 |
| 1:A4:88:TYR:CD2 | 1:A4:88:TYR:C | 2.91 | 0.44 |
| 1:CQ:58:ILE:CG2 | 1:CQ:58:ILE:O | 2.65 | 0.44 |
| 1:CG:7:LEU:HD23 | 1:CU:40:HIS:CE1 | 2.52 | 0.44 |
| 1:AD:75:ILE:HD13 | 1:AD:139:ALA:HA | 1.99 | 0.44 |
| 1:BI:18:VAL:HG23 | 1:BI:51:TRP:CE3 | 2.52 | 0.44 |
| 1:CD:75:ILE:HD13 | 1:CD:139:ALA:HA | 1.99 | 0.44 |
| 1:AA:58:ILE:O | 1:AA:62:ALA:HB2 | 2.18 | 0.44 |
| 1:B2:82:ARG:HG3 | 1:B2:118:GLU:OE2 | 2.18 | 0.44 |
| 1:A2:67:ASN:HA | 1:A2:67:ASN:HD22 | 1.59 | 0.44 |
| 1:BU:58:ILE:O | 1:BU:62:ALA:HB2 | 2.18 | 0.44 |
| 1:BF:58:ILE:O | 1:BF:62:ALA:HB2 | 2.18 | 0.44 |
| 1:BX:149:SER:HB3 | 1:BX:152:TRP:CH2 | 2.52 | 0.44 |
| 1:CC:108:ILE:O | 1:CC:110:VAL:HG23 | 2.17 | 0.44 |
| 1:CC:8:VAL:CG2 | 1:CR:8:VAL:HG13 | 2.48 | 0.44 |
| 1:C1:6:HIS:HB3 | 1:C1:147:HIS:CG | 2.52 | 0.44 |
| 1:B1:129:THR:HG22 | 1:B1:130:LYS:N | 2.33 | 0.44 |
| 1:AG:9:GLY:HA3 | 1:AG:12:LEU:HD12 | 1.99 | 0.44 |
| 1:BH:104:LEU:CD2 | 1:BI:60:LEU:HA | 2.48 | 0.44 |
| 1:BB:70:LYS:HG2 | 1:BB:70:LYS:O | 2.17 | 0.44 |
| 1:CS:34:LEU:O | 1:CS:38:LYS:HG3 | 2.17 | 0.44 |
| 1:AY:88:TYR:CD2 | 1:AY:88:TYR:C | 2.91 | 0.44 |
| 1:BN:148:LEU:HD23 | 1:BN:148:LEU:HA | 1.82 | 0.44 |
| 1:AT:88:TYR:CD2 | 1:AT:88:TYR:C | 2.91 | 0.44 |
| 1:B2:66:ALA:HB2 | 1:B2:74:VAL:HG21 | 1.99 | 0.44 |
| 1:C4:109:PRO:HG3 | 1:C4:149:SER:CB | 2.46 | 0.44 |
| 1:AV:97:LYS:N | 1:AV:100:ALA:HB2 | 2.31 | 0.44 |
| 1:BM:97:LYS:HE3 | 1:BN:97:LYS:NZ | 2.32 | 0.44 |
| 1:C1:55:ALA:CB | 1:C1:95:VAL:HG21 | 2.40 | 0.44 |
| 1:AB:58:ILE:CG2 | 1:AB:58:ILE:O | 2.65 | 0.44 |
| 1:BR:97:LYS:HE3 | 1:BS:97:LYS:NZ | 2.32 | 0.44 |
| 1:B3:75:ILE:HD13 | 1:B3:139:ALA:HA | 1.99 | 0.44 |
| 1:BI:75:ILE:HD13 | 1:BI:139:ALA:HA | 1.99 | 0.44 |
| 1:BW:82:ARG:HG3 | 1:BW:118:GLU:OE2 | 2.18 | 0.44 |
| 1:CH:82:ARG:HG3 | 1:CH:118:GLU:OE2 | 2.17 | 0.44 |
| 1:BA:58:ILE:H | 1:BA:59:PRO:HD2 | 1.80 | 0.44 |
| 1:BK:58:ILE:HG21 | 1:BK:76:THR:OG1 | 2.17 | 0.44 |
| 1:CP:58:ILE:HG21 | 1:CP:76:THR:OG1 | 2.17 | 0.44 |
| 1:AF:58:ILE:HG21 | 1:AF:76:THR:OG1 | 2.17 | 0.44 |
| 1:A3:149:SER:HB3 | 1:A3:152:TRP:CH2 | 2.52 | 0.44 |
| 1:AO:64:LYS:HA | 1:AO:64:LYS:HD3 | 1.85 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:BS:121:GLU:O | 1:BS:125:GLU:HG3 | 2.18 | 0.44 |
| 1:AK:144:GLU:O | 1:AK:148:LEU:HB2 | 2.17 | 0.44 |
| 1:AB:6:HIS:HB3 | 1:AB:147:HIS:CG | 2.52 | 0.44 |
| 1:BA:144:GLU:O | 1:BA:148:LEU:HB2 | 2.18 | 0.44 |
| 1:AU:98:GLY:O | 1:AU:102:LEU:HB2 | 2.18 | 0.44 |
| 1:CV:129:THR:HG22 | 1:CV:130:LYS:N | 2.33 | 0.44 |
| 1:A1:9:GLY:HA3 | 1:A1:12:LEU:HD12 | 1.99 | 0.44 |
| 1:BC:104:LEU:CD2 | 1:BD:60:LEU:HA | 2.48 | 0.44 |
| 1:C2:104:LEU:CD2 | 1:C3:60:LEU:HA | 2.48 | 0.44 |
| 1:BR:83:GLY:HA3 | 2:BR:1001:PO4:O4 | 2.16 | 0.44 |
| 1:AJ:88:TYR:C | 1:AJ:88:TYR:CD2 | 2.91 | 0.44 |
| 1:BC:66:ALA:HB2 | 1:BC:74:VAL:HG21 | 1.99 | 0.44 |
| 1:BU:90:TYR:O | 1:BU:94:GLU:HG2 | 2.18 | 0.44 |
| 1:BE:109:PRO:HG3 | 1:BE:149:SER:CB | 2.46 | 0.44 |
| 1:AY:109:PRO:HG3 | 1:AY:149:SER:CB | 2.46 | 0.44 |
| 1:B1:58:ILE:O | 1:B1:58:ILE:CG2 | 2.65 | 0.44 |
| 1:CL:96:ALA:O | 1:CL:100:ALA:HB2 | 2.06 | 0.44 |
| 1:CH:97:LYS:HE3 | 1:CI:97:LYS:NZ | 2.32 | 0.44 |
| 1:CS:75:ILE:HD13 | 1:CS:139:ALA:HA | 1.99 | 0.44 |
| 1:CS:18:VAL:HG23 | 1:CS:51:TRP:CE3 | 2.52 | 0.44 |
| 1:CR:82:ARG:HG3 | 1:CR:118:GLU:OE2 | 2.17 | 0.44 |
| 1:BZ:58:ILE:H | 1:BZ:59:PRO:HD2 | 1.80 | 0.44 |
| 1:CP:58:ILE:O | 1:CP:62:ALA:HB2 | 2.18 | 0.44 |
| 1:AF:58:ILE:O | 1:AF:62:ALA:HB2 | 2.18 | 0.44 |
| 1:AO:45:ASN:C | 1:AO:47:ILE:H | 2.21 | 0.44 |
| 1:BX:17:VAL:HG13 | 1:BX:65:MET:CE | 2.48 | 0.44 |
| 1:BY:45:ASN:C | 1:BY:47:ILE:H | 2.21 | 0.44 |
| 1:CY:106:THR:O | 1:CY:107:ASP:OD1 | 2.36 | 0.44 |
| 1:C3:121:GLU:O | 1:C3:125:GLU:HG3 | 2.18 | 0.44 |
| 1:AX:121:GLU:O | 1:AX:125:GLU:HG3 | 2.18 | 0.44 |
| 1:CA:144:GLU:O | 1:CA:148:LEU:HB2 | 2.18 | 0.44 |
| 1:CG:6:HIS:HB3 | 1:CG:147:HIS:CG | 2.52 | 0.44 |
| 1:BZ:98:GLY:O | 1:BZ:102:LEU:HB2 | 2.18 | 0.44 |
| 1:CP:98:GLY:O | 1:CP:102:LEU:HB2 | 2.18 | 0.44 |
| 1:CK:98:GLY:O | 1:CK:102:LEU:HB2 | 2.18 | 0.44 |
| 1:AP:98:GLY:O | 1:AP:102:LEU:HB2 | 2.18 | 0.44 |
| 1:AZ:98:GLY:O | 1:AZ:102:LEU:HB2 | 2.18 | 0.44 |
| 1:BL:129:THR:HG22 | 1:BL:130:LYS:N | 2.33 | 0.44 |
| 1:BG:129:THR:CG2 | 1:BG:130:LYS:H | 2.28 | 0.44 |
| 1:CS:9:GLY:HA2 | 1:CS:147:HIS:HE1 | 1.81 | 0.44 |
| 1:BC:28:LYS:NZ | 1:BU:28:LYS:CE | 2.81 | 0.44 |
| 1:AW:104:LEU:CD2 | 1:AX:60:LEU:HA | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CG:9:GLY:HA3 | 1:CG:12:LEU:HD12 | 1.99 | 0.44 |
| 1:CR:104:LEU:CD2 | 1:CS:60:LEU:HA | 2.48 | 0.44 |
| 1:BF:90:TYR:O | 1:BF:94:GLU:HG2 | 2.18 | 0.44 |
| 1:AO:88:TYR:C | 1:AO:88:TYR:CD2 | 2.91 | 0.44 |
| 1:CD:34:LEU:O | 1:CD:38:LYS:HG3 | 2.17 | 0.44 |
| 1:CD:58:ILE:HB | 1:CD:59:PRO:HD3 | 2.00 | 0.44 |
| 1:BL:104:LEU:HD23 | 1:BM:60:LEU:HD13 | 2.00 | 0.44 |
| 1:BG:104:LEU:HD23 | 1:BH:60:LEU:HD13 | 2.00 | 0.44 |
| 1:CT:109:PRO:HG3 | 1:CT:149:SER:CB | 2.46 | 0.44 |
| 1:BB:58:ILE:O | 1:BB:58:ILE:CG2 | 2.65 | 0.44 |
| 1:CQ:97:LYS:HE3 | 1:CR:97:LYS:HZ3 | 1.83 | 0.44 |
| 1:CW:97:LYS:HE3 | 1:CX:97:LYS:NZ | 2.32 | 0.44 |
| 1:AR:52:VAL:CG1 | 1:AR:61:ILE:HD12 | 2.35 | 0.44 |
| 1:CS:18:VAL:HG11 | 1:CS:30:LEU:HD13 | 1.98 | 0.44 |
| 1:AN:75:ILE:HD13 | 1:AN:139:ALA:HA | 1.99 | 0.44 |
| 1:CI:149:SER:HB3 | 1:CI:152:TRP:CH2 | 2.52 | 0.44 |
| 1:BD:17:VAL:HG13 | 1:BD:65:MET:CE | 2.48 | 0.44 |
| 1:AC:108:ILE:O | 1:AC:110:VAL:HG23 | 2.17 | 0.44 |
| 1:A3:17:VAL:HG13 | 1:A3:65:MET:CE | 2.48 | 0.44 |
| 1:C4:45:ASN:C | 1:C4:47:ILE:H | 2.21 | 0.44 |
| 1:AY:45:ASN:C | 1:AY:47:ILE:H | 2.21 | 0.44 |
| 1:CX:121:GLU:O | 1:CX:125:GLU:HG3 | 2.18 | 0.44 |
| 1:C4:106:THR:O | 1:C4:107:ASP:OD1 | 2.36 | 0.44 |
| 1:CS:121:GLU:O | 1:CS:125:GLU:HG3 | 2.18 | 0.44 |
| 1:BP:98:GLY:O | 1:BP:102:LEU:HB2 | 2.18 | 0.44 |
| 1:AA:98:GLY:O | 1:AA:102:LEU:HB2 | 2.18 | 0.44 |
| 1:BU:98:GLY:O | 1:BU:102:LEU:HB2 | 2.18 | 0.44 |
| 1:BF:98:GLY:O | 1:BF:102:LEU:HB2 | 2.18 | 0.44 |
| 1:CQ:129:THR:HG22 | 1:CQ:130:LYS:N | 2.33 | 0.44 |
| 1:BV:9:GLY:HA3 | 1:BV:12:LEU:HD12 | 1.99 | 0.44 |
| 1:AQ:9:GLY:HA3 | 1:AQ:12:LEU:HD12 | 1.99 | 0.44 |
| 1:AL:70:LYS:HG2 | 1:AL:70:LYS:O | 2.17 | 0.44 |
| 1:A2:104:LEU:CD2 | 1:A3:60:LEU:HA | 2.48 | 0.44 |
| 1:C1:70:LYS:HG2 | 1:C1:70:LYS:O | 2.17 | 0.44 |
| 1:BV:70:LYS:O | 1:BV:70:LYS:HG2 | 2.17 | 0.44 |
| 1:B1:70:LYS:O | 1:B1:70:LYS:HG2 | 2.17 | 0.44 |
| 1:BZ:65:MET:HE3 | 1:BZ:71:TYR:CE2 | 2.53 | 0.44 |
| 1:AA:90:TYR:O | 1:AA:94:GLU:HG2 | 2.18 | 0.44 |
| 1:CJ:88:TYR:C | 1:CJ:88:TYR:CD2 | 2.91 | 0.44 |
| 1:CI:148:LEU:HA | 1:CI:148:LEU:HD23 | 1.82 | 0.44 |
| 1:BY:88:TYR:C | 1:BY:88:TYR:CD2 | 2.91 | 0.44 |
| 1:C4:88:TYR:CD2 | 1:C4:88:TYR:C | 2.91 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:CW:148:LEU:HD23 | 1:CW:148:LEU:HA | 1.80 | 0.44 |
| 1:CN:150:LYS:HG3 | 1:CN:150:LYS:H | 1.33 | 0.44 |
| 1:AK:90:TYR:O | 1:AK:94:GLU:HG2 | 2.18 | 0.44 |
| 1:C1:104:LEU:HD23 | 1:C2:60:LEU:HD13 | 2.00 | 0.44 |
| 1:CT:71:TYR:C | 1:CT:150:LYS:HZ3 | 2.19 | 0.44 |
| 1:CR:97:LYS:HE3 | 1:CS:97:LYS:NZ | 2.32 | 0.44 |
| 1:CV:55:ALA:HB1 | 1:CV:95:VAL:CG2 | 2.40 | 0.44 |
| 1:CI:75:ILE:HD13 | 1:CI:139:ALA:HA | 1.99 | 0.44 |
| 1:AR:82:ARG:HG3 | 1:AR:118:GLU:OE2 | 2.18 | 0.44 |
| 1:CK:58:ILE:O | 1:CK:62:ALA:HB2 | 2.18 | 0.44 |
| 1:BZ:58:ILE:O | 1:BZ:62:ALA:HB2 | 2.18 | 0.44 |
| 1:AK:58:ILE:O | 1:AK:62:ALA:HB2 | 2.18 | 0.44 |
| 1:AP:58:ILE:HG21 | 1:AP:76:THR:OG1 | 2.17 | 0.44 |
| 1:B3:17:VAL:HG13 | 1:B3:65:MET:CE | 2.48 | 0.44 |
| 1:BJ:45:ASN:C | 1:BJ:47:ILE:H | 2.21 | 0.44 |
| 1:BT:106:THR:O | 1:BT:107:ASP:OD1 | 2.36 | 0.44 |
| 1:CJ:106:THR:O | 1:CJ:107:ASP:OD1 | 2.36 | 0.44 |
| 1:CD:121:GLU:O | 1:CD:125:GLU:HG3 | 2.17 | 0.44 |
| 1:AA:144:GLU:O | 1:AA:148:LEU:HB2 | 2.18 | 0.44 |
| 1:AD:7:LEU:HD23 | 1:AJ:40:HIS:CE1 | 2.53 | 0.44 |
| 1:AB:129:THR:HG22 | 1:AB:130:LYS:N | 2.33 | 0.44 |
| 1:AL:9:GLY:HA3 | 1:AL:12:LEU:HD12 | 1.99 | 0.44 |
| 1:BR:104:LEU:CD2 | 1:BS:60:LEU:HA | 2.48 | 0.44 |
| 1:BL:65:MET:HE3 | 1:BL:71:TYR:CZ | 2.52 | 0.44 |
| 1:AH:66:ALA:HB2 | 1:AH:74:VAL:HG21 | 1.99 | 0.44 |
| 1:BS:34:LEU:O | 1:BS:38:LYS:HG3 | 2.17 | 0.44 |
| 1:A3:34:LEU:O | 1:A3:38:LYS:HG3 | 2.17 | 0.44 |
| 1:CM:45:ASN:HD22 | 1:CM:45:ASN:HA | 1.63 | 0.44 |
| 1:CR:45:ASN:HD22 | 1:CR:45:ASN:HA | 1.63 | 0.44 |
| 1:BN:58:ILE:HB | 1:BN:59:PRO:HD3 | 2.00 | 0.44 |
| 1:CC:66:ALA:HB2 | 1:CC:74:VAL:HG21 | 1.99 | 0.44 |
| 1:CX:34:LEU:O | 1:CX:38:LYS:HG3 | 2.17 | 0.44 |
| 1:BI:34:LEU:O | 1:BI:38:LYS:HG3 | 2.17 | 0.44 |
| 1:BV:104:LEU:HD23 | 1:BW:60:LEU:HD13 | 2.00 | 0.44 |
| 1:BC:97:LYS:HE3 | 1:BD:97:LYS:NZ | 2.32 | 0.44 |
| 1:BQ:58:ILE:O | 1:BQ:58:ILE:CG2 | 2.65 | 0.44 |
| 1:CG:100:ALA:CA | 1:CH:56:PHE:HZ | 2.28 | 0.44 |
| 1:A1:97:LYS:HA | 1:A1:100:ALA:HB3 | 2.00 | 0.44 |
| 1:A2:52:VAL:CG1 | 1:A2:61:ILE:HD12 | 2.35 | 0.44 |
| 1:B3:18:VAL:HG23 | 1:B3:51:TRP:CE3 | 2.52 | 0.44 |
| 1:CX:75:ILE:HD13 | 1:CX:139:ALA:HA | 1.99 | 0.44 |
| 1:BS:75:ILE:HD13 | 1:BS:139:ALA:HA | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A2:82:ARG:HG3 | 1:A2:118:GLU:OE2 | 2.18 | 0.44 |
| 1:AW:65:MET:HE2 | 1:AW:65:MET:HB3 | 1.79 | 0.44 |
| 1:BA:58:ILE:O | 1:BA:62:ALA:HB2 | 2.18 | 0.44 |
| 1:AP:58:ILE:H | 1:AP:59:PRO:HD2 | 1.80 | 0.44 |
| 1:AP:58:ILE:O | 1:AP:62:ALA:HB2 | 2.18 | 0.44 |
| 1:CS:149:SER:HB3 | 1:CS:152:TRP:CH2 | 2.52 | 0.44 |
| 1:AT:45:ASN:C | 1:AT:47:ILE:H | 2.21 | 0.44 |
| 1:CD:17:VAL:HG13 | 1:CD:65:MET:CE | 2.48 | 0.44 |
| 1:AS:17:VAL:HG13 | 1:AS:65:MET:CE | 2.48 | 0.44 |
| 1:BN:17:VAL:HG13 | 1:BN:65:MET:CE | 2.48 | 0.44 |
| 1:BE:106:THR:O | 1:BE:107:ASP:OD1 | 2.36 | 0.44 |
| 1:AY:106:THR:O | 1:AY:107:ASP:OD1 | 2.36 | 0.44 |
| 1:BP:144:GLU:O | 1:BP:148:LEU:HB2 | 2.18 | 0.44 |
| 1:AG:129:THR:HG22 | 1:AG:130:LYS:N | 2.33 | 0.44 |
| 1:B1:65:MET:HE3 | 1:B1:71:TYR:CE2 | 2.53 | 0.44 |
| 1:CV:13:LYS:HG2 | 1:CV:70:LYS:O | 2.18 | 0.44 |
| 1:B2:104:LEU:CD2 | 1:B3:60:LEU:HA | 2.48 | 0.44 |
| 1:CB:13:LYS:HG2 | 1:CB:70:LYS:O | 2.18 | 0.44 |
| 1:CQ:13:LYS:HG2 | 1:CQ:70:LYS:O | 2.18 | 0.44 |
| 1:CI:34:LEU:O | 1:CI:38:LYS:HG3 | 2.17 | 0.44 |
| 1:AP:90:TYR:O | 1:AP:94:GLU:HG2 | 2.18 | 0.44 |
| 1:BP:90:TYR:O | 1:BP:94:GLU:HG2 | 2.18 | 0.44 |
| 1:AD:58:ILE:HB | 1:AD:59:PRO:HD3 | 2.00 | 0.44 |
| 1:A3:58:ILE:HB | 1:A3:59:PRO:HD3 | 2.00 | 0.44 |
| 1:AZ:51:TRP:O | 1:A4:148:LEU:HD11 | 2.18 | 0.44 |
| 1:AS:34:LEU:O | 1:AS:38:LYS:HG3 | 2.17 | 0.44 |
| 1:AF:90:TYR:O | 1:AF:94:GLU:HG2 | 2.18 | 0.44 |
| 1:AQ:13:LYS:HG2 | 1:AQ:70:LYS:O | 2.18 | 0.43 |
| 1:AO:108:ILE:CG1 | 1:AO:150:LYS:HE3 | 2.42 | 0.43 |
| 1:CQ:104:LEU:HD23 | 1:CR:60:LEU:HD13 | 2.00 | 0.43 |
| 1:AH:97:LYS:HE3 | 1:AI:97:LYS:NZ | 2.32 | 0.43 |
| 1:AM:97:LYS:HE3 | 1:AN:97:LYS:NZ | 2.32 | 0.43 |
| 1:BV:97:LYS:HA | 1:BV:100:ALA:HB3 | 2.00 | 0.43 |
| 1:CN:75:ILE:HD13 | 1:CN:139:ALA:HA | 1.99 | 0.43 |
| 1:BC:82:ARG:NH1 | 1:BC:82:ARG:CG | 2.73 | 0.43 |
| 1:CA:58:ILE:O | 1:CA:62:ALA:HB2 | 2.18 | 0.43 |
| 1:BK:58:ILE:H | 1:BK:59:PRO:HD2 | 1.80 | 0.43 |
| 1:BD:149:SER:HB3 | 1:BD:152:TRP:CH2 | 2.52 | 0.43 |
| 1:CI:17:VAL:HG13 | 1:CI:65:MET:CE | 2.48 | 0.43 |
| 1:CE:106:THR:O | 1:CE:107:ASP:OD1 | 2.36 | 0.43 |
| 1:BY:106:THR:O | 1:BY:107:ASP:C | 2.57 | 0.43 |
| 1:BD:121:GLU:O | 1:BD:125:GLU:HG3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BX:121:GLU:O | 1:BX:125:GLU:HG3 | 2.18 | 0.43 |
| 1:CK:144:GLU:O | 1:CK:148:LEU:HB2 | 2.18 | 0.43 |
| 1:BZ:144:GLU:O | 1:BZ:148:LEU:HB2 | 2.18 | 0.43 |
| 1:AF:144:GLU:O | 1:AF:148:LEU:HB2 | 2.18 | 0.43 |
| 1:CZ:98:GLY:O | 1:CZ:102:LEU:HB2 | 2.18 | 0.43 |
| 1:BK:98:GLY:O | 1:BK:102:LEU:HB2 | 2.18 | 0.43 |
| 1:A1:129:THR:HG22 | 1:A1:130:LYS:N | 2.33 | 0.43 |
| 1:AQ:129:THR:HG22 | 1:AQ:130:LYS:N | 2.33 | 0.43 |
| 1:C1:9:GLY:HA3 | 1:C1:12:LEU:HD12 | 1.99 | 0.43 |
| 1:CB:70:LYS:O | 1:CB:70:LYS:HG2 | 2.16 | 0.43 |
| 1:AV:13:LYS:HG2 | 1:AV:70:LYS:O | 2.18 | 0.43 |
| 1:BY:90:TYR:O | 1:BY:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BZ:90:TYR:O | 1:BZ:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BJ:88:TYR:CD2 | 1:BJ:88:TYR:C | 2.91 | 0.43 |
| 1:CP:51:TRP:O | 1:CT:148:LEU:HD11 | 2.18 | 0.43 |
| 1:CX:58:ILE:HB | 1:CX:59:PRO:HD3 | 2.00 | 0.43 |
| 1:CU:90:TYR:O | 1:CU:94:GLU:HG2 | 2.18 | 0.43 |
| 1:A1:104:LEU:HD23 | 1:A2:60:LEU:HD13 | 2.00 | 0.43 |
| 1:CG:104:LEU:HD23 | 1:CH:60:LEU:HD13 | 2.00 | 0.43 |
| 1:CO:65:MET:HE3 | 1:CO:71:TYR:CE2 | 2.53 | 0.43 |
| 1:BB:100:ALA:CA | 1:BC:56:PHE:HZ | 2.28 | 0.43 |
| 1:AG:100:ALA:CA | 1:AH:56:PHE:HZ | 2.28 | 0.43 |
| 1:CG:55:ALA:HB1 | 1:CG:95:VAL:CG2 | 2.40 | 0.43 |
| 1:CG:58:ILE:CG2 | 1:CG:58:ILE:O | 2.65 | 0.43 |
| 1:C2:82:ARG:HG3 | 1:C2:118:GLU:OE2 | 2.18 | 0.43 |
| 1:CC:67:ASN:HA | 1:CC:67:ASN:HD22 | 1.59 | 0.43 |
| 1:BM:108:ILE:O | 1:BM:110:VAL:HG23 | 2.17 | 0.43 |
| 1:CY:15:GLY:O | 1:CY:74:VAL:HA | 2.18 | 0.43 |
| 1:BI:17:VAL:HG13 | 1:BI:65:MET:CE | 2.48 | 0.43 |
| 1:AJ:106:THR:O | 1:AJ:107:ASP:OD1 | 2.36 | 0.43 |
| 1:AI:121:GLU:O | 1:AI:125:GLU:HG3 | 2.18 | 0.43 |
| 1:CZ:144:GLU:O | 1:CZ:148:LEU:HB2 | 2.18 | 0.43 |
| 1:CA:98:GLY:O | 1:CA:102:LEU:HB2 | 2.18 | 0.43 |
| 1:CB:129:THR:CG2 | 1:CB:130:LYS:H | 2.28 | 0.43 |
| 1:BG:129:THR:HG22 | 1:BG:130:LYS:N | 2.33 | 0.43 |
| 1:BF:28:LYS:HD2 | 1:BR:24:PHE:CE1 | 2.53 | 0.43 |
| 1:BM:104:LEU:CD2 | 1:BN:60:LEU:HA | 2.48 | 0.43 |
| 1:BW:104:LEU:CD2 | 1:BX:60:LEU:HA | 2.48 | 0.43 |
| 1:AB:70:LYS:HG2 | 1:AB:70:LYS:O | 2.17 | 0.43 |
| 1:CL:13:LYS:HG2 | 1:CL:70:LYS:O | 2.18 | 0.43 |
| 1:B1:13:LYS:HG2 | 1:B1:70:LYS:O | 2.18 | 0.43 |
| 1:BI:58:ILE:HB | 1:BI:59:PRO:HD3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B4:90:TYR:O | 1:B4:94:GLU:HG2 | 2.18 | 0.43 |
| 1:CE:90:TYR:O | 1:CE:94:GLU:HG2 | 2.18 | 0.43 |
| 1:CF:90:TYR:O | 1:CF:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BE:88:TYR:CD2 | 1:BE:88:TYR:C | 2.91 | 0.43 |
| 1:BK:90:TYR:O | 1:BK:94:GLU:HG2 | 2.18 | 0.43 |
| 1:CZ:90:TYR:O | 1:CZ:94:GLU:HG2 | 2.18 | 0.43 |
| 1:C2:66:ALA:HB2 | 1:C2:74:VAL:HG21 | 1.99 | 0.43 |
| 1:CU:65:MET:HE3 | 1:CU:71:TYR:CE2 | 2.53 | 0.43 |
| 1:AE:90:TYR:O | 1:AE:94:GLU:HG2 | 2.18 | 0.43 |
| 1:AI:58:ILE:HB | 1:AI:59:PRO:HD3 | 2.00 | 0.43 |
| 1:A2:125:GLU:HA | 1:A2:129:THR:HB | 2.01 | 0.43 |
| 1:CL:104:LEU:HD23 | 1:CM:60:LEU:HD13 | 2.00 | 0.43 |
| 1:CG:97:LYS:N | 1:CG:100:ALA:HB2 | 2.31 | 0.43 |
| 1:CV:58:ILE:CG2 | 1:CV:58:ILE:O | 2.65 | 0.43 |
| 1:CV:97:LYS:HA | 1:CV:100:ALA:HB3 | 2.00 | 0.43 |
| 1:A1:58:ILE:O | 1:A1:58:ILE:CG2 | 2.65 | 0.43 |
| 1:A1:55:ALA:CB | 1:A1:95:VAL:HG21 | 2.40 | 0.43 |
| 1:BM:82:ARG:HG3 | 1:BM:118:GLU:OE2 | 2.17 | 0.43 |
| 1:BF:58:ILE:HG21 | 1:BF:76:THR:OG1 | 2.17 | 0.43 |
| 1:BN:149:SER:HB3 | 1:BN:152:TRP:CH2 | 2.52 | 0.43 |
| 1:BQ:129:THR:HG22 | 1:BQ:130:LYS:N | 2.33 | 0.43 |
| 1:BF:7:LEU:HA | 1:BF:7:LEU:HD12 | 1.84 | 0.43 |
| 1:AX:17:VAL:HG13 | 1:AX:65:MET:CE | 2.48 | 0.43 |
| 1:C4:15:GLY:O | 1:C4:74:VAL:HA | 2.19 | 0.43 |
| 1:BJ:106:THR:O | 1:BJ:107:ASP:OD1 | 2.36 | 0.43 |
| 1:BO:106:THR:O | 1:BO:107:ASP:OD1 | 2.36 | 0.43 |
| 1:AU:7:LEU:HA | 1:AU:7:LEU:HD12 | 1.84 | 0.43 |
| 1:BU:144:GLU:O | 1:BU:148:LEU:HB2 | 2.18 | 0.43 |
| 1:CB:9:GLY:HA3 | 1:CB:12:LEU:HD12 | 1.99 | 0.43 |
| 1:AC:104:LEU:CD2 | 1:AD:60:LEU:HA | 2.48 | 0.43 |
| 1:CC:104:LEU:CD2 | 1:CD:60:LEU:HA | 2.48 | 0.43 |
| 1:BE:90:TYR:O | 1:BE:94:GLU:HG2 | 2.18 | 0.43 |
| 1:AK:51:TRP:O | 1:AO:148:LEU:HD11 | 2.18 | 0.43 |
| 1:AA:51:TRP:O | 1:AE:148:LEU:HD11 | 2.18 | 0.43 |
| 1:AR:66:ALA:HB2 | 1:AR:74:VAL:HG21 | 1.99 | 0.43 |
| 1:AZ:90:TYR:O | 1:AZ:94:GLU:HG2 | 2.18 | 0.43 |
| 1:AA:65:MET:HE3 | 1:AA:71:TYR:CE2 | 2.53 | 0.43 |
| 1:CK:51:TRP:O | 1:CO:148:LEU:HD11 | 2.18 | 0.43 |
| 1:AU:90:TYR:O | 1:AU:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BT:90:TYR:O | 1:BT:94:GLU:HG2 | 2.18 | 0.43 |
| 1:CA:65:MET:HE3 | 1:CA:71:TYR:CE2 | 2.54 | 0.43 |
| 1:BQ:104:LEU:HD23 | 1:BR:60:LEU:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:AT:65:MET:HE3 | 1:AT:71:TYR:CE2 | 2.54 | 0.43 |
| 1:BB:97:LYS:HA | 1:BB:100:ALA:HB3 | 2.00 | 0.43 |
| 1:AH:97:LYS:HE3 | 1:AI:97:LYS:HZ1 | 1.83 | 0.43 |
| 1:BL:58:ILE:O | 1:BL:58:ILE:CG2 | 2.65 | 0.43 |
| 1:C2:97:LYS:HE3 | 1:C3:97:LYS:NZ | 2.32 | 0.43 |
| 1:AQ:58:ILE:O | 1:AQ:58:ILE:CG2 | 2.65 | 0.43 |
| 1:CQ:55:ALA:HB1 | 1:CQ:95:VAL:CG2 | 2.40 | 0.43 |
| 1:AS:75:ILE:HD13 | 1:AS:139:ALA:HA | 1.99 | 0.43 |
| 1:BI:75:ILE:HG22 | 1:BI:77:LEU:CD1 | 2.48 | 0.43 |
| 1:CI:75:ILE:HG22 | 1:CI:77:LEU:CD1 | 2.49 | 0.43 |
| 1:AW:82:ARG:HG3 | 1:AW:118:GLU:OE2 | 2.17 | 0.43 |
| 1:AI:75:ILE:HD13 | 1:AI:139:ALA:HA | 1.99 | 0.43 |
| 1:C2:34:LEU:HD22 | 1:C2:38:LYS:CE | 2.43 | 0.43 |
| 1:CZ:58:ILE:O | 1:CZ:62:ALA:HB2 | 2.18 | 0.43 |
| 1:CU:7:LEU:HD12 | 1:CU:7:LEU:HA | 1.84 | 0.43 |
| 1:CN:17:VAL:HG13 | 1:CN:65:MET:CE | 2.48 | 0.43 |
| 1:C3:17:VAL:HG13 | 1:C3:65:MET:CE | 2.48 | 0.43 |
| 1:CS:17:VAL:HG13 | 1:CS:65:MET:CE | 2.48 | 0.43 |
| 1:CX:17:VAL:HG13 | 1:CX:65:MET:CE | 2.48 | 0.43 |
| 1:CT:106:THR:O | 1:CT:107:ASP:OD1 | 2.36 | 0.43 |
| 1:A4:106:THR:O | 1:A4:107:ASP:C | 2.57 | 0.43 |
| 1:AO:106:THR:O | 1:AO:107:ASP:C | 2.57 | 0.43 |
| 1:BN:121:GLU:O | 1:BN:125:GLU:HG3 | 2.18 | 0.43 |
| 1:AS:121:GLU:O | 1:AS:125:GLU:HG3 | 2.17 | 0.43 |
| 1:CF:98:GLY:O | 1:CF:102:LEU:HB2 | 2.18 | 0.43 |
| 1:BN:48:ASP:HB2 | 1:BN:71:TYR:CE1 | 2.50 | 0.43 |
| 1:BV:129:THR:HG22 | 1:BV:130:LYS:N | 2.33 | 0.43 |
| 1:CG:129:THR:HG22 | 1:CG:130:LYS:N | 2.33 | 0.43 |
| 1:AB:9:GLY:HA3 | 1:AB:12:LEU:HD12 | 1.99 | 0.43 |
| 1:BB:65:MET:HE3 | 1:BB:71:TYR:CZ | 2.53 | 0.43 |
| 1:AL:13:LYS:HG2 | 1:AL:70:LYS:O | 2.18 | 0.43 |
| 1:C1:13:LYS:HG2 | 1:C1:70:LYS:O | 2.18 | 0.43 |
| 1:CT:15:GLY:O | 1:CT:74:VAL:HA | 2.19 | 0.43 |
| 1:B4:88:TYR:CD2 | 1:B4:88:TYR:C | 2.91 | 0.43 |
| 1:BO:88:TYR:CD2 | 1:BO:88:TYR:C | 2.91 | 0.43 |
| 1:CA:90:TYR:O | 1:CA:94:GLU:HG2 | 2.18 | 0.43 |
| 1:A2:66:ALA:HB2 | 1:A2:74:VAL:HG21 | 1.99 | 0.43 |
| 1:BT:15:GLY:O | 1:BT:74:VAL:HA | 2.18 | 0.43 |
| 1:CR:125:GLU:HA | 1:CR:129:THR:HB | 2.01 | 0.43 |
| 1:BM:125:GLU:HA | 1:BM:129:THR:HB | 2.01 | 0.43 |
| 1:AG:104:LEU:HD23 | 1:AH:60:LEU:HD13 | 2.00 | 0.43 |
| 1:CB:104:LEU:HD23 | 1:CC:60:LEU:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CT:71:TYR:O | 1:CT:150:LYS:NZ | 2.44 | 0.43 |
| 1:AB:97:LYS:N | 1:AB:100:ALA:HB2 | 2.31 | 0.43 |
| 1:BG:97:LYS:HA | 1:BG:100:ALA:HB3 | 2.00 | 0.43 |
| 1:CV:100:ALA:CA | 1:CW:56:PHE:HZ | 2.28 | 0.43 |
| 1:C3:52:VAL:CG1 | 1:C3:61:ILE:HD12 | 2.35 | 0.43 |
| 1:BH:82:ARG:HG3 | 1:BH:118:GLU:OE2 | 2.18 | 0.43 |
| 1:AC:82:ARG:HG3 | 1:AC:118:GLU:OE2 | 2.17 | 0.43 |
| 1:BP:58:ILE:O | 1:BP:62:ALA:HB2 | 2.18 | 0.43 |
| 1:CT:106:THR:O | 1:CT:107:ASP:C | 2.57 | 0.43 |
| 1:BY:106:THR:O | 1:BY:107:ASP:OD1 | 2.36 | 0.43 |
| 1:C4:106:THR:O | 1:C4:107:ASP:C | 2.57 | 0.43 |
| 1:AT:106:THR:O | 1:AT:107:ASP:OD1 | 2.36 | 0.43 |
| 1:AU:144:GLU:O | 1:AU:148:LEU:HB2 | 2.18 | 0.43 |
| 1:CP:144:GLU:O | 1:CP:148:LEU:HB2 | 2.18 | 0.43 |
| 1:BA:98:GLY:O | 1:BA:102:LEU:HB2 | 2.18 | 0.43 |
| 1:AF:98:GLY:O | 1:AF:102:LEU:HB2 | 2.18 | 0.43 |
| 1:AK:98:GLY:O | 1:AK:102:LEU:HB2 | 2.18 | 0.43 |
| 1:BB:129:THR:HG22 | 1:BB:130:LYS:N | 2.33 | 0.43 |
| 1:BY:7:LEU:HD11 | 1:BY:140:VAL:HG22 | 2.01 | 0.43 |
| 1:CO:7:LEU:HD11 | 1:CO:140:VAL:HG22 | 2.01 | 0.43 |
| 1:AE:7:LEU:HD11 | 1:AE:140:VAL:HG22 | 2.01 | 0.43 |
| 1:BQ:13:LYS:HG2 | 1:BQ:70:LYS:O | 2.18 | 0.43 |
| 1:BA:51:TRP:O | 1:BE:148:LEU:HD11 | 2.18 | 0.43 |
| 1:BX:34:LEU:O | 1:BX:38:LYS:HG3 | 2.17 | 0.43 |
| 1:BE:15:GLY:O | 1:BE:74:VAL:HA | 2.18 | 0.43 |
| 1:BU:51:TRP:O | 1:BY:148:LEU:HD11 | 2.18 | 0.43 |
| 1:BE:21:PHE:O | 1:BE:22:ASN:HB2 | 2.19 | 0.43 |
| 1:CR:66:ALA:HB2 | 1:CR:74:VAL:HG21 | 2.00 | 0.43 |
| 1:AF:51:TRP:O | 1:AJ:148:LEU:HD11 | 2.18 | 0.43 |
| 1:CT:88:TYR:CD2 | 1:CT:88:TYR:C | 2.91 | 0.43 |
| 1:CO:88:TYR:C | 1:CO:88:TYR:CD2 | 2.91 | 0.43 |
| 1:BW:66:ALA:HB2 | 1:BW:74:VAL:HG21 | 2.00 | 0.43 |
| 1:AM:125:GLU:HA | 1:AM:129:THR:HB | 2.01 | 0.43 |
| 1:CC:125:GLU:HA | 1:CC:129:THR:HB | 2.01 | 0.43 |
| 1:AL:104:LEU:HD23 | 1:AM:60:LEU:HD13 | 2.00 | 0.43 |
| 1:AB:104:LEU:HD23 | 1:AC:60:LEU:HD13 | 2.00 | 0.43 |
| 1:AL:97:LYS:HE3 | 1:AM:97:LYS:HZ3 | 1.83 | 0.43 |
| 1:C1:55:ALA:HB1 | 1:C1:95:VAL:CG2 | 2.40 | 0.43 |
| 1:CP:39:ARG:NH1 | 1:CV:7:LEU:HD22 | 2.33 | 0.43 |
| 1:CX:75:ILE:HG22 | 1:CX:77:LEU:CD1 | 2.48 | 0.43 |
| 1:BR:82:ARG:HG3 | 1:BR:118:GLU:OE2 | 2.18 | 0.43 |
| 1:AA:58:ILE:H | 1:AA:59:PRO:HD2 | 1.80 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BE:45:ASN:C | 1:BE:47:ILE:H | 2.21 | 0.43 |
| 1:CT:64:LYS:HD3 | 1:CT:64:LYS:HA | 1.85 | 0.43 |
| 1:B4:45:ASN:C | 1:B4:47:ILE:H | 2.21 | 0.43 |
| 1:BQ:4:GLU:CG | 1:BR:51:TRP:HD1 | 2.29 | 0.43 |
| 1:CB:4:GLU:CG | 1:CC:51:TRP:HD1 | 2.29 | 0.43 |
| 1:AO:106:THR:O | 1:AO:107:ASP:OD1 | 2.36 | 0.43 |
| 1:CO:106:THR:O | 1:CO:107:ASP:OD1 | 2.36 | 0.43 |
| 1:BF:144:GLU:O | 1:BF:148:LEU:HB2 | 2.18 | 0.43 |
| 1:AD:7:LEU:HB3 | 1:AJ:39:ARG:O | 2.19 | 0.43 |
| 1:AV:129:THR:HG22 | 1:AV:130:LYS:N | 2.33 | 0.43 |
| 1:AR:104:LEU:CD2 | 1:AS:60:LEU:HA | 2.48 | 0.43 |
| 1:AH:104:LEU:CD2 | 1:AI:60:LEU:HA | 2.48 | 0.43 |
| 1:CJ:21:PHE:O | 1:CJ:22:ASN:HB2 | 2.19 | 0.43 |
| 1:AU:51:TRP:O | 1:AY:148:LEU:HD11 | 2.19 | 0.43 |
| 1:BJ:90:TYR:O | 1:BJ:94:GLU:HG2 | 2.18 | 0.43 |
| 1:CE:21:PHE:O | 1:CE:22:ASN:HB2 | 2.19 | 0.43 |
| 1:CZ:51:TRP:O | 1:C4:148:LEU:HD11 | 2.18 | 0.43 |
| 1:AT:15:GLY:O | 1:AT:74:VAL:HA | 2.18 | 0.43 |
| 1:AC:66:ALA:HB2 | 1:AC:74:VAL:HG21 | 1.99 | 0.43 |
| 1:CQ:24:PHE:CD1 | 1:CV:28:LYS:HG3 | 2.53 | 0.43 |
| 1:CY:88:TYR:CD2 | 1:CY:88:TYR:C | 2.91 | 0.43 |
| 1:BM:66:ALA:HB2 | 1:BM:74:VAL:HG21 | 1.99 | 0.43 |
| 1:CF:51:TRP:O | 1:CJ:148:LEU:HD11 | 2.19 | 0.43 |
| 1:C2:125:GLU:HA | 1:C2:129:THR:HB | 2.01 | 0.43 |
| 1:CJ:108:ILE:CG1 | 1:CJ:150:LYS:HE3 | 2.42 | 0.43 |
| 1:CJ:65:MET:HE3 | 1:CJ:71:TYR:CE2 | 2.54 | 0.43 |
| 1:BV:58:ILE:CG2 | 1:BV:58:ILE:O | 2.65 | 0.43 |
| 1:AM:38:LYS:HZ2 | 1:AM:44:GLU:HA | 1.83 | 0.43 |
| 1:AX:75:ILE:HG22 | 1:AX:77:LEU:CD1 | 2.49 | 0.43 |
| 1:CZ:58:ILE:H | 1:CZ:59:PRO:HD2 | 1.80 | 0.43 |
| 1:AZ:58:ILE:HG21 | 1:AZ:76:THR:OG1 | 2.17 | 0.43 |
| 1:AD:17:VAL:HG13 | 1:AD:65:MET:CE | 2.48 | 0.43 |
| 1:BT:45:ASN:C | 1:BT:47:ILE:H | 2.21 | 0.43 |
| 1:AI:17:VAL:HG13 | 1:AI:65:MET:CE | 2.48 | 0.43 |
| 1:BL:4:GLU:CG | 1:BM:51:TRP:HD1 | 2.29 | 0.43 |
| 1:AO:7:LEU:HD11 | 1:AO:140:VAL:HG22 | 2.01 | 0.43 |
| 1:B2:18:VAL:HA | 1:B2:77:LEU:O | 2.19 | 0.43 |
| 1:BG:9:GLY:HA3 | 1:BG:12:LEU:HD12 | 1.99 | 0.43 |
| 1:BL:13:LYS:HG2 | 1:BL:70:LYS:O | 2.18 | 0.43 |
| 1:AY:90:TYR:O | 1:AY:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BK:51:TRP:O | 1:BO:148:LEU:HD11 | 2.18 | 0.43 |
| 1:C4:7:LEU:HD11 | 1:C4:140:VAL:HG22 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:BO:15:GLY:O | 1:BO:74:VAL:HA | 2.19 | 0.43 |
| 1:BT:88:TYR:C | 1:BT:88:TYR:CD2 | 2.91 | 0.43 |
| 1:CS:150:LYS:H | 1:CS:150:LYS:HG3 | 1.33 | 0.43 |
| 1:C2:148:LEU:HD23 | 1:C2:148:LEU:HA | 1.80 | 0.43 |
| 1:AW:45:ASN:HA | 1:AW:45:ASN:HD22 | 1.64 | 0.43 |
| 1:CO:21:PHE:O | 1:CO:22:ASN:HB2 | 2.19 | 0.43 |
| 1:CJ:90:TYR:O | 1:CJ:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BX:58:ILE:HB | 1:BX:59:PRO:HD3 | 2.00 | 0.43 |
| 1:AO:90:TYR:O | 1:AO:94:GLU:HG2 | 2.18 | 0.43 |
| 1:AH:125:GLU:HA | 1:AH:129:THR:HB | 2.01 | 0.43 |
| 1:AO:65:MET:HE3 | 1:AO:71:TYR:CE2 | 2.54 | 0.43 |
| 1:BE:65:MET:HE3 | 1:BE:71:TYR:CE2 | 2.53 | 0.43 |
| 1:CL:97:LYS:HA | 1:CL:100:ALA:HB3 | 2.00 | 0.43 |
| 1:CN:75:ILE:HG22 | 1:CN:77:LEU:CD1 | 2.49 | 0.43 |
| 1:AN:75:ILE:HG22 | 1:AN:77:LEU:CD1 | 2.49 | 0.43 |
| 1:C3:75:ILE:HG22 | 1:C3:77:LEU:CD1 | 2.49 | 0.43 |
| 1:AI:75:ILE:HG22 | 1:AI:77:LEU:CD1 | 2.49 | 0.43 |
| 1:CE:45:ASN:C | 1:CE:47:ILE:H | 2.21 | 0.43 |
| 1:AE:106:THR:O | 1:AE:107:ASP:OD1 | 2.36 | 0.43 |
| 1:A4:106:THR:O | 1:A4:107:ASP:OD1 | 2.36 | 0.43 |
| 1:BR:18:VAL:HA | 1:BR:77:LEU:O | 2.19 | 0.43 |
| 1:AC:18:VAL:HA | 1:AC:77:LEU:O | 2.19 | 0.43 |
| 1:CW:18:VAL:HA | 1:CW:77:LEU:O | 2.19 | 0.43 |
| 1:CC:18:VAL:HA | 1:CC:77:LEU:O | 2.19 | 0.43 |
| 1:B4:7:LEU:HD11 | 1:B4:140:VAL:HG22 | 2.01 | 0.43 |
| 1:CT:8:VAL:CG2 | 1:C3:8:VAL:HG13 | 2.48 | 0.43 |
| 1:AB:13:LYS:HG2 | 1:AB:70:LYS:O | 2.18 | 0.43 |
| 1:CQ:9:GLY:HA3 | 1:CQ:12:LEU:HD12 | 1.99 | 0.43 |
| 1:BO:90:TYR:O | 1:BO:94:GLU:HG2 | 2.18 | 0.43 |
| 1:AD:34:LEU:O | 1:AD:38:LYS:HG3 | 2.17 | 0.43 |
| 1:CI:128:GLY:O | 1:CK:22:ASN:HA | 2.19 | 0.43 |
| 1:AJ:90:TYR:O | 1:AJ:94:GLU:HG2 | 2.18 | 0.43 |
| 1:CE:88:TYR:CD2 | 1:CE:88:TYR:C | 2.91 | 0.43 |
| 1:AT:90:TYR:O | 1:AT:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BP:51:TRP:O | 1:BT:148:LEU:HD11 | 2.18 | 0.43 |
| 1:AJ:21:PHE:O | 1:AJ:22:ASN:HB2 | 2.19 | 0.43 |
| 1:C3:58:ILE:HB | 1:C3:59:PRO:HD3 | 2.00 | 0.43 |
| 1:CK:90:TYR:O | 1:CK:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BB:55:ALA:HB1 | 1:BB:95:VAL:CG2 | 2.40 | 0.43 |
| 1:AG:97:LYS:HA | 1:AG:100:ALA:HB3 | 2.00 | 0.43 |
| 1:CL:100:ALA:CA | 1:CM:56:PHE:HZ | 2.28 | 0.43 |
| 1:CV:97:LYS:N | 1:CV:100:ALA:HB2 | 2.31 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AD:75:ILE:HG22 | 1:AD:77:LEU:CD1 | 2.49 | 0.43 |
| 1:BX:75:ILE:HG22 | 1:BX:77:LEU:CD1 | 2.49 | 0.43 |
| 1:BH:34:LEU:HD22 | 1:BH:38:LYS:CE | 2.43 | 0.43 |
| 1:AU:58:ILE:HG22 | 1:AU:58:ILE:O | 2.11 | 0.43 |
| 1:BG:120:ILE:CD1 | 1:BQ:125:GLU:HG2 | 2.49 | 0.43 |
| 1:BO:45:ASN:C | 1:BO:47:ILE:H | 2.21 | 0.43 |
| 1:AE:45:ASN:C | 1:AE:47:ILE:H | 2.21 | 0.43 |
| 1:CI:121:GLU:O | 1:CI:125:GLU:HG3 | 2.18 | 0.43 |
| 1:CT:7:LEU:HD11 | 1:CT:140:VAL:HG22 | 2.01 | 0.43 |
| 1:CO:106:THR:O | 1:CO:107:ASP:C | 2.57 | 0.43 |
| 1:A2:18:VAL:HA | 1:A2:77:LEU:O | 2.19 | 0.43 |
| 1:BE:7:LEU:HD11 | 1:BE:140:VAL:HG22 | 2.01 | 0.43 |
| 1:B1:9:GLY:HA3 | 1:B1:12:LEU:HD12 | 1.99 | 0.43 |
| 1:BB:13:LYS:HG2 | 1:BB:70:LYS:O | 2.18 | 0.43 |
| 1:AS:58:ILE:HB | 1:AS:59:PRO:HD3 | 2.00 | 0.43 |
| 1:BA:90:TYR:O | 1:BA:94:GLU:HG2 | 2.18 | 0.43 |
| 1:BZ:51:TRP:O | 1:B4:148:LEU:HD11 | 2.19 | 0.43 |
| 1:CY:90:TYR:O | 1:CY:94:GLU:HG2 | 2.18 | 0.43 |
| 1:AY:21:PHE:O | 1:AY:22:ASN:HB2 | 2.19 | 0.43 |
| 1:BI:150:LYS:H | 1:BI:150:LYS:HG3 | 1.33 | 0.43 |
| 1:AW:148:LEU:HD23 | 1:AW:148:LEU:HA | 1.80 | 0.43 |
| 1:CW:28:LYS:HZ1 | 1:C3:28:LYS:NZ | 2.16 | 0.43 |
| 1:B2:125:GLU:HA | 1:B2:129:THR:HB | 2.01 | 0.43 |
| 1:AQ:104:LEU:HD23 | 1:AR:60:LEU:HD13 | 2.00 | 0.43 |
| 1:C1:97:LYS:HA | 1:C1:100:ALA:HB3 | 2.00 | 0.43 |
| 1:AQ:97:LYS:HA | 1:AQ:100:ALA:HB3 | 2.00 | 0.43 |
| 1:AQ:55:ALA:CB | 1:AQ:95:VAL:HG21 | 2.40 | 0.43 |
| 1:AB:97:LYS:HA | 1:AB:100:ALA:HB3 | 2.00 | 0.43 |
| 1:CQ:55:ALA:CB | 1:CQ:95:VAL:HG21 | 2.40 | 0.43 |
| 1:A1:97:LYS:HE3 | 1:A2:97:LYS:HZ1 | 1.82 | 0.43 |
| 1:BD:75:ILE:HG22 | 1:BD:77:LEU:CD1 | 2.49 | 0.43 |
| 1:BS:75:ILE:HG22 | 1:BS:77:LEU:CD1 | 2.49 | 0.43 |
| 1:CD:75:ILE:HG22 | 1:CD:77:LEU:CD1 | 2.49 | 0.43 |
| 1:C3:75:ILE:HD13 | 1:C3:139:ALA:HA | 1.99 | 0.43 |
| 1:AO:15:GLY:O | 1:AO:74:VAL:HA | 2.19 | 0.43 |
| 1:CY:45:ASN:C | 1:CY:47:ILE:H | 2.21 | 0.43 |
| 1:BS:17:VAL:HG13 | 1:BS:65:MET:CE | 2.48 | 0.43 |
| 1:AJ:15:GLY:O | 1:AJ:74:VAL:HA | 2.18 | 0.43 |
| 1:CY:106:THR:O | 1:CY:107:ASP:C | 2.57 | 0.43 |
| 1:AJ:106:THR:O | 1:AJ:107:ASP:C | 2.57 | 0.43 |
| 1:BE:106:THR:O | 1:BE:107:ASP:C | 2.57 | 0.43 |
| 1:BE:40:HIS:CE1 | 1:BN:7:LEU:HD23 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AN:48:ASP:HB2 | 1:AN:71:TYR:CE1 | 2.50 | 0.43 |
| 1:AW:18:VAL:HA | 1:AW:77:LEU:O | 2.19 | 0.43 |
| 1:AY:7:LEU:HD11 | 1:AY:140:VAL:HG22 | 2.01 | 0.43 |
| 1:CT:21:PHE:O | 1:CT:22:ASN:HB2 | 2.19 | 0.43 |
| 1:AP:51:TRP:O | 1:AT:148:LEU:HD11 | 2.18 | 0.43 |
| 1:AR:91:VAL:O | 1:AR:95:VAL:HG23 | 2.19 | 0.43 |
| 1:BJ:15:GLY:O | 1:BJ:74:VAL:HA | 2.19 | 0.43 |
| 1:BR:91:VAL:O | 1:BR:95:VAL:HG23 | 2.19 | 0.43 |
| 1:AE:88:TYR:CD2 | 1:AE:88:TYR:C | 2.91 | 0.43 |
| 1:AI:148:LEU:HD23 | 1:AI:148:LEU:HA | 1.82 | 0.43 |
| 1:BW:91:VAL:O | 1:BW:95:VAL:HG23 | 2.19 | 0.43 |
| 1:AT:21:PHE:O | 1:AT:22:ASN:HB2 | 2.19 | 0.43 |
| 1:CJ:145:MET:O | 1:CJ:149:SER:HB3 | 2.20 | 0.42 |
| 1:CT:145:MET:O | 1:CT:149:SER:HB3 | 2.19 | 0.42 |
| 1:AG:58:ILE:CG2 | 1:AG:58:ILE:O | 2.65 | 0.42 |
| 1:BL:97:LYS:HA | 1:BL:100:ALA:HB3 | 2.00 | 0.42 |
| 1:BW:97:LYS:HE3 | 1:BX:97:LYS:NZ | 2.32 | 0.42 |
| 1:AH:52:VAL:CG1 | 1:AH:61:ILE:HD12 | 2.35 | 0.42 |
| 1:CR:52:VAL:CG1 | 1:CR:61:ILE:HD12 | 2.35 | 0.42 |
| 1:A2:34:LEU:HD22 | 1:A2:38:LYS:CE | 2.43 | 0.42 |
| 1:BQ:129:THR:CG2 | 1:BQ:130:LYS:H | 2.28 | 0.42 |
| 1:AT:106:THR:O | 1:AT:107:ASP:C | 2.57 | 0.42 |
| 1:CJ:106:THR:O | 1:CJ:107:ASP:C | 2.57 | 0.42 |
| 1:AY:106:THR:O | 1:AY:107:ASP:C | 2.57 | 0.42 |
| 1:CB:129:THR:HG22 | 1:CB:130:LYS:N | 2.33 | 0.42 |
| 1:BW:18:VAL:HA | 1:BW:77:LEU:O | 2.19 | 0.42 |
| 1:C2:18:VAL:HA | 1:C2:77:LEU:O | 2.19 | 0.42 |
| 1:CR:18:VAL:HA | 1:CR:77:LEU:O | 2.19 | 0.42 |
| 1:CM:104:LEU:CD2 | 1:CN:60:LEU:HA | 2.48 | 0.42 |
| 1:CW:66:ALA:HB2 | 1:CW:74:VAL:HG21 | 1.99 | 0.42 |
| 1:AH:91:VAL:O | 1:AH:95:VAL:HG23 | 2.19 | 0.42 |
| 1:CA:51:TRP:O | 1:CE:148:LEU:HD11 | 2.18 | 0.42 |
| 1:C4:90:TYR:O | 1:C4:94:GLU:HG2 | 2.18 | 0.42 |
| 1:A4:21:PHE:O | 1:A4:22:ASN:HB2 | 2.19 | 0.42 |
| 1:CS:58:ILE:HB | 1:CS:59:PRO:HD3 | 2.00 | 0.42 |
| 1:AM:148:LEU:HA | 1:AM:148:LEU:HD23 | 1.80 | 0.42 |
| 1:BX:148:LEU:HD23 | 1:BX:148:LEU:HA | 1.82 | 0.42 |
| 1:AM:45:ASN:HD22 | 1:AM:45:ASN:HA | 1.64 | 0.42 |
| 1:CX:148:LEU:HD23 | 1:CX:148:LEU:HA | 1.82 | 0.42 |
| 1:CT:90:TYR:O | 1:CT:94:GLU:HG2 | 2.18 | 0.42 |
| 1:BM:91:VAL:O | 1:BM:95:VAL:HG23 | 2.19 | 0.42 |
| 1:BW:125:GLU:HA | 1:BW:129:THR:HB | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AQ:13:LYS:NZ | 1:BU:43:GLU:CB | 2.67 | 0.42 |
| 1:CO:145:MET:O | 1:CO:149:SER:HB3 | 2.19 | 0.42 |
| 1:A4:65:MET:HE3 | 1:A4:71:TYR:CE2 | 2.54 | 0.42 |
| 1:B4:145:MET:O | 1:B4:149:SER:HB3 | 2.19 | 0.42 |
| 1:AV:97:LYS:HA | 1:AV:100:ALA:HB3 | 2.00 | 0.42 |
| 1:CB:97:LYS:HA | 1:CB:100:ALA:HB3 | 2.00 | 0.42 |
| 1:CL:55:ALA:HB1 | 1:CL:95:VAL:CG2 | 2.40 | 0.42 |
| 1:BV:55:ALA:HB1 | 1:BV:95:VAL:CG2 | 2.40 | 0.42 |
| 1:B3:75:ILE:HG22 | 1:B3:77:LEU:CD1 | 2.49 | 0.42 |
| 1:A3:75:ILE:HG22 | 1:A3:77:LEU:CD1 | 2.49 | 0.42 |
| 1:CE:106:THR:O | 1:CE:107:ASP:C | 2.57 | 0.42 |
| 1:AE:106:THR:O | 1:AE:107:ASP:C | 2.57 | 0.42 |
| 1:B4:106:THR:O | 1:B4:107:ASP:OD1 | 2.36 | 0.42 |
| 1:BO:106:THR:O | 1:BO:107:ASP:C | 2.57 | 0.42 |
| 1:CD:20:ARG:NH1 | 1:CR:39:ARG:NH1 | 2.67 | 0.42 |
| 1:AR:18:VAL:HA | 1:AR:77:LEU:O | 2.19 | 0.42 |
| 1:A4:7:LEU:HD11 | 1:A4:140:VAL:HG22 | 2.01 | 0.42 |
| 1:AM:104:LEU:CD2 | 1:AN:60:LEU:HA | 2.48 | 0.42 |
| 1:CH:66:ALA:HB2 | 1:CH:74:VAL:HG21 | 1.99 | 0.42 |
| 1:BF:51:TRP:O | 1:BJ:148:LEU:HD11 | 2.18 | 0.42 |
| 1:BJ:21:PHE:O | 1:BJ:22:ASN:HB2 | 2.19 | 0.42 |
| 1:AR:125:GLU:HA | 1:AR:129:THR:HB | 2.01 | 0.42 |
| 1:AD:120:ILE:CG1 | 1:AR:129:THR:HG21 | 2.49 | 0.42 |
| 1:AV:104:LEU:HD23 | 1:AW:60:LEU:HD13 | 2.00 | 0.42 |
| 1:CH:125:GLU:HA | 1:CH:129:THR:HB | 2.01 | 0.42 |
| 1:AO:145:MET:O | 1:AO:149:SER:HB3 | 2.20 | 0.42 |
| 1:CO:108:ILE:CG1 | 1:CO:150:LYS:HE3 | 2.42 | 0.42 |
| 1:BE:145:MET:O | 1:BE:149:SER:HB3 | 2.20 | 0.42 |
| 1:BT:145:MET:O | 1:BT:149:SER:HB3 | 2.19 | 0.42 |
| 1:C4:108:ILE:CG1 | 1:C4:150:LYS:HE3 | 2.42 | 0.42 |
| 1:CR:97:LYS:HE3 | 1:CS:97:LYS:HZ1 | 1.84 | 0.42 |
| 1:CA:58:ILE:H | 1:CA:59:PRO:HD2 | 1.80 | 0.42 |
| 1:AN:17:VAL:HG13 | 1:AN:65:MET:CE | 2.48 | 0.42 |
| 1:CT:45:ASN:C | 1:CT:47:ILE:H | 2.21 | 0.42 |
| 1:BD:7:LEU:CB | 1:BJ:39:ARG:O | 2.67 | 0.42 |
| 1:BC:18:VAL:HA | 1:BC:77:LEU:O | 2.19 | 0.42 |
| 1:CP:18:VAL:HG22 | 1:CP:77:LEU:HB2 | 2.02 | 0.42 |
| 1:BM:18:VAL:HA | 1:BM:77:LEU:O | 2.19 | 0.42 |
| 1:CL:129:THR:HG22 | 1:CL:130:LYS:N | 2.33 | 0.42 |
| 1:CW:104:LEU:CD2 | 1:CX:60:LEU:HA | 2.48 | 0.42 |
| 1:CG:13:LYS:HG2 | 1:CG:70:LYS:O | 2.18 | 0.42 |
| 1:CM:83:GLY:HA3 | 2:CM:2201:PO4:P | 2.60 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:C2:83:GLY:HA3 | 2:C2:2201:PO4:P | 2.60 | 0.42 |
| 1:AE:21:PHE:O | 1:AE:22:ASN:HB2 | 2.19 | 0.42 |
| 1:B3:58:ILE:HB | 1:B3:59:PRO:HD3 | 2.00 | 0.42 |
| 1:CG:31:GLY:O | 1:CG:35:ASP:HB2 | 2.20 | 0.42 |
| 1:B2:91:VAL:O | 1:B2:95:VAL:HG23 | 2.19 | 0.42 |
| 1:CW:125:GLU:HA | 1:CW:129:THR:HB | 2.01 | 0.42 |
| 1:BR:125:GLU:HA | 1:BR:129:THR:HB | 2.01 | 0.42 |
| 1:B1:104:LEU:HD23 | 1:B2:60:LEU:HD13 | 2.00 | 0.42 |
| 1:BC:125:GLU:HA | 1:BC:129:THR:HB | 2.01 | 0.42 |
| 1:AE:145:MET:O | 1:AE:149:SER:HB3 | 2.20 | 0.42 |
| 1:BB:104:LEU:HD23 | 1:BC:60:LEU:HD13 | 2.00 | 0.42 |
| 1:B1:97:LYS:HA | 1:B1:100:ALA:HB3 | 2.00 | 0.42 |
| 1:BG:55:ALA:HB1 | 1:BG:95:VAL:CG2 | 2.40 | 0.42 |
| 1:BF:39:ARG:NH2 | 1:BQ:144:GLU:CD | 2.73 | 0.42 |
| 1:AS:75:ILE:HG22 | 1:AS:77:LEU:CD1 | 2.49 | 0.42 |
| 1:BH:15:GLY:HA3 | 1:BH:65:MET:HE1 | 2.01 | 0.42 |
| 1:BU:58:ILE:H | 1:BU:59:PRO:HD2 | 1.80 | 0.42 |
| 1:AT:95:VAL:HG12 | 1:AT:112:PHE:HE1 | 1.85 | 0.42 |
| 1:AE:95:VAL:HG12 | 1:AE:112:PHE:HE1 | 1.85 | 0.42 |
| 1:CO:15:GLY:O | 1:CO:74:VAL:HA | 2.19 | 0.42 |
| 1:BY:15:GLY:O | 1:BY:74:VAL:HA | 2.18 | 0.42 |
| 1:BO:95:VAL:HG12 | 1:BO:112:PHE:HE1 | 1.85 | 0.42 |
| 1:B4:106:THR:O | 1:B4:107:ASP:C | 2.57 | 0.42 |
| 1:CP:7:LEU:HD12 | 1:CP:7:LEU:HA | 1.84 | 0.42 |
| 1:BZ:18:VAL:HG22 | 1:BZ:77:LEU:HB2 | 2.02 | 0.42 |
| 1:CM:18:VAL:HA | 1:CM:77:LEU:O | 2.19 | 0.42 |
| 1:A1:129:THR:CG2 | 1:A1:130:LYS:H | 2.28 | 0.42 |
| 1:AZ:18:VAL:HG22 | 1:AZ:77:LEU:HB2 | 2.02 | 0.42 |
| 1:CP:21:PHE:O | 1:CP:22:ASN:HB2 | 2.20 | 0.42 |
| 1:AD:40:HIS:CE1 | 1:AJ:7:LEU:HD23 | 2.54 | 0.42 |
| 1:BG:13:LYS:HG2 | 1:BG:70:LYS:O | 2.18 | 0.42 |
| 1:AG:13:LYS:HG2 | 1:AG:70:LYS:O | 2.18 | 0.42 |
| 1:A1:13:LYS:HG2 | 1:A1:70:LYS:O | 2.18 | 0.42 |
| 1:CC:83:GLY:HA3 | 2:CC:1001:PO4:O3 | 2.20 | 0.42 |
| 1:CA:21:PHE:O | 1:CA:22:ASN:HB2 | 2.20 | 0.42 |
| 1:BC:83:GLY:HA3 | 2:BC:1001:PO4:O3 | 2.20 | 0.42 |
| 1:BB:31:GLY:O | 1:BB:35:ASP:HB2 | 2.20 | 0.42 |
| 1:AY:6:HIS:HB3 | 1:AY:147:HIS:CG | 2.55 | 0.42 |
| 1:CW:91:VAL:O | 1:CW:95:VAL:HG23 | 2.19 | 0.42 |
| 1:A4:15:GLY:O | 1:A4:74:VAL:HA | 2.19 | 0.42 |
| 1:CI:58:ILE:HB | 1:CI:59:PRO:HD3 | 2.00 | 0.42 |
| 1:BY:21:PHE:O | 1:BY:22:ASN:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:B4:21:PHE:O | 1:B4:22:ASN:HB2 | 2.19 | 0.42 |
| 1:B2:45:ASN:HD22 | 1:B2:45:ASN:HA | 1.63 | 0.42 |
| 1:BZ:21:PHE:O | 1:BZ:22:ASN:HB2 | 2.20 | 0.42 |
| 1:BT:7:LEU:HD11 | 1:BT:140:VAL:HG22 | 2.01 | 0.42 |
| 1:AA:21:PHE:O | 1:AA:22:ASN:HB2 | 2.20 | 0.42 |
| 1:AM:91:VAL:O | 1:AM:95:VAL:HG23 | 2.19 | 0.42 |
| 1:AZ:21:PHE:O | 1:AZ:22:ASN:HB2 | 2.20 | 0.42 |
| 1:CN:58:ILE:HB | 1:CN:59:PRO:HD3 | 2.00 | 0.42 |
| 1:AW:91:VAL:O | 1:AW:95:VAL:HG23 | 2.19 | 0.42 |
| 1:BH:125:GLU:HA | 1:BH:129:THR:HB | 2.01 | 0.42 |
| 1:AJ:145:MET:O | 1:AJ:149:SER:HB3 | 2.19 | 0.42 |
| 1:AY:65:MET:HE3 | 1:AY:71:TYR:CE2 | 2.55 | 0.42 |
| 1:BJ:145:MET:O | 1:BJ:149:SER:HB3 | 2.20 | 0.42 |
| 1:AV:55:ALA:HB1 | 1:AV:95:VAL:CG2 | 2.40 | 0.42 |
| 1:AL:97:LYS:HA | 1:AL:100:ALA:HB3 | 2.00 | 0.42 |
| 1:BG:100:ALA:CA | 1:BH:56:PHE:HZ | 2.28 | 0.42 |
| 1:CG:97:LYS:HA | 1:CG:100:ALA:HB3 | 2.00 | 0.42 |
| 1:BX:52:VAL:CG1 | 1:BX:61:ILE:HD12 | 2.35 | 0.42 |
| 1:CF:28:LYS:HD2 | 1:CR:24:PHE:CD1 | 2.55 | 0.42 |
| 1:CW:39:ARG:CZ | 1:C3:20:ARG:CZ | 2.97 | 0.42 |
| 1:BO:64:LYS:HD3 | 1:BO:64:LYS:HA | 1.85 | 0.42 |
| 1:CO:45:ASN:C | 1:CO:47:ILE:H | 2.21 | 0.42 |
| 1:BT:106:THR:O | 1:BT:107:ASP:C | 2.57 | 0.42 |
| 1:BJ:106:THR:O | 1:BJ:107:ASP:C | 2.57 | 0.42 |
| 1:CI:48:ASP:HB2 | 1:CI:71:TYR:CE1 | 2.50 | 0.42 |
| 1:AP:18:VAL:HG22 | 1:AP:77:LEU:HB2 | 2.02 | 0.42 |
| 1:AH:18:VAL:HA | 1:AH:77:LEU:O | 2.19 | 0.42 |
| 1:BU:18:VAL:HG22 | 1:BU:77:LEU:HB2 | 2.02 | 0.42 |
| 1:BI:98:GLY:HA2 | 1:BI:102:LEU:HD23 | 2.02 | 0.42 |
| 1:BV:65:MET:HE3 | 1:BV:71:TYR:CE2 | 2.55 | 0.42 |
| 1:CC:83:GLY:HA3 | 2:CC:1001:PO4:P | 2.60 | 0.42 |
| 1:AR:83:GLY:HA3 | 2:AR:1001:PO4:P | 2.60 | 0.42 |
| 1:AH:83:GLY:HA3 | 2:AH:1001:PO4:O3 | 2.20 | 0.42 |
| 1:BH:83:GLY:HA3 | 2:BH:1001:PO4:O3 | 2.20 | 0.42 |
| 1:CH:83:GLY:HA3 | 2:CH:2201:PO4:P | 2.60 | 0.42 |
| 1:A1:31:GLY:O | 1:A1:35:ASP:HB2 | 2.20 | 0.42 |
| 1:BJ:6:HIS:HB3 | 1:BJ:147:HIS:CG | 2.55 | 0.42 |
| 1:BS:58:ILE:HB | 1:BS:59:PRO:HD3 | 2.00 | 0.42 |
| 1:CO:6:HIS:HB3 | 1:CO:147:HIS:CG | 2.55 | 0.42 |
| 1:AS:29:LEU:HD11 | 1:AS:134:LYS:HB3 | 2.02 | 0.42 |
| 1:CU:51:TRP:O | 1:CY:148:LEU:HD11 | 2.19 | 0.42 |
| 1:AN:58:ILE:HB | 1:AN:59:PRO:HD3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AG:31:GLY:O | 1:AG:35:ASP:HB2 | 2.20 | 0.42 |
| 1:CY:21:PHE:O | 1:CY:22:ASN:HB2 | 2.19 | 0.42 |
| 1:C2:91:VAL:O | 1:C2:95:VAL:HG23 | 2.19 | 0.42 |
| 1:BA:21:PHE:O | 1:BA:22:ASN:HB2 | 2.20 | 0.42 |
| 1:CC:91:VAL:O | 1:CC:95:VAL:HG23 | 2.19 | 0.42 |
| 1:A4:90:TYR:O | 1:A4:94:GLU:HG2 | 2.18 | 0.42 |
| 1:AQ:104:LEU:HD13 | 1:AR:102:LEU:CD2 | 2.46 | 0.42 |
| 1:A4:108:ILE:CG1 | 1:A4:150:LYS:HE3 | 2.42 | 0.42 |
| 1:AY:145:MET:O | 1:AY:149:SER:HB3 | 2.19 | 0.42 |
| 1:CY:145:MET:O | 1:CY:149:SER:HB3 | 2.20 | 0.42 |
| 1:BB:97:LYS:N | 1:BB:100:ALA:HB2 | 2.31 | 0.42 |
| 1:C1:55:ALA:HA | 1:C1:58:ILE:HG13 | 2.02 | 0.42 |
| 1:CQ:97:LYS:HE3 | 1:CR:97:LYS:HZ1 | 1.84 | 0.42 |
| 1:CK:53:PRO:HD2 | 1:CK:57:GLU:CB | 2.49 | 0.42 |
| 1:AA:18:VAL:HG22 | 1:AA:77:LEU:HB2 | 2.02 | 0.42 |
| 1:AJ:7:LEU:HD11 | 1:AJ:140:VAL:HG22 | 2.01 | 0.42 |
| 1:AX:6:HIS:HB3 | 1:AX:147:HIS:CG | 2.55 | 0.42 |
| 1:C3:6:HIS:HB3 | 1:C3:147:HIS:CG | 2.55 | 0.42 |
| 1:CX:6:HIS:HB3 | 1:CX:147:HIS:CG | 2.55 | 0.42 |
| 1:BE:7:LEU:HA | 1:BE:7:LEU:HD12 | 1.91 | 0.42 |
| 1:AD:98:GLY:HA2 | 1:AD:102:LEU:HD23 | 2.02 | 0.42 |
| 1:CR:83:GLY:HA3 | 2:CR:2201:PO4:P | 2.60 | 0.42 |
| 1:A4:6:HIS:HB3 | 1:A4:147:HIS:CG | 2.55 | 0.42 |
| 1:CO:90:TYR:O | 1:CO:94:GLU:HG2 | 2.18 | 0.42 |
| 1:BP:21:PHE:O | 1:BP:22:ASN:HB2 | 2.20 | 0.42 |
| 1:AJ:6:HIS:HB3 | 1:AJ:147:HIS:CG | 2.55 | 0.42 |
| 1:CN:148:LEU:HA | 1:CN:148:LEU:HD23 | 1.82 | 0.42 |
| 1:AX:58:ILE:HB | 1:AX:59:PRO:HD3 | 2.00 | 0.42 |
| 1:BD:58:ILE:HB | 1:BD:59:PRO:HD3 | 2.00 | 0.42 |
| 1:BQ:31:GLY:O | 1:BQ:35:ASP:HB2 | 2.20 | 0.42 |
| 1:BC:91:VAL:O | 1:BC:95:VAL:HG23 | 2.19 | 0.42 |
| 1:AN:29:LEU:HD11 | 1:AN:134:LYS:HB3 | 2.02 | 0.42 |
| 1:BY:145:MET:O | 1:BY:149:SER:HB3 | 2.20 | 0.42 |
| 1:BL:55:ALA:CB | 1:BL:95:VAL:HG21 | 2.40 | 0.42 |
| 1:B1:55:ALA:HA | 1:B1:58:ILE:HG13 | 2.02 | 0.42 |
| 1:CQ:97:LYS:HA | 1:CQ:100:ALA:HB3 | 2.00 | 0.42 |
| 1:CM:67:ASN:HD22 | 1:CM:67:ASN:HA | 1.60 | 0.42 |
| 1:AJ:45:ASN:C | 1:AJ:47:ILE:H | 2.21 | 0.42 |
| 1:BE:95:VAL:HG12 | 1:BE:112:PHE:HE1 | 1.85 | 0.42 |
| 1:CE:95:VAL:HG12 | 1:CE:112:PHE:HE1 | 1.85 | 0.42 |
| 1:AL:129:THR:HG22 | 1:AL:130:LYS:N | 2.33 | 0.42 |
| 1:CF:18:VAL:HG22 | 1:CF:77:LEU:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AX:98:GLY:HA2 | 1:AX:102:LEU:HD23 | 2.02 | 0.42 |
| 1:BS:98:GLY:HA2 | 1:BS:102:LEU:HD23 | 2.02 | 0.42 |
| 1:CM:83:GLY:HA3 | 2:CM:2201:PO4:O3 | 2.20 | 0.42 |
| 1:CA:24:PHE:CD1 | 1:CN:28:LYS:HG3 | 2.54 | 0.42 |
| 1:AH:83:GLY:HA3 | 2:AH:1001:PO4:P | 2.60 | 0.42 |
| 1:BC:83:GLY:HA3 | 2:BC:1001:PO4:P | 2.60 | 0.42 |
| 1:AM:83:GLY:HA3 | 2:AM:1001:PO4:P | 2.60 | 0.42 |
| 1:CK:21:PHE:O | 1:CK:22:ASN:HB2 | 2.20 | 0.42 |
| 1:BK:21:PHE:O | 1:BK:22:ASN:HB2 | 2.20 | 0.42 |
| 1:A3:29:LEU:HD11 | 1:A3:134:LYS:HB3 | 2.02 | 0.42 |
| 1:B1:31:GLY:O | 1:B1:35:ASP:HB2 | 2.20 | 0.42 |
| 1:BL:31:GLY:O | 1:BL:35:ASP:HB2 | 2.20 | 0.42 |
| 1:CZ:116:THR:O | 1:C1:85:THR:HB | 2.20 | 0.42 |
| 1:BY:6:HIS:HB3 | 1:BY:147:HIS:CG | 2.55 | 0.42 |
| 1:BI:29:LEU:HD11 | 1:BI:134:LYS:HB3 | 2.02 | 0.42 |
| 1:CP:90:TYR:O | 1:CP:94:GLU:HG2 | 2.18 | 0.42 |
| 1:BU:65:MET:HE3 | 1:BU:71:TYR:CE2 | 2.54 | 0.42 |
| 1:AQ:31:GLY:O | 1:AQ:35:ASP:HB2 | 2.20 | 0.42 |
| 1:BE:6:HIS:HB3 | 1:BE:147:HIS:CG | 2.55 | 0.42 |
| 1:BT:6:HIS:HB3 | 1:BT:147:HIS:CG | 2.55 | 0.42 |
| 1:CJ:6:HIS:HB3 | 1:CJ:147:HIS:CG | 2.55 | 0.42 |
| 1:AE:6:HIS:HB3 | 1:AE:147:HIS:CG | 2.55 | 0.42 |
| 1:C4:6:HIS:HB3 | 1:C4:147:HIS:CG | 2.55 | 0.42 |
| 1:B4:15:GLY:O | 1:B4:74:VAL:HA | 2.18 | 0.42 |
| 1:AU:21:PHE:O | 1:AU:22:ASN:HB2 | 2.20 | 0.42 |
| 1:CV:104:LEU:HD23 | 1:CW:60:LEU:HD13 | 2.00 | 0.42 |
| 1:CE:145:MET:O | 1:CE:149:SER:HB3 | 2.20 | 0.42 |
| 1:BT:65:MET:HE3 | 1:BT:71:TYR:CE2 | 2.55 | 0.42 |
| 1:AL:55:ALA:HA | 1:AL:58:ILE:HG13 | 2.02 | 0.42 |
| 1:BV:55:ALA:HA | 1:BV:58:ILE:HG13 | 2.02 | 0.42 |
| 1:BQ:55:ALA:HA | 1:BQ:58:ILE:HG13 | 2.02 | 0.42 |
| 1:BH:97:LYS:HE3 | 1:BI:97:LYS:HZ3 | 1.84 | 0.42 |
| 1:A4:95:VAL:HG12 | 1:A4:112:PHE:HE1 | 1.85 | 0.42 |
| 1:CY:95:VAL:HG12 | 1:CY:112:PHE:HE1 | 1.85 | 0.42 |
| 1:C1:129:THR:HG22 | 1:C1:130:LYS:N | 2.33 | 0.42 |
| 1:CN:6:HIS:HB3 | 1:CN:147:HIS:CG | 2.55 | 0.42 |
| 1:CE:7:LEU:HD11 | 1:CE:140:VAL:HG22 | 2.01 | 0.42 |
| 1:AK:21:PHE:O | 1:AK:22:ASN:HB2 | 2.20 | 0.42 |
| 1:AW:83:GLY:HA3 | 2:AW:201:PO4:O3 | 2.20 | 0.42 |
| 1:AO:6:HIS:HB3 | 1:AO:147:HIS:CG | 2.55 | 0.42 |
| 1:BT:21:PHE:O | 1:BT:22:ASN:HB2 | 2.19 | 0.42 |
| 1:CM:91:VAL:O | 1:CM:95:VAL:HG23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:CX:29:LEU:HD11 | 1:CX:134:LYS:HB3 | 2.02 | 0.42 |
| 1:AU:116:THR:O | 1:AV:85:THR:HB | 2.20 | 0.42 |
| 1:A3:150:LYS:HG3 | 1:A3:150:LYS:H | 1.33 | 0.42 |
| 1:AZ:116:THR:O | 1:A1:85:THR:HB | 2.20 | 0.42 |
| 1:BN:29:LEU:HD11 | 1:BN:134:LYS:HB3 | 2.02 | 0.42 |
| 1:CE:15:GLY:O | 1:CE:74:VAL:HA | 2.18 | 0.42 |
| 1:BC:129:THR:O | 1:BC:131:ALA:N | 2.53 | 0.42 |
| 1:BL:55:ALA:HA | 1:BL:58:ILE:HG13 | 2.02 | 0.42 |
| 1:AQ:55:ALA:HA | 1:AQ:58:ILE:HG13 | 2.02 | 0.42 |
| 1:AB:96:ALA:O | 1:AB:100:ALA:HB2 | 2.06 | 0.42 |
| 1:BV:100:ALA:O | 1:BW:56:PHE:CE1 | 2.73 | 0.42 |
| 1:AP:53:PRO:HD2 | 1:AP:57:GLU:CB | 2.49 | 0.42 |
| 1:CW:34:LEU:HD22 | 1:CW:38:LYS:CE | 2.44 | 0.42 |
| 1:AW:15:GLY:HA3 | 1:AW:65:MET:HE3 | 2.01 | 0.42 |
| 1:BR:63:LYS:O | 1:BR:65:MET:N | 2.53 | 0.42 |
| 1:B4:64:LYS:HD3 | 1:B4:64:LYS:HA | 1.85 | 0.42 |
| 1:AY:95:VAL:HG12 | 1:AY:112:PHE:HE1 | 1.85 | 0.42 |
| 1:BJ:95:VAL:HG12 | 1:BJ:112:PHE:HE1 | 1.85 | 0.42 |
| 1:CJ:15:GLY:O | 1:CJ:74:VAL:HA | 2.19 | 0.42 |
| 1:BI:48:ASP:HB2 | 1:BI:71:TYR:CE1 | 2.50 | 0.42 |
| 1:AU:18:VAL:HG22 | 1:AU:77:LEU:HB2 | 2.02 | 0.42 |
| 1:BI:6:HIS:HB3 | 1:BI:147:HIS:CG | 2.55 | 0.42 |
| 1:BO:7:LEU:HD11 | 1:BO:140:VAL:HG22 | 2.01 | 0.42 |
| 1:CD:6:HIS:HB3 | 1:CD:147:HIS:CG | 2.55 | 0.42 |
| 1:CG:65:MET:HE3 | 1:CG:71:TYR:CE2 | 2.55 | 0.42 |
| 1:AI:98:GLY:HA2 | 1:AI:102:LEU:HD23 | 2.02 | 0.42 |
| 1:BD:98:GLY:HA2 | 1:BD:102:LEU:HD23 | 2.02 | 0.42 |
| 1:BV:13:LYS:HG2 | 1:BV:70:LYS:O | 2.18 | 0.42 |
| 1:CX:98:GLY:HA2 | 1:CX:102:LEU:HD23 | 2.02 | 0.42 |
| 1:BH:83:GLY:HA3 | 2:BH:1001:PO4:P | 2.60 | 0.42 |
| 1:BW:83:GLY:HA3 | 2:BW:1001:PO4:P | 2.60 | 0.42 |
| 1:A2:83:GLY:HA3 | 2:A2:1001:PO4:O3 | 2.20 | 0.42 |
| 1:BM:83:GLY:HA3 | 2:BM:1001:PO4:P | 2.60 | 0.42 |
| 1:BR:83:GLY:HA3 | 2:BR:1001:PO4:O3 | 2.20 | 0.42 |
| 1:CS:29:LEU:HD11 | 1:CS:134:LYS:HB3 | 2.02 | 0.42 |
| 1:BX:29:LEU:HD11 | 1:BX:134:LYS:HB3 | 2.02 | 0.42 |
| 1:AT:7:LEU:HD11 | 1:AT:140:VAL:HG22 | 2.01 | 0.42 |
| 1:AO:21:PHE:O | 1:AO:22:ASN:HB2 | 2.19 | 0.42 |
| 1:BO:21:PHE:O | 1:BO:22:ASN:HB2 | 2.19 | 0.42 |
| 1:A2:91:VAL:O | 1:A2:95:VAL:HG23 | 2.19 | 0.42 |
| 1:CJ:7:LEU:HD11 | 1:CJ:140:VAL:HG22 | 2.01 | 0.42 |
| 1:AP:116:THR:O | 1:AQ:85:THR:HB | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CJ:52:VAL:CB | 1:CJ:53:PRO:CD | 2.98 | 0.42 |
| 1:CE:52:VAL:CB | 1:CE:53:PRO:CD | 2.98 | 0.42 |
| 1:AQ:69:GLY:C | 1:BU:10:THR:CG2 | 2.86 | 0.42 |
| 1:AR:129:THR:O | 1:AR:131:ALA:N | 2.53 | 0.42 |
| 1:A2:129:THR:O | 1:A2:131:ALA:N | 2.53 | 0.42 |
| 1:BO:145:MET:O | 1:BO:149:SER:HB3 | 2.20 | 0.42 |
| 1:CB:100:ALA:O | 1:CC:56:PHE:CE1 | 2.73 | 0.42 |
| 1:CB:55:ALA:CB | 1:CB:95:VAL:HG21 | 2.40 | 0.42 |
| 1:AB:100:ALA:O | 1:AC:56:PHE:CE1 | 2.73 | 0.42 |
| 1:BQ:97:LYS:HA | 1:BQ:100:ALA:HB3 | 2.00 | 0.42 |
| 1:A3:52:VAL:CG1 | 1:A3:61:ILE:HD12 | 2.35 | 0.42 |
| 1:AK:52:VAL:HB | 1:AK:53:PRO:CD | 2.50 | 0.42 |
| 1:BA:52:VAL:HB | 1:BA:53:PRO:CD | 2.50 | 0.42 |
| 1:BU:53:PRO:HD2 | 1:BU:57:GLU:CB | 2.49 | 0.42 |
| 1:AZ:52:VAL:HB | 1:AZ:53:PRO:CD | 2.50 | 0.42 |
| 1:AH:63:LYS:O | 1:AH:65:MET:N | 2.53 | 0.42 |
| 1:BH:63:LYS:O | 1:BH:65:MET:N | 2.53 | 0.42 |
| 1:AY:15:GLY:O | 1:AY:74:VAL:HA | 2.19 | 0.42 |
| 1:BK:7:LEU:HA | 1:BK:7:LEU:HD12 | 1.84 | 0.42 |
| 1:CJ:45:ASN:C | 1:CJ:47:ILE:H | 2.21 | 0.42 |
| 1:AI:39:ARG:O | 1:AO:7:LEU:CB | 2.67 | 0.42 |
| 1:BH:18:VAL:HA | 1:BH:77:LEU:O | 2.19 | 0.42 |
| 1:BX:6:HIS:HB3 | 1:BX:147:HIS:CG | 2.55 | 0.42 |
| 1:CB:65:MET:HE3 | 1:CB:71:TYR:CE2 | 2.55 | 0.42 |
| 1:C2:83:GLY:HA3 | 2:C2:2201:PO4:O3 | 2.20 | 0.42 |
| 1:B2:83:GLY:HA3 | 2:B2:1001:PO4:O3 | 2.20 | 0.42 |
| 1:BR:83:GLY:HA3 | 2:BR:1001:PO4:P | 2.60 | 0.42 |
| 1:C3:29:LEU:HD11 | 1:C3:134:LYS:HB3 | 2.02 | 0.42 |
| 1:CP:116:THR:O | 1:CQ:85:THR:HB | 2.20 | 0.42 |
| 1:BO:6:HIS:HB3 | 1:BO:147:HIS:CG | 2.55 | 0.42 |
| 1:BU:106:THR:C | 1:BU:108:ILE:H | 2.23 | 0.42 |
| 1:BG:31:GLY:O | 1:BG:35:ASP:HB2 | 2.20 | 0.42 |
| 1:BD:29:LEU:HD11 | 1:BD:134:LYS:HB3 | 2.02 | 0.42 |
| 1:AZ:106:THR:C | 1:AZ:108:ILE:H | 2.23 | 0.42 |
| 1:BP:106:THR:C | 1:BP:108:ILE:H | 2.23 | 0.42 |
| 1:B3:29:LEU:HD11 | 1:B3:134:LYS:HB3 | 2.02 | 0.42 |
| 1:AD:120:ILE:HG12 | 1:AR:129:THR:HG21 | 2.02 | 0.41 |
| 1:B2:129:THR:O | 1:B2:131:ALA:N | 2.53 | 0.41 |
| 1:BM:129:THR:O | 1:BM:131:ALA:N | 2.53 | 0.41 |
| 1:CC:129:THR:O | 1:CC:131:ALA:N | 2.53 | 0.41 |
| 1:AW:125:GLU:HA | 1:AW:129:THR:HB | 2.01 | 0.41 |
| 1:AQ:70:LYS:HE3 | 1:BU:43:GLU:CD | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A4:145:MET:O | 1:A4:149:SER:HB3 | 2.19 | 0.41 |
| 1:CY:65:MET:HE3 | 1:CY:71:TYR:CE2 | 2.55 | 0.41 |
| 1:CB:97:LYS:N | 1:CB:100:ALA:HB2 | 2.31 | 0.41 |
| 1:CV:100:ALA:O | 1:CW:56:PHE:CE1 | 2.73 | 0.41 |
| 1:CV:55:ALA:HA | 1:CV:58:ILE:HG13 | 2.02 | 0.41 |
| 1:AU:52:VAL:HB | 1:AU:53:PRO:CD | 2.50 | 0.41 |
| 1:AF:53:PRO:HD2 | 1:AF:57:GLU:CB | 2.49 | 0.41 |
| 1:CU:53:PRO:HD2 | 1:CU:57:GLU:CB | 2.49 | 0.41 |
| 1:CS:75:ILE:HG22 | 1:CS:77:LEU:CD1 | 2.49 | 0.41 |
| 1:AW:67:ASN:HA | 1:AW:67:ASN:HD22 | 1.59 | 0.41 |
| 1:C4:30:LEU:HA | 1:C4:77:LEU:HD23 | 2.02 | 0.41 |
| 1:CT:95:VAL:HG12 | 1:CT:112:PHE:HE1 | 1.85 | 0.41 |
| 1:A4:45:ASN:C | 1:A4:47:ILE:H | 2.21 | 0.41 |
| 1:BJ:7:LEU:HD11 | 1:BJ:140:VAL:HG22 | 2.01 | 0.41 |
| 1:AM:18:VAL:HA | 1:AM:77:LEU:O | 2.19 | 0.41 |
| 1:AK:18:VAL:HG22 | 1:AK:77:LEU:HB2 | 2.02 | 0.41 |
| 1:BS:6:HIS:HB3 | 1:BS:147:HIS:CG | 2.55 | 0.41 |
| 1:BQ:71:TYR:O | 1:BQ:108:ILE:HD13 | 2.21 | 0.41 |
| 1:CR:83:GLY:HA3 | 2:CR:2201:PO4:O3 | 2.20 | 0.41 |
| 1:CI:29:LEU:HD11 | 1:CI:134:LYS:HB3 | 2.02 | 0.41 |
| 1:CZ:106:THR:C | 1:CZ:108:ILE:H | 2.24 | 0.41 |
| 1:CT:28:LYS:NZ | 1:C4:28:LYS:NZ | 2.67 | 0.41 |
| 1:BH:91:VAL:O | 1:BH:95:VAL:HG23 | 2.19 | 0.41 |
| 1:AS:148:LEU:HA | 1:AS:148:LEU:HD23 | 1.82 | 0.41 |
| 1:CF:21:PHE:O | 1:CF:22:ASN:HB2 | 2.20 | 0.41 |
| 1:CR:91:VAL:O | 1:CR:95:VAL:HG23 | 2.19 | 0.41 |
| 1:CH:91:VAL:O | 1:CH:95:VAL:HG23 | 2.19 | 0.41 |
| 1:CQ:31:GLY:O | 1:CQ:35:ASP:HB2 | 2.20 | 0.41 |
| 1:AV:104:LEU:HD13 | 1:AW:102:LEU:CD2 | 2.46 | 0.41 |
| 1:AT:145:MET:O | 1:AT:149:SER:HB3 | 2.19 | 0.41 |
| 1:AL:97:LYS:HE3 | 1:AM:97:LYS:HZ1 | 1.84 | 0.41 |
| 1:C1:58:ILE:CG2 | 1:C1:58:ILE:O | 2.65 | 0.41 |
| 1:CQ:55:ALA:HA | 1:CQ:58:ILE:HG13 | 2.02 | 0.41 |
| 1:A1:55:ALA:HA | 1:A1:58:ILE:HG13 | 2.02 | 0.41 |
| 1:A1:100:ALA:O | 1:A2:56:PHE:CE1 | 2.73 | 0.41 |
| 1:BK:52:VAL:HB | 1:BK:53:PRO:CD | 2.51 | 0.41 |
| 1:BF:53:PRO:HD2 | 1:BF:57:GLU:CB | 2.49 | 0.41 |
| 1:AA:53:PRO:HD2 | 1:AA:57:GLU:CB | 2.49 | 0.41 |
| 1:AT:30:LEU:HA | 1:AT:77:LEU:HD23 | 2.02 | 0.41 |
| 1:A2:63:LYS:O | 1:A2:65:MET:N | 2.53 | 0.41 |
| 1:CH:67:ASN:HD22 | 1:CH:67:ASN:HA | 1.59 | 0.41 |
| 1:C2:63:LYS:O | 1:C2:65:MET:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:CY:64:LYS:HA | 1:CY:64:LYS:HD3 | 1.85 | 0.41 |
| 1:AE:15:GLY:O | 1:AE:74:VAL:HA | 2.18 | 0.41 |
| 1:B4:95:VAL:HG12 | 1:B4:112:PHE:HE1 | 1.85 | 0.41 |
| 1:CA:18:VAL:HG22 | 1:CA:77:LEU:HB2 | 2.02 | 0.41 |
| 1:B3:6:HIS:HB3 | 1:B3:147:HIS:CG | 2.55 | 0.41 |
| 1:BN:6:HIS:HB3 | 1:BN:147:HIS:CG | 2.55 | 0.41 |
| 1:AC:83:GLY:HA3 | 2:AC:1001:PO4:O3 | 2.20 | 0.41 |
| 1:AC:83:GLY:HA3 | 2:AC:1001:PO4:P | 2.60 | 0.41 |
| 1:B2:83:GLY:HA3 | 2:B2:1001:PO4:P | 2.60 | 0.41 |
| 1:CW:83:GLY:HA3 | 2:CW:2201:PO4:O3 | 2.20 | 0.41 |
| 1:CW:83:GLY:HA3 | 2:CW:2201:PO4:P | 2.60 | 0.41 |
| 1:A2:83:GLY:HA3 | 2:A2:1001:PO4:P | 2.60 | 0.41 |
| 1:BM:83:GLY:HA3 | 2:BM:1001:PO4:O3 | 2.20 | 0.41 |
| 1:CY:7:LEU:HD11 | 1:CY:140:VAL:HG22 | 2.01 | 0.41 |
| 1:BP:116:THR:O | 1:BQ:85:THR:HB | 2.20 | 0.41 |
| 1:BR:148:LEU:HA | 1:BR:148:LEU:HD23 | 1.80 | 0.41 |
| 1:BS:29:LEU:HD11 | 1:BS:134:LYS:HB3 | 2.02 | 0.41 |
| 1:BH:129:THR:O | 1:BH:131:ALA:N | 2.53 | 0.41 |
| 1:BW:129:THR:O | 1:BW:131:ALA:N | 2.53 | 0.41 |
| 1:AV:100:ALA:O | 1:AW:56:PHE:CE1 | 2.73 | 0.41 |
| 1:CB:55:ALA:HA | 1:CB:58:ILE:HG13 | 2.02 | 0.41 |
| 1:AL:55:ALA:HB1 | 1:AL:95:VAL:CG2 | 2.40 | 0.41 |
| 1:BQ:100:ALA:O | 1:BR:56:PHE:CE1 | 2.73 | 0.41 |
| 1:BG:55:ALA:HA | 1:BG:58:ILE:HG13 | 2.02 | 0.41 |
| 1:CG:100:ALA:O | 1:CH:56:PHE:CE1 | 2.73 | 0.41 |
| 1:CU:52:VAL:HB | 1:CU:53:PRO:CD | 2.50 | 0.41 |
| 1:BN:75:ILE:HG22 | 1:BN:77:LEU:CD1 | 2.49 | 0.41 |
| 1:CC:39:ARG:CZ | 1:CS:20:ARG:CZ | 2.98 | 0.41 |
| 1:CJ:30:LEU:HA | 1:CJ:77:LEU:HD23 | 2.02 | 0.41 |
| 1:CT:39:ARG:O | 1:C3:7:LEU:CB | 2.68 | 0.41 |
| 1:CG:120:ILE:CD1 | 1:CQ:125:GLU:HG2 | 2.50 | 0.41 |
| 1:CE:64:LYS:HD3 | 1:CE:64:LYS:HA | 1.85 | 0.41 |
| 1:CO:95:VAL:HG12 | 1:CO:112:PHE:HE1 | 1.85 | 0.41 |
| 1:CV:4:GLU:CG | 1:CW:51:TRP:HD1 | 2.29 | 0.41 |
| 1:CZ:18:VAL:HG22 | 1:CZ:77:LEU:HB2 | 2.02 | 0.41 |
| 1:BF:18:VAL:HG22 | 1:BF:77:LEU:HB2 | 2.02 | 0.41 |
| 1:CH:18:VAL:HA | 1:CH:77:LEU:O | 2.19 | 0.41 |
| 1:A3:6:HIS:HB3 | 1:A3:147:HIS:CG | 2.55 | 0.41 |
| 1:BC:24:PHE:CE1 | 1:BU:28:LYS:HD2 | 2.53 | 0.41 |
| 1:AL:65:MET:HE3 | 1:AL:71:TYR:CE2 | 2.54 | 0.41 |
| 1:A1:71:TYR:O | 1:A1:108:ILE:HD13 | 2.21 | 0.41 |
| 1:CG:71:TYR:O | 1:CG:108:ILE:HD13 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:C1:71:TYR:O | 1:C1:108:ILE:HD13 | 2.21 | 0.41 |
| 1:AM:83:GLY:HA3 | 2:AM:1001:PO4:O3 | 2.20 | 0.41 |
| 1:AL:31:GLY:O | 1:AL:35:ASP:HB2 | 2.20 | 0.41 |
| 1:AT:6:HIS:HB3 | 1:AT:147:HIS:CG | 2.55 | 0.41 |
| 1:CU:21:PHE:O | 1:CU:22:ASN:HB2 | 2.20 | 0.41 |
| 1:C1:31:GLY:O | 1:C1:35:ASP:HB2 | 2.20 | 0.41 |
| 1:CL:31:GLY:O | 1:CL:35:ASP:HB2 | 2.20 | 0.41 |
| 1:CD:148:LEU:HA | 1:CD:148:LEU:HD23 | 1.82 | 0.41 |
| 1:AC:91:VAL:O | 1:AC:95:VAL:HG23 | 2.19 | 0.41 |
| 1:AF:106:THR:C | 1:AF:108:ILE:H | 2.23 | 0.41 |
| 1:AJ:52:VAL:CB | 1:AJ:53:PRO:CD | 2.98 | 0.41 |
| 1:CM:125:GLU:HA | 1:CM:129:THR:HB | 2.01 | 0.41 |
| 1:CM:129:THR:O | 1:CM:131:ALA:N | 2.53 | 0.41 |
| 1:AG:55:ALA:HA | 1:AG:58:ILE:HG13 | 2.02 | 0.41 |
| 1:CP:52:VAL:HB | 1:CP:53:PRO:CD | 2.50 | 0.41 |
| 1:BY:129:THR:O | 1:BY:130:LYS:C | 2.59 | 0.41 |
| 1:CO:129:THR:O | 1:CO:130:LYS:C | 2.59 | 0.41 |
| 1:AJ:30:LEU:HA | 1:AJ:77:LEU:HD23 | 2.03 | 0.41 |
| 1:CC:63:LYS:O | 1:CC:65:MET:N | 2.53 | 0.41 |
| 1:BM:63:LYS:O | 1:BM:65:MET:N | 2.53 | 0.41 |
| 1:CM:63:LYS:O | 1:CM:65:MET:N | 2.53 | 0.41 |
| 1:AM:63:LYS:O | 1:AM:65:MET:N | 2.53 | 0.41 |
| 1:AE:64:LYS:HA | 1:AE:64:LYS:HD3 | 1.85 | 0.41 |
| 1:AI:48:ASP:HB2 | 1:AI:71:TYR:CE1 | 2.50 | 0.41 |
| 1:BK:18:VAL:HG22 | 1:BK:77:LEU:HB2 | 2.02 | 0.41 |
| 1:AF:18:VAL:HG22 | 1:AF:77:LEU:HB2 | 2.02 | 0.41 |
| 1:AD:6:HIS:HB3 | 1:AD:147:HIS:CG | 2.55 | 0.41 |
| 1:C1:65:MET:HE3 | 1:C1:71:TYR:CE2 | 2.54 | 0.41 |
| 1:BG:71:TYR:O | 1:BG:108:ILE:HD13 | 2.21 | 0.41 |
| 1:CS:98:GLY:HA2 | 1:CS:102:LEU:HD23 | 2.02 | 0.41 |
| 1:AR:83:GLY:HA3 | 2:AR:1001:PO4:O3 | 2.20 | 0.41 |
| 1:CH:83:GLY:HA3 | 2:CH:2201:PO4:O3 | 2.20 | 0.41 |
| 1:BM:95:VAL:HG12 | 1:BM:112:PHE:HE1 | 1.86 | 0.41 |
| 1:AG:25:ILE:HG23 | 1:AG:127:ALA:HB2 | 2.03 | 0.41 |
| 1:BK:116:THR:O | 1:BL:85:THR:HB | 2.20 | 0.41 |
| 1:AN:150:LYS:HG3 | 1:AN:150:LYS:H | 1.33 | 0.41 |
| 1:AG:24:PHE:CD1 | 1:AQ:28:LYS:HG3 | 2.55 | 0.41 |
| 1:AX:29:LEU:HD11 | 1:AX:134:LYS:HB3 | 2.02 | 0.41 |
| 1:AC:125:GLU:HA | 1:AC:129:THR:HB | 2.01 | 0.41 |
| 1:BR:129:THR:O | 1:BR:131:ALA:N | 2.53 | 0.41 |
| 1:CE:65:MET:HE3 | 1:CE:71:TYR:CE2 | 2.55 | 0.41 |
| 1:BJ:65:MET:HE3 | 1:BJ:71:TYR:CE2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:AV:55:ALA:HA | 1:AV:58:ILE:HG13 | 2.02 | 0.41 |
| 1:CL:100:ALA:O | 1:CM:56:PHE:CE1 | 2.73 | 0.41 |
| 1:BV:97:LYS:N | 1:BV:100:ALA:HB2 | 2.31 | 0.41 |
| 1:AP:52:VAL:HB | 1:AP:53:PRO:CD | 2.50 | 0.41 |
| 1:BU:52:VAL:HB | 1:BU:53:PRO:CD | 2.50 | 0.41 |
| 1:CZ:52:VAL:HB | 1:CZ:53:PRO:CD | 2.50 | 0.41 |
| 1:CY:129:THR:O | 1:CY:130:LYS:C | 2.59 | 0.41 |
| 1:CJ:129:THR:O | 1:CJ:130:LYS:C | 2.59 | 0.41 |
| 1:C4:129:THR:O | 1:C4:130:LYS:C | 2.59 | 0.41 |
| 1:CD:28:LYS:HG3 | 1:CF:24:PHE:CD1 | 2.55 | 0.41 |
| 1:AO:30:LEU:HA | 1:AO:77:LEU:HD23 | 2.02 | 0.41 |
| 1:AR:63:LYS:O | 1:AR:65:MET:N | 2.53 | 0.41 |
| 1:A2:15:GLY:HA3 | 1:A2:65:MET:HE1 | 2.03 | 0.41 |
| 1:CW:63:LYS:O | 1:CW:65:MET:N | 2.53 | 0.41 |
| 1:AT:64:LYS:HA | 1:AT:64:LYS:HD3 | 1.85 | 0.41 |
| 1:BA:18:VAL:HG22 | 1:BA:77:LEU:HB2 | 2.02 | 0.41 |
| 1:BF:21:PHE:O | 1:BF:22:ASN:HB2 | 2.20 | 0.41 |
| 1:AE:7:LEU:HD12 | 1:AE:7:LEU:HA | 1.91 | 0.41 |
| 1:AS:39:ARG:O | 1:AY:7:LEU:HB3 | 2.21 | 0.41 |
| 1:CI:6:HIS:HB3 | 1:CI:147:HIS:CG | 2.55 | 0.41 |
| 1:BG:65:MET:HE3 | 1:BG:71:TYR:CE2 | 2.56 | 0.41 |
| 1:CJ:7:LEU:HD12 | 1:CJ:7:LEU:HA | 1.91 | 0.41 |
| 1:CY:6:HIS:HB3 | 1:CY:147:HIS:CG | 2.55 | 0.41 |
| 1:AK:106:THR:C | 1:AK:108:ILE:H | 2.23 | 0.41 |
| 1:CA:106:THR:C | 1:CA:108:ILE:H | 2.24 | 0.41 |
| 1:BA:116:THR:O | 1:BB:85:THR:HB | 2.20 | 0.41 |
| 1:AP:21:PHE:O | 1:AP:22:ASN:HB2 | 2.20 | 0.41 |
| 1:AD:148:LEU:HD23 | 1:AD:148:LEU:HA | 1.82 | 0.41 |
| 1:BC:148:LEU:HD23 | 1:BC:148:LEU:HA | 1.80 | 0.41 |
| 1:BF:106:THR:C | 1:BF:108:ILE:H | 2.24 | 0.41 |
| 1:BU:116:THR:O | 1:BV:85:THR:HB | 2.20 | 0.41 |
| 1:AB:31:GLY:O | 1:AB:35:ASP:HB2 | 2.20 | 0.41 |
| 1:CU:116:THR:O | 1:CV:85:THR:HB | 2.20 | 0.41 |
| 1:AW:129:THR:O | 1:AW:131:ALA:N | 2.53 | 0.41 |
| 1:AH:129:THR:O | 1:AH:131:ALA:N | 2.53 | 0.41 |
| 1:CB:104:LEU:HD13 | 1:CC:102:LEU:CD2 | 2.46 | 0.41 |
| 1:AE:108:ILE:CG1 | 1:AE:150:LYS:HE3 | 2.42 | 0.41 |
| 1:AE:65:MET:HE3 | 1:AE:71:TYR:CE2 | 2.55 | 0.41 |
| 1:AY:71:TYR:O | 1:AY:150:LYS:NZ | 2.44 | 0.41 |
| 1:C4:145:MET:O | 1:C4:149:SER:HB3 | 2.20 | 0.41 |
| 1:BB:100:ALA:O | 1:BC:56:PHE:CE1 | 2.73 | 0.41 |
| 1:AQ:100:ALA:O | 1:AR:56:PHE:CE1 | 2.73 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:AB:55:ALA:HB1 | 1:AB:95:VAL:CG2 | 2.40 | 0.41 |
| 1:AB:55:ALA:HA | 1:AB:58:ILE:HG13 | 2.02 | 0.41 |
| 1:CQ:100:ALA:O | 1:CR:56:PHE:CE1 | 2.73 | 0.41 |
| 1:BG:100:ALA:O | 1:BH:56:PHE:CE1 | 2.73 | 0.41 |
| 1:CN:52:VAL:CG1 | 1:CN:61:ILE:HD12 | 2.35 | 0.41 |
| 1:BP:52:VAL:HB | 1:BP:53:PRO:CD | 2.51 | 0.41 |
| 1:CK:52:VAL:HB | 1:CK:53:PRO:CD | 2.51 | 0.41 |
| 1:BO:129:THR:O | 1:BO:130:LYS:C | 2.59 | 0.41 |
| 1:AY:129:THR:O | 1:AY:130:LYS:C | 2.59 | 0.41 |
| 1:BJ:129:THR:O | 1:BJ:130:LYS:C | 2.59 | 0.41 |
| 1:CE:129:THR:O | 1:CE:130:LYS:C | 2.59 | 0.41 |
| 1:B2:34:LEU:HD22 | 1:B2:38:LYS:CE | 2.43 | 0.41 |
| 1:CK:76:THR:CG2 | 1:CK:112:PHE:HA | 2.51 | 0.41 |
| 1:BK:76:THR:CG2 | 1:BK:112:PHE:HA | 2.51 | 0.41 |
| 1:CO:64:LYS:HA | 1:CO:64:LYS:HD3 | 1.85 | 0.41 |
| 1:BT:95:VAL:HG12 | 1:BT:112:PHE:HE1 | 1.85 | 0.41 |
| 1:BY:14:VAL:HG21 | 1:BY:37:LEU:HD22 | 2.03 | 0.41 |
| 1:BG:4:GLU:CG | 1:BH:51:TRP:HD1 | 2.29 | 0.41 |
| 1:AO:95:VAL:HG12 | 1:AO:112:PHE:HE1 | 1.85 | 0.41 |
| 1:BW:63:LYS:O | 1:BW:65:MET:N | 2.53 | 0.41 |
| 1:AN:6:HIS:HB3 | 1:AN:147:HIS:CG | 2.55 | 0.41 |
| 1:BD:6:HIS:HB3 | 1:BD:147:HIS:CG | 2.55 | 0.41 |
| 1:AI:6:HIS:HB3 | 1:AI:147:HIS:CG | 2.55 | 0.41 |
| 1:B1:71:TYR:O | 1:B1:108:ILE:HD13 | 2.21 | 0.41 |
| 1:AV:71:TYR:O | 1:AV:108:ILE:HD13 | 2.21 | 0.41 |
| 1:CL:65:MET:HE3 | 1:CL:71:TYR:CE2 | 2.56 | 0.41 |
| 1:CL:71:TYR:O | 1:CL:108:ILE:HD13 | 2.21 | 0.41 |
| 1:CW:95:VAL:HG12 | 1:CW:112:PHE:HE1 | 1.86 | 0.41 |
| 1:CM:95:VAL:HG12 | 1:CM:112:PHE:HE1 | 1.86 | 0.41 |
| 1:BZ:116:THR:O | 1:B1:85:THR:HB | 2.20 | 0.41 |
| 1:BL:25:ILE:HG23 | 1:BL:127:ALA:HB2 | 2.03 | 0.41 |
| 1:BQ:25:ILE:HG23 | 1:BQ:127:ALA:HB2 | 2.03 | 0.41 |
| 1:CE:6:HIS:HB3 | 1:CE:147:HIS:CG | 2.55 | 0.41 |
| 1:BV:31:GLY:O | 1:BV:35:ASP:HB2 | 2.20 | 0.41 |
| 1:CU:106:THR:C | 1:CU:108:ILE:H | 2.23 | 0.41 |
| 1:B4:6:HIS:HB3 | 1:B4:147:HIS:CG | 2.55 | 0.41 |
| 1:CZ:21:PHE:O | 1:CZ:22:ASN:HB2 | 2.20 | 0.41 |
| 1:BF:116:THR:O | 1:BG:85:THR:HB | 2.20 | 0.41 |
| 1:BT:52:VAL:CB | 1:BT:53:PRO:CD | 2.98 | 0.41 |
| 1:AG:100:ALA:O | 1:AH:56:PHE:CE1 | 2.73 | 0.41 |
| 1:BL:100:ALA:O | 1:BM:56:PHE:CE1 | 2.73 | 0.41 |
| 1:AA:52:VAL:HB | 1:AA:53:PRO:CD | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A4:129:THR:O | 1:A4:130:LYS:C | 2.59 | 0.41 |
| 1:BT:30:LEU:HA | 1:BT:77:LEU:HD23 | 2.03 | 0.41 |
| 1:BW:34:LEU:HD22 | 1:BW:38:LYS:CE | 2.43 | 0.41 |
| 1:CH:65:MET:HB3 | 1:CH:65:MET:HE3 | 1.91 | 0.41 |
| 1:CU:76:THR:CG2 | 1:CU:112:PHE:HA | 2.51 | 0.41 |
| 1:C2:67:ASN:HD22 | 1:C2:67:ASN:HA | 1.59 | 0.41 |
| 1:BF:76:THR:CG2 | 1:BF:112:PHE:HA | 2.51 | 0.41 |
| 1:CF:76:THR:CG2 | 1:CF:112:PHE:HA | 2.51 | 0.41 |
| 1:CT:14:VAL:HG21 | 1:CT:37:LEU:HD22 | 2.03 | 0.41 |
| 1:BY:95:VAL:HG12 | 1:BY:112:PHE:HE1 | 1.85 | 0.41 |
| 1:C4:95:VAL:HG12 | 1:C4:112:PHE:HE1 | 1.85 | 0.41 |
| 1:CR:63:LYS:O | 1:CR:65:MET:N | 2.53 | 0.41 |
| 1:C4:21:PHE:O | 1:C4:22:ASN:HB2 | 2.19 | 0.41 |
| 1:CU:18:VAL:HG22 | 1:CU:77:LEU:HB2 | 2.02 | 0.41 |
| 1:AS:6:HIS:HB3 | 1:AS:147:HIS:CG | 2.55 | 0.41 |
| 1:CS:6:HIS:HB3 | 1:CS:147:HIS:CG | 2.55 | 0.41 |
| 1:AN:98:GLY:HA2 | 1:AN:102:LEU:HD23 | 2.02 | 0.41 |
| 1:BX:98:GLY:HA2 | 1:BX:102:LEU:HD23 | 2.02 | 0.41 |
| 1:BV:71:TYR:O | 1:BV:108:ILE:HD13 | 2.21 | 0.41 |
| 1:CI:98:GLY:HA2 | 1:CI:102:LEU:HD23 | 2.02 | 0.41 |
| 1:AR:95:VAL:HG12 | 1:AR:112:PHE:HE1 | 1.86 | 0.41 |
| 1:AH:95:VAL:HG12 | 1:AH:112:PHE:HE1 | 1.86 | 0.41 |
| 1:BC:95:VAL:HG12 | 1:BC:112:PHE:HE1 | 1.86 | 0.41 |
| 1:CH:95:VAL:HG12 | 1:CH:112:PHE:HE1 | 1.86 | 0.41 |
| 1:BU:21:PHE:O | 1:BU:22:ASN:HB2 | 2.20 | 0.41 |
| 1:BA:106:THR:C | 1:BA:108:ILE:H | 2.24 | 0.41 |
| 1:BV:25:ILE:HG23 | 1:BV:127:ALA:HB2 | 2.03 | 0.41 |
| 1:AK:116:THR:O | 1:AL:85:THR:HB | 2.20 | 0.41 |
| 1:CH:45:ASN:HD22 | 1:CH:45:ASN:HA | 1.64 | 0.41 |
| 1:CG:25:ILE:HG23 | 1:CG:127:ALA:HB2 | 2.03 | 0.41 |
| 1:AP:106:THR:C | 1:AP:108:ILE:H | 2.24 | 0.41 |
| 1:BB:25:ILE:HG23 | 1:BB:127:ALA:HB2 | 2.03 | 0.41 |
| 1:AC:129:THR:O | 1:AC:131:ALA:N | 2.53 | 0.41 |
| 1:AM:129:THR:O | 1:AM:131:ALA:N | 2.53 | 0.41 |
| 1:CE:71:TYR:O | 1:CE:150:LYS:NZ | 2.44 | 0.41 |
| 1:BO:65:MET:HE3 | 1:BO:71:TYR:CE2 | 2.55 | 0.41 |
| 1:C1:100:ALA:O | 1:C2:56:PHE:CE1 | 2.73 | 0.41 |
| 1:A1:97:LYS:HE3 | 1:A2:97:LYS:HZ3 | 1.85 | 0.41 |
| 1:AU:53:PRO:HD2 | 1:AU:57:GLU:CB | 2.49 | 0.41 |
| 1:CX:20:ARG:HD3 | 1:C2:39:ARG:NH2 | 2.35 | 0.41 |
| 1:BR:34:LEU:HD22 | 1:BR:38:LYS:CE | 2.43 | 0.41 |
| 1:BO:30:LEU:HA | 1:BO:77:LEU:HD23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CE:30:LEU:HA | 1:CE:77:LEU:HD23 | 2.02 | 0.41 |
| 1:AW:63:LYS:O | 1:AW:65:MET:N | 2.53 | 0.41 |
| 1:AJ:64:LYS:HA | 1:AJ:64:LYS:HD3 | 1.85 | 0.41 |
| 1:CJ:14:VAL:HG21 | 1:CJ:37:LEU:HD22 | 2.03 | 0.41 |
| 1:CV:71:TYR:O | 1:CV:108:ILE:HD13 | 2.21 | 0.41 |
| 1:CB:71:TYR:O | 1:CB:108:ILE:HD13 | 2.21 | 0.41 |
| 1:A3:98:GLY:HA2 | 1:A3:102:LEU:HD23 | 2.02 | 0.41 |
| 1:AA:106:THR:C | 1:AA:108:ILE:H | 2.23 | 0.41 |
| 1:AV:31:GLY:O | 1:AV:35:ASP:HB2 | 2.20 | 0.41 |
| 1:AE:28:LYS:HG3 | 1:AO:24:PHE:CD1 | 2.56 | 0.41 |
| 1:AF:21:PHE:O | 1:AF:22:ASN:HB2 | 2.20 | 0.41 |
| 1:CB:83:GLY:HA3 | 2:CB:1001:PO4:O1 | 2.21 | 0.41 |
| 1:A1:25:ILE:HG23 | 1:A1:127:ALA:HB2 | 2.03 | 0.41 |
| 1:CK:106:THR:C | 1:CK:108:ILE:H | 2.24 | 0.41 |
| 1:AF:116:THR:O | 1:AG:85:THR:HB | 2.20 | 0.41 |
| 1:CK:116:THR:O | 1:CL:85:THR:HB | 2.20 | 0.41 |
| 1:C2:129:THR:O | 1:C2:131:ALA:N | 2.53 | 0.41 |
| 1:CR:129:THR:O | 1:CR:131:ALA:N | 2.53 | 0.41 |
| 1:CW:129:THR:O | 1:CW:131:ALA:N | 2.53 | 0.41 |
| 1:AQ:70:LYS:HG3 | 1:BU:43:GLU:OE1 | 2.20 | 0.41 |
| 1:BB:104:LEU:HD13 | 1:BC:102:LEU:CD2 | 2.46 | 0.41 |
| 1:AJ:65:MET:HE3 | 1:AJ:71:TYR:CE2 | 2.56 | 0.41 |
| 1:AT:108:ILE:CG1 | 1:AT:150:LYS:HE3 | 2.42 | 0.41 |
| 1:BB:55:ALA:HA | 1:BB:58:ILE:HG13 | 2.02 | 0.41 |
| 1:AL:100:ALA:O | 1:AM:56:PHE:CE1 | 2.73 | 0.41 |
| 1:AB:58:ILE:O | 1:AB:62:ALA:CB | 2.69 | 0.41 |
| 1:B1:55:ALA:HB1 | 1:B1:95:VAL:CG2 | 2.40 | 0.41 |
| 1:B1:100:ALA:O | 1:B2:56:PHE:CE1 | 2.73 | 0.41 |
| 1:B2:97:LYS:HE3 | 1:B3:97:LYS:HZ3 | 1.85 | 0.41 |
| 1:BF:40:HIS:CE1 | 1:BQ:7:LEU:HD23 | 2.56 | 0.41 |
| 1:BF:52:VAL:HB | 1:BF:53:PRO:CD | 2.50 | 0.41 |
| 1:CF:52:VAL:HB | 1:CF:53:PRO:CD | 2.51 | 0.41 |
| 1:CA:52:VAL:HB | 1:CA:53:PRO:CD | 2.50 | 0.41 |
| 1:BZ:52:VAL:HB | 1:BZ:53:PRO:CD | 2.50 | 0.41 |
| 1:BT:129:THR:O | 1:BT:130:LYS:C | 2.59 | 0.41 |
| 1:AJ:129:THR:O | 1:AJ:130:LYS:C | 2.59 | 0.41 |
| 1:AE:129:THR:O | 1:AE:130:LYS:C | 2.59 | 0.41 |
| 1:AM:34:LEU:HD22 | 1:AM:38:LYS:CE | 2.43 | 0.41 |
| 1:AE:30:LEU:HA | 1:AE:77:LEU:HD23 | 2.02 | 0.41 |
| 1:CO:30:LEU:HA | 1:CO:77:LEU:HD23 | 2.02 | 0.41 |
| 1:BJ:30:LEU:HA | 1:BJ:77:LEU:HD23 | 2.02 | 0.41 |
| 1:BZ:76:THR:CG2 | 1:BZ:112:PHE:HA | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AM:67:ASN:HD22 | 1:AM:67:ASN:HA | 1.59 | 0.41 |
| 1:AM:15:GLY:HA3 | 1:AM:65:MET:HE1 | 2.03 | 0.41 |
| 1:CH:63:LYS:O | 1:CH:65:MET:N | 2.53 | 0.41 |
| 1:CT:30:LEU:HA | 1:CT:77:LEU:HD23 | 2.02 | 0.41 |
| 1:AC:63:LYS:O | 1:AC:65:MET:N | 2.53 | 0.41 |
| 1:BU:76:THR:CG2 | 1:BU:112:PHE:HA | 2.51 | 0.41 |
| 1:AK:76:THR:CG2 | 1:AK:112:PHE:HA | 2.51 | 0.41 |
| 1:CA:76:THR:CG2 | 1:CA:112:PHE:HA | 2.51 | 0.41 |
| 1:AF:76:THR:CG2 | 1:AF:112:PHE:HA | 2.51 | 0.41 |
| 1:CP:76:THR:CG2 | 1:CP:112:PHE:HA | 2.51 | 0.41 |
| 1:AY:14:VAL:HG12 | 1:AY:15:GLY:N | 2.36 | 0.41 |
| 1:CJ:95:VAL:HG12 | 1:CJ:112:PHE:HE1 | 1.85 | 0.41 |
| 1:BC:63:LYS:O | 1:BC:65:MET:N | 2.53 | 0.41 |
| 1:CL:129:THR:CG2 | 1:CL:130:LYS:H | 2.28 | 0.41 |
| 1:AE:7:LEU:HD23 | 1:AN:40:HIS:CE1 | 2.56 | 0.41 |
| 1:AS:98:GLY:HA2 | 1:AS:102:LEU:HD23 | 2.02 | 0.41 |
| 1:AG:71:TYR:O | 1:AG:108:ILE:HD13 | 2.21 | 0.41 |
| 1:BL:71:TYR:O | 1:BL:108:ILE:HD13 | 2.21 | 0.41 |
| 1:C3:98:GLY:HA2 | 1:C3:102:LEU:HD23 | 2.02 | 0.41 |
| 1:AM:95:VAL:HG12 | 1:AM:112:PHE:HE1 | 1.86 | 0.41 |
| 1:C2:95:VAL:HG12 | 1:C2:112:PHE:HE1 | 1.86 | 0.41 |
| 1:AC:95:VAL:HG12 | 1:AC:112:PHE:HE1 | 1.86 | 0.41 |
| 1:AQ:25:ILE:HG23 | 1:AQ:127:ALA:HB2 | 2.03 | 0.41 |
| 1:CN:29:LEU:HD11 | 1:CN:134:LYS:HB3 | 2.02 | 0.41 |
| 1:AA:116:THR:O | 1:AB:85:THR:HB | 2.20 | 0.41 |
| 1:AU:32:GLY:HA3 | 1:AU:135:GLY:C | 2.42 | 0.41 |
| 1:CA:116:THR:O | 1:CB:85:THR:HB | 2.20 | 0.41 |
| 1:BC:45:ASN:HD22 | 1:BC:45:ASN:HA | 1.64 | 0.41 |
| 1:AD:29:LEU:HD11 | 1:AD:134:LYS:HB3 | 2.02 | 0.41 |
| 1:CT:6:HIS:HB3 | 1:CT:147:HIS:CG | 2.55 | 0.41 |
| 1:CF:106:THR:C | 1:CF:108:ILE:H | 2.24 | 0.41 |
| 1:CA:26:THR:HA | 1:CA:29:LEU:HB3 | 2.03 | 0.41 |
| 1:AB:83:GLY:HA3 | 2:AB:1001:PO4:O1 | 2.21 | 0.41 |
| 1:CL:25:ILE:HG23 | 1:CL:127:ALA:HB2 | 2.03 | 0.41 |
| 1:AB:25:ILE:HG23 | 1:AB:127:ALA:HB2 | 2.03 | 0.41 |
| 1:AL:111:ILE:N | 1:AL:111:ILE:HD12 | 2.36 | 0.41 |
| 1:CL:83:GLY:HA3 | 2:CL:1201:PO4:O1 | 2.21 | 0.41 |
| 1:A1:104:LEU:HD13 | 1:A2:102:LEU:CD2 | 2.46 | 0.41 |
| 1:CH:129:THR:O | 1:CH:131:ALA:N | 2.53 | 0.41 |
| 1:BL:55:ALA:HB1 | 1:BL:95:VAL:CG2 | 2.40 | 0.41 |
| 1:CL:55:ALA:CB | 1:CL:95:VAL:HG21 | 2.40 | 0.41 |
| 1:CG:58:ILE:O | 1:CG:62:ALA:CB | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A1:58:ILE:O | 1:A1:62:ALA:CB | 2.69 | 0.41 |
| 1:AF:52:VAL:HB | 1:AF:53:PRO:CD | 2.50 | 0.41 |
| 1:CC:39:ARG:NE | 1:CS:20:ARG:CZ | 2.84 | 0.41 |
| 1:CH:34:LEU:HD22 | 1:CH:38:LYS:CE | 2.43 | 0.41 |
| 1:AA:58:ILE:N | 1:AA:59:PRO:CD | 2.84 | 0.41 |
| 1:AZ:76:THR:CG2 | 1:AZ:112:PHE:HA | 2.51 | 0.41 |
| 1:BJ:64:LYS:HD3 | 1:BJ:64:LYS:HA | 1.85 | 0.41 |
| 1:AE:14:VAL:HG21 | 1:AE:37:LEU:HD22 | 2.03 | 0.41 |
| 1:C4:14:VAL:HG12 | 1:C4:15:GLY:N | 2.36 | 0.41 |
| 1:AY:14:VAL:HG21 | 1:AY:37:LEU:HD22 | 2.03 | 0.41 |
| 1:AJ:95:VAL:HG12 | 1:AJ:112:PHE:HE1 | 1.85 | 0.41 |
| 1:AJ:14:VAL:HG12 | 1:AJ:15:GLY:N | 2.36 | 0.41 |
| 1:BY:14:VAL:HG12 | 1:BY:15:GLY:N | 2.36 | 0.41 |
| 1:B3:7:LEU:HD12 | 1:B3:7:LEU:HA | 1.96 | 0.41 |
| 1:BP:18:VAL:HG22 | 1:BP:77:LEU:HB2 | 2.02 | 0.41 |
| 1:CG:129:THR:CG2 | 1:CG:130:LYS:H | 2.28 | 0.41 |
| 1:C1:129:THR:CG2 | 1:C1:130:LYS:H | 2.28 | 0.41 |
| 1:AQ:71:TYR:O | 1:AQ:108:ILE:HD13 | 2.21 | 0.41 |
| 1:AQ:65:MET:HE3 | 1:AQ:71:TYR:CE2 | 2.56 | 0.41 |
| 1:CQ:65:MET:HE3 | 1:CQ:71:TYR:CE2 | 2.56 | 0.41 |
| 1:AB:71:TYR:O | 1:AB:108:ILE:HD13 | 2.21 | 0.41 |
| 1:BW:83:GLY:HA3 | 2:BW:1001:PO4:O3 | 2.20 | 0.41 |
| 1:AW:83:GLY:HA3 | 2:AW:201:PO4:P | 2.60 | 0.41 |
| 1:BO:14:VAL:HG12 | 1:BO:15:GLY:N | 2.36 | 0.41 |
| 1:B2:95:VAL:HG12 | 1:B2:112:PHE:HE1 | 1.86 | 0.41 |
| 1:CP:106:THR:C | 1:CP:108:ILE:H | 2.23 | 0.41 |
| 1:BG:83:GLY:HA3 | 2:BG:1001:PO4:O1 | 2.21 | 0.41 |
| 1:AI:29:LEU:HD11 | 1:AI:134:LYS:HB3 | 2.02 | 0.41 |
| 1:BQ:83:GLY:HA3 | 2:BQ:1001:PO4:O1 | 2.21 | 0.41 |
| 1:CB:31:GLY:O | 1:CB:35:ASP:HB2 | 2.20 | 0.41 |
| 1:BB:83:GLY:HA3 | 2:BB:1001:PO4:O1 | 2.21 | 0.41 |
| 1:AP:26:THR:HA | 1:AP:29:LEU:HB3 | 2.03 | 0.41 |
| 1:CV:31:GLY:O | 1:CV:35:ASP:HB2 | 2.20 | 0.41 |
| 1:BG:111:ILE:HD12 | 1:BG:111:ILE:N | 2.36 | 0.41 |
| 1:CF:26:THR:HA | 1:CF:29:LEU:HB3 | 2.03 | 0.41 |
| 1:C1:83:GLY:HA3 | 2:C1:1201:PO4:O1 | 2.21 | 0.41 |
| 1:AS:97:LYS:HG3 | 1:AT:97:LYS:HZ1 | 1.86 | 0.40 |
| 1:BQ:58:ILE:O | 1:BQ:62:ALA:CB | 2.69 | 0.40 |
| 1:AY:30:LEU:HA | 1:AY:77:LEU:HD23 | 2.02 | 0.40 |
| 1:BR:15:GLY:HA3 | 1:BR:65:MET:HE1 | 2.02 | 0.40 |
| 1:AC:15:GLY:HA3 | 1:AC:65:MET:HE1 | 2.03 | 0.40 |
| 1:AP:76:THR:CG2 | 1:AP:112:PHE:HA | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AE:14:VAL:HG12 | 1:AE:15:GLY:N | 2.36 | 0.40 |
| 1:CZ:7:LEU:HA | 1:CZ:7:LEU:HD12 | 1.84 | 0.40 |
| 1:CK:18:VAL:HG22 | 1:CK:77:LEU:HB2 | 2.02 | 0.40 |
| 1:CQ:71:TYR:O | 1:CQ:108:ILE:HD13 | 2.21 | 0.40 |
| 1:CD:98:GLY:HA2 | 1:CD:102:LEU:HD23 | 2.02 | 0.40 |
| 1:BJ:14:VAL:HG12 | 1:BJ:15:GLY:N | 2.36 | 0.40 |
| 1:AQ:83:GLY:HA3 | 2:AQ:1001:PO4:O1 | 2.21 | 0.40 |
| 1:B1:25:ILE:HG23 | 1:B1:127:ALA:HB2 | 2.03 | 0.40 |
| 1:CB:25:ILE:HG23 | 1:CB:127:ALA:HB2 | 2.03 | 0.40 |
| 1:CD:29:LEU:HD11 | 1:CD:134:LYS:HB3 | 2.02 | 0.40 |
| 1:BQ:111:ILE:HD12 | 1:BQ:111:ILE:N | 2.36 | 0.40 |
| 1:CG:111:ILE:N | 1:CG:111:ILE:HD12 | 2.37 | 0.40 |
| 1:AV:25:ILE:HG23 | 1:AV:127:ALA:HB2 | 2.03 | 0.40 |
| 1:B1:83:GLY:HA3 | 2:B1:1001:PO4:O1 | 2.21 | 0.40 |
| 1:CP:32:GLY:HA3 | 1:CP:135:GLY:C | 2.42 | 0.40 |
| 1:AK:26:THR:HA | 1:AK:29:LEU:HB3 | 2.04 | 0.40 |
| 1:A1:23:GLU:HA | 1:A1:26:THR:OG1 | 2.22 | 0.40 |
| 1:AL:23:GLU:HA | 1:AL:26:THR:OG1 | 2.21 | 0.40 |
| 1:CY:108:ILE:CG1 | 1:CY:150:LYS:HE3 | 2.42 | 0.40 |
| 1:BG:58:ILE:O | 1:BG:62:ALA:CB | 2.69 | 0.40 |
| 1:CG:55:ALA:HA | 1:CG:58:ILE:HG13 | 2.02 | 0.40 |
| 1:A3:97:LYS:HG3 | 1:A4:97:LYS:HZ1 | 1.86 | 0.40 |
| 1:BM:20:ARG:HH11 | 1:BM:20:ARG:HB3 | 1.87 | 0.40 |
| 1:CZ:76:THR:CG2 | 1:CZ:112:PHE:HA | 2.51 | 0.40 |
| 1:AO:14:VAL:HG21 | 1:AO:37:LEU:HD22 | 2.03 | 0.40 |
| 1:CY:14:VAL:HG21 | 1:CY:37:LEU:HD22 | 2.03 | 0.40 |
| 1:B2:63:LYS:O | 1:B2:65:MET:N | 2.53 | 0.40 |
| 1:BW:95:VAL:HG12 | 1:BW:112:PHE:HE1 | 1.86 | 0.40 |
| 1:A4:14:VAL:HG12 | 1:A4:15:GLY:N | 2.36 | 0.40 |
| 1:CR:95:VAL:HG12 | 1:CR:112:PHE:HE1 | 1.86 | 0.40 |
| 1:BF:32:GLY:HA3 | 1:BF:135:GLY:C | 2.42 | 0.40 |
| 1:CF:116:THR:O | 1:CG:85:THR:HB | 2.20 | 0.40 |
| 1:CU:32:GLY:HA3 | 1:CU:135:GLY:C | 2.42 | 0.40 |
| 1:CV:25:ILE:HG23 | 1:CV:127:ALA:HB2 | 2.03 | 0.40 |
| 1:AQ:111:ILE:N | 1:AQ:111:ILE:HD12 | 2.36 | 0.40 |
| 1:BW:148:LEU:HA | 1:BW:148:LEU:HD23 | 1.80 | 0.40 |
| 1:AG:83:GLY:HA3 | 2:AG:1001:PO4:O1 | 2.21 | 0.40 |
| 1:AT:53:PRO:HD2 | 1:AT:57:GLU:CB | 2.52 | 0.40 |
| 1:BW:121:GLU:O | 1:BW:125:GLU:HB2 | 2.22 | 0.40 |
| 1:AG:58:ILE:O | 1:AG:62:ALA:CB | 2.69 | 0.40 |
| 1:AL:58:ILE:O | 1:AL:62:ALA:CB | 2.69 | 0.40 |
| 1:B1:58:ILE:O | 1:B1:62:ALA:CB | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CL:55:ALA:HA | 1:CL:58:ILE:HG13 | 2.02 | 0.40 |
| 1:AK:53:PRO:HD2 | 1:AK:57:GLU:CB | 2.49 | 0.40 |
| 1:B4:129:THR:O | 1:B4:130:LYS:C | 2.59 | 0.40 |
| 1:CZ:58:ILE:N | 1:CZ:59:PRO:CD | 2.84 | 0.40 |
| 1:CW:15:GLY:HA3 | 1:CW:65:MET:HE1 | 2.04 | 0.40 |
| 1:CM:106:THR:HG23 | 1:CM:107:ASP:N | 2.37 | 0.40 |
| 1:AO:14:VAL:HG12 | 1:AO:15:GLY:N | 2.36 | 0.40 |
| 1:BH:106:THR:HG23 | 1:BH:107:ASP:N | 2.37 | 0.40 |
| 1:CO:14:VAL:HG12 | 1:CO:15:GLY:N | 2.36 | 0.40 |
| 1:CO:14:VAL:HG21 | 1:CO:37:LEU:HD22 | 2.03 | 0.40 |
| 1:AH:106:THR:HG23 | 1:AH:107:ASP:N | 2.37 | 0.40 |
| 1:CJ:14:VAL:HG12 | 1:CJ:15:GLY:N | 2.36 | 0.40 |
| 1:CI:7:LEU:HD12 | 1:CI:7:LEU:HA | 1.96 | 0.40 |
| 1:BF:28:LYS:HE3 | 1:BR:28:LYS:NZ | 2.37 | 0.40 |
| 1:AL:71:TYR:O | 1:AL:108:ILE:HD13 | 2.21 | 0.40 |
| 1:BN:98:GLY:HA2 | 1:BN:102:LEU:HD23 | 2.02 | 0.40 |
| 1:BB:71:TYR:O | 1:BB:108:ILE:HD13 | 2.21 | 0.40 |
| 1:BE:14:VAL:HG12 | 1:BE:15:GLY:N | 2.36 | 0.40 |
| 1:BL:23:GLU:HA | 1:BL:26:THR:OG1 | 2.22 | 0.40 |
| 1:BV:23:GLU:HA | 1:BV:26:THR:OG1 | 2.22 | 0.40 |
| 1:BK:106:THR:C | 1:BK:108:ILE:H | 2.23 | 0.40 |
| 1:CQ:122:GLN:O | 1:CQ:126:ARG:HD2 | 2.22 | 0.40 |
| 1:AP:67:ASN:HA | 1:AP:67:ASN:HD22 | 1.69 | 0.40 |
| 1:AV:83:GLY:HA3 | 2:AV:1001:PO4:O1 | 2.21 | 0.40 |
| 1:CG:23:GLU:HA | 1:CG:26:THR:OG1 | 2.22 | 0.40 |
| 1:C1:122:GLN:O | 1:C1:126:ARG:HD2 | 2.22 | 0.40 |
| 1:CK:32:GLY:HA3 | 1:CK:135:GLY:C | 2.42 | 0.40 |
| 1:AE:52:VAL:CB | 1:AE:53:PRO:CD | 2.98 | 0.40 |
| 1:AJ:53:PRO:HD2 | 1:AJ:57:GLU:CB | 2.52 | 0.40 |
| 1:BY:53:PRO:HD2 | 1:BY:57:GLU:CB | 2.52 | 0.40 |
| 1:C2:121:GLU:O | 1:C2:125:GLU:HB2 | 2.22 | 0.40 |
| 1:BE:71:TYR:O | 1:BE:150:LYS:NZ | 2.44 | 0.40 |
| 1:B4:65:MET:HE3 | 1:B4:71:TYR:CE2 | 2.56 | 0.40 |
| 1:CT:65:MET:HE3 | 1:CT:71:TYR:CE2 | 2.57 | 0.40 |
| 1:BB:58:ILE:O | 1:BB:62:ALA:CB | 2.69 | 0.40 |
| 1:CA:97:LYS:NZ | 1:CE:97:LYS:HG3 | 2.37 | 0.40 |
| 1:AO:129:THR:O | 1:AO:130:LYS:C | 2.59 | 0.40 |
| 1:CT:129:THR:O | 1:CT:130:LYS:C | 2.59 | 0.40 |
| 1:CM:34:LEU:HD22 | 1:CM:38:LYS:CE | 2.43 | 0.40 |
| 1:BY:30:LEU:HA | 1:BY:77:LEU:HD23 | 2.02 | 0.40 |
| 1:AA:76:THR:CG2 | 1:AA:112:PHE:HA | 2.51 | 0.40 |
| 1:AF:58:ILE:N | 1:AF:59:PRO:CD | 2.84 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AW:106:THR:HG23 | 1:AW:107:ASP:N | 2.37 | 0.40 |
| 1:C3:17:VAL:CG2 | 1:C3:76:THR:HG22 | 2.52 | 0.40 |
| 1:C4:14:VAL:HG21 | 1:C4:37:LEU:HD22 | 2.03 | 0.40 |
| 1:AJ:14:VAL:HG21 | 1:AJ:37:LEU:HD22 | 2.03 | 0.40 |
| 1:BN:17:VAL:CG2 | 1:BN:76:THR:HG22 | 2.52 | 0.40 |
| 1:CN:98:GLY:HA2 | 1:CN:102:LEU:HD23 | 2.02 | 0.40 |
| 1:AW:95:VAL:HG12 | 1:AW:112:PHE:HE1 | 1.86 | 0.40 |
| 1:CG:83:GLY:HA3 | 2:CG:1201:PO4:O1 | 2.21 | 0.40 |
| 1:BU:26:THR:HA | 1:BU:29:LEU:HB3 | 2.04 | 0.40 |
| 1:CB:23:GLU:HA | 1:CB:26:THR:OG1 | 2.21 | 0.40 |
| 1:CL:23:GLU:HA | 1:CL:26:THR:OG1 | 2.21 | 0.40 |
| 1:BL:83:GLY:HA3 | 2:BL:1001:PO4:O1 | 2.21 | 0.40 |
| 1:AB:122:GLN:O | 1:AB:126:ARG:HD2 | 2.22 | 0.40 |
| 1:CQ:25:ILE:HG23 | 1:CQ:127:ALA:HB2 | 2.03 | 0.40 |
| 1:AU:151:HIS:O | 1:AU:151:HIS:CD2 | 2.75 | 0.40 |
| 1:BF:151:HIS:CD2 | 1:BF:151:HIS:O | 2.75 | 0.40 |
| 1:CF:151:HIS:CD2 | 1:CF:151:HIS:O | 2.75 | 0.40 |
| 1:AE:53:PRO:HD2 | 1:AE:57:GLU:CB | 2.52 | 0.40 |
| 1:BO:53:PRO:HD2 | 1:BO:57:GLU:CB | 2.52 | 0.40 |
| 1:CE:53:PRO:HD2 | 1:CE:57:GLU:CB | 2.52 | 0.40 |
| 1:AY:53:PRO:HD2 | 1:AY:57:GLU:CB | 2.52 | 0.40 |
| 1:CW:121:GLU:O | 1:CW:125:GLU:HB2 | 2.22 | 0.40 |
| 1:CH:121:GLU:O | 1:CH:125:GLU:HB2 | 2.22 | 0.40 |
| 1:AB:104:LEU:HD23 | 1:AC:60:LEU:CD1 | 2.52 | 0.40 |
| 1:BQ:104:LEU:HD23 | 1:BR:60:LEU:CD1 | 2.52 | 0.40 |
| 1:BY:65:MET:HE3 | 1:BY:71:TYR:CE2 | 2.56 | 0.40 |
| 1:AF:97:LYS:NZ | 1:AJ:97:LYS:HG3 | 2.37 | 0.40 |
| 1:AU:76:THR:CG2 | 1:AU:112:PHE:HA | 2.51 | 0.40 |
| 1:B4:30:LEU:HA | 1:B4:77:LEU:HD23 | 2.02 | 0.40 |
| 1:CU:129:THR:HB | 1:CU:130:LYS:H | 1.75 | 0.40 |
| 1:CH:15:GLY:HA3 | 1:CH:65:MET:HE1 | 2.02 | 0.40 |
| 1:BU:58:ILE:N | 1:BU:59:PRO:CD | 2.84 | 0.40 |
| 1:BP:76:THR:CG2 | 1:BP:112:PHE:HA | 2.51 | 0.40 |
| 1:C2:106:THR:HG23 | 1:C2:107:ASP:N | 2.37 | 0.40 |
| 1:B2:106:THR:HG23 | 1:B2:107:ASP:N | 2.37 | 0.40 |
| 1:CN:17:VAL:CG2 | 1:CN:76:THR:HG22 | 2.52 | 0.40 |
| 1:BT:64:LYS:HA | 1:BT:64:LYS:HD3 | 1.85 | 0.40 |
| 1:AR:106:THR:HG23 | 1:AR:107:ASP:N | 2.37 | 0.40 |
| 1:AT:14:VAL:HG21 | 1:AT:37:LEU:HD22 | 2.03 | 0.40 |
| 1:AC:106:THR:HG23 | 1:AC:107:ASP:N | 2.37 | 0.40 |
| 1:CY:14:VAL:HG12 | 1:CY:15:GLY:N | 2.36 | 0.40 |
| 1:CD:17:VAL:CG2 | 1:CD:76:THR:HG22 | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:CX:17:VAL:CG2 | 1:CX:76:THR:HG22 | 2.52 | 0.40 |
| 1:BS:40:HIS:CE1 | 1:BY:7:LEU:HD23 | 2.57 | 0.40 |
| 1:CT:8:VAL:HG22 | 1:C3:8:VAL:HG13 | 2.01 | 0.40 |
| 1:CH:28:LYS:HZ3 | 1:CU:28:LYS:CE | 2.34 | 0.40 |
| 1:BA:15:GLY:HA3 | 1:BA:65:MET:CE | 2.52 | 0.40 |
| 1:BB:23:GLU:HA | 1:BB:26:THR:OG1 | 2.22 | 0.40 |
| 1:BZ:106:THR:C | 1:BZ:108:ILE:H | 2.23 | 0.40 |
| 1:BK:26:THR:HA | 1:BK:29:LEU:HB3 | 2.04 | 0.40 |
| 1:BU:32:GLY:HA3 | 1:BU:135:GLY:C | 2.42 | 0.40 |
| 1:CF:32:GLY:HA3 | 1:CF:135:GLY:C | 2.42 | 0.40 |
| 1:BH:80:VAL:HG12 | 1:BH:88:TYR:CD1 | 2.57 | 0.40 |
| 1:C1:25:ILE:HG23 | 1:C1:127:ALA:HB2 | 2.03 | 0.40 |
| 1:BF:26:THR:HA | 1:BF:29:LEU:HB3 | 2.03 | 0.40 |
| 1:AV:111:ILE:N | 1:AV:111:ILE:HD12 | 2.36 | 0.40 |
| 1:CZ:151:HIS:O | 1:CZ:151:HIS:CG | 2.75 | 0.40 |
| 1:AF:151:HIS:CD2 | 1:AF:151:HIS:O | 2.75 | 0.40 |
| 1:AP:151:HIS:CD2 | 1:AP:151:HIS:O | 2.75 | 0.40 |
| 1:AG:122:GLN:O | 1:AG:126:ARG:HD2 | 2.22 | 0.40 |
| 1:BW:80:VAL:HG12 | 1:BW:88:TYR:CD1 | 2.57 | 0.40 |
| 1:CM:80:VAL:HG12 | 1:CM:88:TYR:CD1 | 2.57 | 0.40 |
| 1:AU:26:THR:HA | 1:AU:29:LEU:HB3 | 2.03 | 0.40 |

All (13) 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 | Distance(Å) | Clash(Å) |
|------------------|------------------------|-------------|----------|
| 1:AG:153:ALA:O | 1:AH:46:ASP:OD1[2_565] | 1.84 | 0.36 |
| 1:AH:69:GLY:O | 1:AH:69:GLY:O[2_565] | 1.90 | 0.30 |
| 1:BJ:151:HIS:CE1 | 1:CY:13:LYS:CE[2_665] | 1.91 | 0.29 |
| 1:CB:153:ALA:O | 1:CC:69:GLY:CA[2_565] | 1.94 | 0.26 |
| 1:CH:39:ARG:NH2 | 1:CM:20:ARG:NH1[2_665] | 1.96 | 0.24 |
| 1:BL:11:GLY:O | 1:CG:153:ALA:C[1_545] | 1.99 | 0.21 |
| 1:BL:72:ASP:OD2 | 1:CG:153:ALA:O[1_545] | 2.03 | 0.17 |
| 1:CB:153:ALA:O | 1:CC:69:GLY:N[2_565] | 2.10 | 0.10 |
| 1:CZ:24:PHE:CB | 1:C4:128:GLY:O[2_665] | 2.12 | 0.08 |
| 1:BL:72:ASP:OD2 | 1:CG:153:ALA:CB[1_545] | 2.13 | 0.07 |
| 1:CH:39:ARG:NH2 | 1:CM:20:ARG:NH2[2_665] | 2.17 | 0.03 |
| 1:AG:153:ALA:CB | 1:AH:46:ASP:OD1[2_565] | 2.18 | 0.02 |
| 1:CH:39:ARG:NH2 | 1:CM:20:ARG:CZ[2_665] | 2.19 | 0.01 |

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 | A1 | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | A2 | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | A3 | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | A4 | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | AA | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | AB | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | AC | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | AD | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | AE | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | AF | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | AG | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | AH | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | AI | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | AJ | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | AK | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | AL | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | AM | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | AN | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | AO | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | AP | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | AQ | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | AR | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | AS | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | AT | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | AU | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | AV | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | AW | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | AX | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | AY | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | AZ | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | B1 | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | B2 | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | B3 | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | B4 | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | BA | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | BB | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | BC | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | BD | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | BE | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | BF | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | BG | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | BH | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | BI | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | BJ | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | BK | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | BL | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | BM | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | BN | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | BO | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | BP | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | BQ | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | BR | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | BS | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | BT | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | BU | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | BV | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | BW | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | BX | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | BY | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | BZ | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | C1 | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | C2 | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | C3 | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | C4 | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | CA | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | CB | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | CC | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | CD | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | CE | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | CF | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | CG | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | CH | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | CI | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | CJ | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | CK | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | CL | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | CM | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | CN | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | CO | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | CP | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | CQ | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | CR | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |
| 1 | CS | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | CT | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | CU | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| 1 | CV | 150/153 (98%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 1 | CW | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%) | 6 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 1 | CX | 150/153 (98%) | 137 (91%) | 11 (7%) | 2 (1%) | 18 | 72 |
| 1 | CY | 150/153 (98%) | 133 (89%) | 17 (11%) | 0 | 100 | 100 |
| 1 | CZ | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%) | 18 | 72 |
| All | All | 13500/13770 (98%) | 11826 (88%) | 1512 (11%) | 162 (1%) | 19 | 75 |

All (162) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AC | 130 | LYS |
| 1 | AH | 130 | LYS |
| 1 | AM | 130 | LYS |
| 1 | AR | 130 | LYS |
| 1 | AW | 130 | LYS |
| 1 | A2 | 130 | LYS |
| 1 | BC | 130 | LYS |
| 1 | BH | 130 | LYS |
| 1 | BM | 130 | LYS |
| 1 | BR | 130 | LYS |
| 1 | BW | 130 | LYS |
| 1 | B2 | 130 | LYS |
| 1 | CC | 130 | LYS |
| 1 | CH | 130 | LYS |
| 1 | CM | 130 | LYS |
| 1 | CR | 130 | LYS |
| 1 | CW | 130 | LYS |
| 1 | C2 | 130 | LYS |
| 1 | AA | 33 | ALA |
| 1 | AA | 36 | GLY |
| 1 | AC | 64 | LYS |
| 1 | AF | 33 | ALA |
| 1 | AF | 36 | GLY |
| 1 | AH | 64 | LYS |
| 1 | AK | 33 | ALA |
| 1 | AK | 36 | GLY |
| 1 | AM | 64 | LYS |
| 1 | AP | 33 | ALA |
| 1 | AP | 36 | GLY |
| 1 | AR | 64 | LYS |
| 1 | AU | 33 | ALA |
| 1 | AU | 36 | GLY |
| 1 | AW | 64 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AZ | 33 | ALA |
| 1 | AZ | 36 | GLY |
| 1 | A2 | 64 | LYS |
| 1 | BA | 33 | ALA |
| 1 | BA | 36 | GLY |
| 1 | BC | 64 | LYS |
| 1 | BF | 33 | ALA |
| 1 | BF | 36 | GLY |
| 1 | BH | 64 | LYS |
| 1 | BK | 33 | ALA |
| 1 | BK | 36 | GLY |
| 1 | BM | 64 | LYS |
| 1 | BP | 33 | ALA |
| 1 | BP | 36 | GLY |
| 1 | BR | 64 | LYS |
| 1 | BU | 33 | ALA |
| 1 | BU | 36 | GLY |
| 1 | BW | 64 | LYS |
| 1 | BZ | 33 | ALA |
| 1 | BZ | 36 | GLY |
| 1 | B2 | 64 | LYS |
| 1 | CA | 33 | ALA |
| 1 | CA | 36 | GLY |
| 1 | CC | 64 | LYS |
| 1 | CF | 33 | ALA |
| 1 | CF | 36 | GLY |
| 1 | CH | 64 | LYS |
| 1 | CK | 33 | ALA |
| 1 | CK | 36 | GLY |
| 1 | CM | 64 | LYS |
| 1 | CP | 33 | ALA |
| 1 | CP | 36 | GLY |
| 1 | CR | 64 | LYS |
| 1 | CU | 33 | ALA |
| 1 | CU | 36 | GLY |
| 1 | CW | 64 | LYS |
| 1 | CZ | 33 | ALA |
| 1 | CZ | 36 | GLY |
| 1 | C2 | 64 | LYS |
| 1 | AD | 53 | PRO |
| 1 | AI | 53 | PRO |
| 1 | AN | 53 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AS | 53 | PRO |
| 1 | AX | 53 | PRO |
| 1 | A3 | 53 | PRO |
| 1 | BD | 53 | PRO |
| 1 | BI | 53 | PRO |
| 1 | BN | 53 | PRO |
| 1 | BS | 53 | PRO |
| 1 | BX | 53 | PRO |
| 1 | B3 | 53 | PRO |
| 1 | CD | 53 | PRO |
| 1 | CI | 53 | PRO |
| 1 | CN | 53 | PRO |
| 1 | CS | 53 | PRO |
| 1 | CX | 53 | PRO |
| 1 | C3 | 53 | PRO |
| 1 | AC | 36 | GLY |
| 1 | AC | 53 | PRO |
| 1 | AH | 36 | GLY |
| 1 | AH | 53 | PRO |
| 1 | AM | 36 | GLY |
| 1 | AM | 53 | PRO |
| 1 | AR | 36 | GLY |
| 1 | AR | 53 | PRO |
| 1 | AW | 36 | GLY |
| 1 | AW | 53 | PRO |
| 1 | A2 | 36 | GLY |
| 1 | A2 | 53 | PRO |
| 1 | BC | 36 | GLY |
| 1 | BC | 53 | PRO |
| 1 | BH | 36 | GLY |
| 1 | BH | 53 | PRO |
| 1 | BM | 36 | GLY |
| 1 | BM | 53 | PRO |
| 1 | BR | 36 | GLY |
| 1 | BR | 53 | PRO |
| 1 | BW | 36 | GLY |
| 1 | BW | 53 | PRO |
| 1 | B2 | 36 | GLY |
| 1 | B2 | 53 | PRO |
| 1 | CC | 36 | GLY |
| 1 | CC | 53 | PRO |
| 1 | CH | 36 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CH | 53 | PRO |
| 1 | CM | 36 | GLY |
| 1 | CM | 53 | PRO |
| 1 | CR | 36 | GLY |
| 1 | CR | 53 | PRO |
| 1 | CW | 36 | GLY |
| 1 | CW | 53 | PRO |
| 1 | C2 | 36 | GLY |
| 1 | C2 | 53 | PRO |
| 1 | AD | 130 | LYS |
| 1 | AI | 130 | LYS |
| 1 | AN | 130 | LYS |
| 1 | AS | 130 | LYS |
| 1 | AX | 130 | LYS |
| 1 | A3 | 130 | LYS |
| 1 | BD | 130 | LYS |
| 1 | BI | 130 | LYS |
| 1 | BN | 130 | LYS |
| 1 | BS | 130 | LYS |
| 1 | BX | 130 | LYS |
| 1 | B3 | 130 | LYS |
| 1 | CD | 130 | LYS |
| 1 | CI | 130 | LYS |
| 1 | CN | 130 | LYS |
| 1 | CS | 130 | LYS |
| 1 | CX | 130 | LYS |
| 1 | C3 | 130 | LYS |
| 1 | AC | 69 | GLY |
| 1 | AH | 69 | GLY |
| 1 | AM | 69 | GLY |
| 1 | AR | 69 | GLY |
| 1 | AW | 69 | GLY |
| 1 | A2 | 69 | GLY |
| 1 | BC | 69 | GLY |
| 1 | BH | 69 | GLY |
| 1 | BM | 69 | GLY |
| 1 | BR | 69 | GLY |
| 1 | BW | 69 | GLY |
| 1 | B2 | 69 | GLY |
| 1 | CC | 69 | GLY |
| 1 | CH | 69 | GLY |
| 1 | CM | 69 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CR | 69 | GLY |
| 1 | CW | 69 | GLY |
| 1 | C2 | 69 | 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 | A1 | 115/118 (98%) | 105 (91%) | 10 (9%) | 15 | 57 |
| 1 | A2 | 116/118 (98%) | 112 (97%) | 4 (3%) | 49 | 88 |
| 1 | A3 | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | A4 | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AA | 115/118 (98%) | 110 (96%) | 5 (4%) | 40 | 84 |
| 1 | AB | 115/118 (98%) | 105 (91%) | 10 (9%) | 15 | 57 |
| 1 | AC | 116/118 (98%) | 112 (97%) | 4 (3%) | 49 | 88 |
| 1 | AD | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AE | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AF | 115/118 (98%) | 110 (96%) | 5 (4%) | 40 | 84 |
| 1 | AG | 115/118 (98%) | 105 (91%) | 10 (9%) | 15 | 57 |
| 1 | AH | 116/118 (98%) | 112 (97%) | 4 (3%) | 49 | 88 |
| 1 | AI | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AJ | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AK | 115/118 (98%) | 110 (96%) | 5 (4%) | 40 | 84 |
| 1 | AL | 115/118 (98%) | 105 (91%) | 10 (9%) | 15 | 57 |
| 1 | AM | 116/118 (98%) | 112 (97%) | 4 (3%) | 49 | 88 |
| 1 | AN | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AO | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AP | 115/118 (98%) | 110 (96%) | 5 (4%) | 40 | 84 |
| 1 | AQ | 115/118 (98%) | 105 (91%) | 10 (9%) | 15 | 57 |
| 1 | AR | 116/118 (98%) | 112 (97%) | 4 (3%) | 49 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | AS | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AT | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AU | 115/118 (98%) | 110 (96%) | 5 (4%) | 40 | 84 |
| 1 | AV | 115/118 (98%) | 105 (91%) | 10 (9%) | 15 | 57 |
| 1 | AW | 116/118 (98%) | 112 (97%) | 4 (3%) | 49 | 88 |
| 1 | AX | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AY | 116/118 (98%) | 108 (93%) | 8 (7%) | 22 | 69 |
| 1 | AZ | 115/118 (98%) | 110 (96%) | 5 (4%) | 40 | 84 |
| 1 | B1 | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | B2 | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | B3 | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | B4 | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BA | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | BB | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | BC | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | BD | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BE | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BF | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | BG | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | BH | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | BI | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BJ | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BK | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | BL | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | BM | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | BN | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BO | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BP | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | BQ | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | BR | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | BS | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | BT | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BU | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | BV | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | BW | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | BX | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BY | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | BZ | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | C1 | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | C2 | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | C3 | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | C4 | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CA | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | CB | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | CC | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | CD | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CE | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CF | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | CG | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | CH | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | CI | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CJ | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CK | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | CL | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | CM | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | CN | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CO | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CP | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | CQ | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | CR | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | CS | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CT | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|------------|----------|-------------|----|
| 1 | CU | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| 1 | CV | 117/118 (99%) | 107 (92%) | 10 (8%) | 15 | 58 |
| 1 | CW | 117/118 (99%) | 113 (97%) | 4 (3%) | 49 | 88 |
| 1 | CX | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CY | 117/118 (99%) | 109 (93%) | 8 (7%) | 22 | 70 |
| 1 | CZ | 117/118 (99%) | 112 (96%) | 5 (4%) | 40 | 84 |
| All | All | 10488/10620 (99%) | 9858 (94%) | 630 (6%) | 27 | 74 |

All (630) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 6 | HIS |
| 1 | AA | 21 | PHE |
| 1 | AA | 116 | THR |
| 1 | AA | 147 | HIS |
| 1 | AA | 150 | LYS |
| 1 | AB | 34 | LEU |
| 1 | AB | 43 | GLU |
| 1 | AB | 77 | LEU |
| 1 | AB | 88 | TYR |
| 1 | AB | 103 | SER |
| 1 | AB | 104 | LEU |
| 1 | AB | 106 | THR |
| 1 | AB | 109 | PRO |
| 1 | AB | 116 | THR |
| 1 | AB | 152 | TRP |
| 1 | AC | 45 | ASN |
| 1 | AC | 67 | ASN |
| 1 | AC | 82 | ARG |
| 1 | AC | 109 | PRO |
| 1 | AD | 67 | ASN |
| 1 | AD | 77 | LEU |
| 1 | AD | 106 | THR |
| 1 | AD | 109 | PRO |
| 1 | AD | 116 | THR |
| 1 | AD | 129 | THR |
| 1 | AD | 130 | LYS |
| 1 | AD | 152 | TRP |
| 1 | AE | 77 | LEU |
| 1 | AE | 88 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AE | 107 | ASP |
| 1 | AE | 116 | THR |
| 1 | AE | 129 | THR |
| 1 | AE | 149 | SER |
| 1 | AE | 150 | LYS |
| 1 | AE | 152 | TRP |
| 1 | AF | 6 | HIS |
| 1 | AF | 21 | PHE |
| 1 | AF | 116 | THR |
| 1 | AF | 147 | HIS |
| 1 | AF | 150 | LYS |
| 1 | AG | 34 | LEU |
| 1 | AG | 43 | GLU |
| 1 | AG | 77 | LEU |
| 1 | AG | 88 | TYR |
| 1 | AG | 103 | SER |
| 1 | AG | 104 | LEU |
| 1 | AG | 106 | THR |
| 1 | AG | 109 | PRO |
| 1 | AG | 116 | THR |
| 1 | AG | 152 | TRP |
| 1 | AH | 45 | ASN |
| 1 | AH | 67 | ASN |
| 1 | AH | 82 | ARG |
| 1 | AH | 109 | PRO |
| 1 | AI | 67 | ASN |
| 1 | AI | 77 | LEU |
| 1 | AI | 106 | THR |
| 1 | AI | 109 | PRO |
| 1 | AI | 116 | THR |
| 1 | AI | 129 | THR |
| 1 | AI | 130 | LYS |
| 1 | AI | 152 | TRP |
| 1 | AJ | 77 | LEU |
| 1 | AJ | 88 | TYR |
| 1 | AJ | 107 | ASP |
| 1 | AJ | 116 | THR |
| 1 | AJ | 129 | THR |
| 1 | AJ | 149 | SER |
| 1 | AJ | 150 | LYS |
| 1 | AJ | 152 | TRP |
| 1 | AK | 6 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AK | 21 | PHE |
| 1 | AK | 116 | THR |
| 1 | AK | 147 | HIS |
| 1 | AK | 150 | LYS |
| 1 | AL | 34 | LEU |
| 1 | AL | 43 | GLU |
| 1 | AL | 77 | LEU |
| 1 | AL | 88 | TYR |
| 1 | AL | 103 | SER |
| 1 | AL | 104 | LEU |
| 1 | AL | 106 | THR |
| 1 | AL | 109 | PRO |
| 1 | AL | 116 | THR |
| 1 | AL | 152 | TRP |
| 1 | AM | 45 | ASN |
| 1 | AM | 67 | ASN |
| 1 | AM | 82 | ARG |
| 1 | AM | 109 | PRO |
| 1 | AN | 67 | ASN |
| 1 | AN | 77 | LEU |
| 1 | AN | 106 | THR |
| 1 | AN | 109 | PRO |
| 1 | AN | 116 | THR |
| 1 | AN | 129 | THR |
| 1 | AN | 130 | LYS |
| 1 | AN | 152 | TRP |
| 1 | AO | 77 | LEU |
| 1 | AO | 88 | TYR |
| 1 | AO | 107 | ASP |
| 1 | AO | 116 | THR |
| 1 | AO | 129 | THR |
| 1 | AO | 149 | SER |
| 1 | AO | 150 | LYS |
| 1 | AO | 152 | TRP |
| 1 | AP | 6 | HIS |
| 1 | AP | 21 | PHE |
| 1 | AP | 116 | THR |
| 1 | AP | 147 | HIS |
| 1 | AP | 150 | LYS |
| 1 | AQ | 34 | LEU |
| 1 | AQ | 43 | GLU |
| 1 | AQ | 77 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AQ | 88 | TYR |
| 1 | AQ | 103 | SER |
| 1 | AQ | 104 | LEU |
| 1 | AQ | 106 | THR |
| 1 | AQ | 109 | PRO |
| 1 | AQ | 116 | THR |
| 1 | AQ | 152 | TRP |
| 1 | AR | 45 | ASN |
| 1 | AR | 67 | ASN |
| 1 | AR | 82 | ARG |
| 1 | AR | 109 | PRO |
| 1 | AS | 67 | ASN |
| 1 | AS | 77 | LEU |
| 1 | AS | 106 | THR |
| 1 | AS | 109 | PRO |
| 1 | AS | 116 | THR |
| 1 | AS | 129 | THR |
| 1 | AS | 130 | LYS |
| 1 | AS | 152 | TRP |
| 1 | AT | 77 | LEU |
| 1 | AT | 88 | TYR |
| 1 | AT | 107 | ASP |
| 1 | AT | 116 | THR |
| 1 | AT | 129 | THR |
| 1 | AT | 149 | SER |
| 1 | AT | 150 | LYS |
| 1 | AT | 152 | TRP |
| 1 | AU | 6 | HIS |
| 1 | AU | 21 | PHE |
| 1 | AU | 116 | THR |
| 1 | AU | 147 | HIS |
| 1 | AU | 150 | LYS |
| 1 | AV | 34 | LEU |
| 1 | AV | 43 | GLU |
| 1 | AV | 77 | LEU |
| 1 | AV | 88 | TYR |
| 1 | AV | 103 | SER |
| 1 | AV | 104 | LEU |
| 1 | AV | 106 | THR |
| 1 | AV | 109 | PRO |
| 1 | AV | 116 | THR |
| 1 | AV | 152 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AW | 45 | ASN |
| 1 | AW | 67 | ASN |
| 1 | AW | 82 | ARG |
| 1 | AW | 109 | PRO |
| 1 | AX | 67 | ASN |
| 1 | AX | 77 | LEU |
| 1 | AX | 106 | THR |
| 1 | AX | 109 | PRO |
| 1 | AX | 116 | THR |
| 1 | AX | 129 | THR |
| 1 | AX | 130 | LYS |
| 1 | AX | 152 | TRP |
| 1 | AY | 77 | LEU |
| 1 | AY | 88 | TYR |
| 1 | AY | 107 | ASP |
| 1 | AY | 116 | THR |
| 1 | AY | 129 | THR |
| 1 | AY | 149 | SER |
| 1 | AY | 150 | LYS |
| 1 | AY | 152 | TRP |
| 1 | AZ | 6 | HIS |
| 1 | AZ | 21 | PHE |
| 1 | AZ | 116 | THR |
| 1 | AZ | 147 | HIS |
| 1 | AZ | 150 | LYS |
| 1 | A1 | 34 | LEU |
| 1 | A1 | 43 | GLU |
| 1 | A1 | 77 | LEU |
| 1 | A1 | 88 | TYR |
| 1 | A1 | 103 | SER |
| 1 | A1 | 104 | LEU |
| 1 | A1 | 106 | THR |
| 1 | A1 | 109 | PRO |
| 1 | A1 | 116 | THR |
| 1 | A1 | 152 | TRP |
| 1 | A2 | 45 | ASN |
| 1 | A2 | 67 | ASN |
| 1 | A2 | 82 | ARG |
| 1 | A2 | 109 | PRO |
| 1 | A3 | 67 | ASN |
| 1 | A3 | 77 | LEU |
| 1 | A3 | 106 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A3 | 109 | PRO |
| 1 | A3 | 116 | THR |
| 1 | A3 | 129 | THR |
| 1 | A3 | 130 | LYS |
| 1 | A3 | 152 | TRP |
| 1 | A4 | 77 | LEU |
| 1 | A4 | 88 | TYR |
| 1 | A4 | 107 | ASP |
| 1 | A4 | 116 | THR |
| 1 | A4 | 129 | THR |
| 1 | A4 | 149 | SER |
| 1 | A4 | 150 | LYS |
| 1 | A4 | 152 | TRP |
| 1 | BA | 6 | HIS |
| 1 | BA | 21 | PHE |
| 1 | BA | 116 | THR |
| 1 | BA | 147 | HIS |
| 1 | BA | 150 | LYS |
| 1 | BB | 34 | LEU |
| 1 | BB | 43 | GLU |
| 1 | BB | 77 | LEU |
| 1 | BB | 88 | TYR |
| 1 | BB | 103 | SER |
| 1 | BB | 104 | LEU |
| 1 | BB | 106 | THR |
| 1 | BB | 109 | PRO |
| 1 | BB | 116 | THR |
| 1 | BB | 152 | TRP |
| 1 | BC | 45 | ASN |
| 1 | BC | 67 | ASN |
| 1 | BC | 82 | ARG |
| 1 | BC | 109 | PRO |
| 1 | BD | 67 | ASN |
| 1 | BD | 77 | LEU |
| 1 | BD | 106 | THR |
| 1 | BD | 109 | PRO |
| 1 | BD | 116 | THR |
| 1 | BD | 129 | THR |
| 1 | BD | 130 | LYS |
| 1 | BD | 152 | TRP |
| 1 | BE | 77 | LEU |
| 1 | BE | 88 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BE | 107 | ASP |
| 1 | BE | 116 | THR |
| 1 | BE | 129 | THR |
| 1 | BE | 149 | SER |
| 1 | BE | 150 | LYS |
| 1 | BE | 152 | TRP |
| 1 | BF | 6 | HIS |
| 1 | BF | 21 | PHE |
| 1 | BF | 116 | THR |
| 1 | BF | 147 | HIS |
| 1 | BF | 150 | LYS |
| 1 | BG | 34 | LEU |
| 1 | BG | 43 | GLU |
| 1 | BG | 77 | LEU |
| 1 | BG | 88 | TYR |
| 1 | BG | 103 | SER |
| 1 | BG | 104 | LEU |
| 1 | BG | 106 | THR |
| 1 | BG | 109 | PRO |
| 1 | BG | 116 | THR |
| 1 | BG | 152 | TRP |
| 1 | BH | 45 | ASN |
| 1 | BH | 67 | ASN |
| 1 | BH | 82 | ARG |
| 1 | BH | 109 | PRO |
| 1 | BI | 67 | ASN |
| 1 | BI | 77 | LEU |
| 1 | BI | 106 | THR |
| 1 | BI | 109 | PRO |
| 1 | BI | 116 | THR |
| 1 | BI | 129 | THR |
| 1 | BI | 130 | LYS |
| 1 | BI | 152 | TRP |
| 1 | BJ | 77 | LEU |
| 1 | BJ | 88 | TYR |
| 1 | BJ | 107 | ASP |
| 1 | BJ | 116 | THR |
| 1 | BJ | 129 | THR |
| 1 | BJ | 149 | SER |
| 1 | BJ | 150 | LYS |
| 1 | BJ | 152 | TRP |
| 1 | BK | 6 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BK | 21 | PHE |
| 1 | BK | 116 | THR |
| 1 | BK | 147 | HIS |
| 1 | BK | 150 | LYS |
| 1 | BL | 34 | LEU |
| 1 | BL | 43 | GLU |
| 1 | BL | 77 | LEU |
| 1 | BL | 88 | TYR |
| 1 | BL | 103 | SER |
| 1 | BL | 104 | LEU |
| 1 | BL | 106 | THR |
| 1 | BL | 109 | PRO |
| 1 | BL | 116 | THR |
| 1 | BL | 152 | TRP |
| 1 | BM | 45 | ASN |
| 1 | BM | 67 | ASN |
| 1 | BM | 82 | ARG |
| 1 | BM | 109 | PRO |
| 1 | BN | 67 | ASN |
| 1 | BN | 77 | LEU |
| 1 | BN | 106 | THR |
| 1 | BN | 109 | PRO |
| 1 | BN | 116 | THR |
| 1 | BN | 129 | THR |
| 1 | BN | 130 | LYS |
| 1 | BN | 152 | TRP |
| 1 | BO | 77 | LEU |
| 1 | BO | 88 | TYR |
| 1 | BO | 107 | ASP |
| 1 | BO | 116 | THR |
| 1 | BO | 129 | THR |
| 1 | BO | 149 | SER |
| 1 | BO | 150 | LYS |
| 1 | BO | 152 | TRP |
| 1 | BP | 6 | HIS |
| 1 | BP | 21 | PHE |
| 1 | BP | 116 | THR |
| 1 | BP | 147 | HIS |
| 1 | BP | 150 | LYS |
| 1 | BQ | 34 | LEU |
| 1 | BQ | 43 | GLU |
| 1 | BQ | 77 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BQ | 88 | TYR |
| 1 | BQ | 103 | SER |
| 1 | BQ | 104 | LEU |
| 1 | BQ | 106 | THR |
| 1 | BQ | 109 | PRO |
| 1 | BQ | 116 | THR |
| 1 | BQ | 152 | TRP |
| 1 | BR | 45 | ASN |
| 1 | BR | 67 | ASN |
| 1 | BR | 82 | ARG |
| 1 | BR | 109 | PRO |
| 1 | BS | 67 | ASN |
| 1 | BS | 77 | LEU |
| 1 | BS | 106 | THR |
| 1 | BS | 109 | PRO |
| 1 | BS | 116 | THR |
| 1 | BS | 129 | THR |
| 1 | BS | 130 | LYS |
| 1 | BS | 152 | TRP |
| 1 | BT | 77 | LEU |
| 1 | BT | 88 | TYR |
| 1 | BT | 107 | ASP |
| 1 | BT | 116 | THR |
| 1 | BT | 129 | THR |
| 1 | BT | 149 | SER |
| 1 | BT | 150 | LYS |
| 1 | BT | 152 | TRP |
| 1 | BU | 6 | HIS |
| 1 | BU | 21 | PHE |
| 1 | BU | 116 | THR |
| 1 | BU | 147 | HIS |
| 1 | BU | 150 | LYS |
| 1 | BV | 34 | LEU |
| 1 | BV | 43 | GLU |
| 1 | BV | 77 | LEU |
| 1 | BV | 88 | TYR |
| 1 | BV | 103 | SER |
| 1 | BV | 104 | LEU |
| 1 | BV | 106 | THR |
| 1 | BV | 109 | PRO |
| 1 | BV | 116 | THR |
| 1 | BV | 152 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BW | 45 | ASN |
| 1 | BW | 67 | ASN |
| 1 | BW | 82 | ARG |
| 1 | BW | 109 | PRO |
| 1 | BX | 67 | ASN |
| 1 | BX | 77 | LEU |
| 1 | BX | 106 | THR |
| 1 | BX | 109 | PRO |
| 1 | BX | 116 | THR |
| 1 | BX | 129 | THR |
| 1 | BX | 130 | LYS |
| 1 | BX | 152 | TRP |
| 1 | BY | 77 | LEU |
| 1 | BY | 88 | TYR |
| 1 | BY | 107 | ASP |
| 1 | BY | 116 | THR |
| 1 | BY | 129 | THR |
| 1 | BY | 149 | SER |
| 1 | BY | 150 | LYS |
| 1 | BY | 152 | TRP |
| 1 | BZ | 6 | HIS |
| 1 | BZ | 21 | PHE |
| 1 | BZ | 116 | THR |
| 1 | BZ | 147 | HIS |
| 1 | BZ | 150 | LYS |
| 1 | B1 | 34 | LEU |
| 1 | B1 | 43 | GLU |
| 1 | B1 | 77 | LEU |
| 1 | B1 | 88 | TYR |
| 1 | B1 | 103 | SER |
| 1 | B1 | 104 | LEU |
| 1 | B1 | 106 | THR |
| 1 | B1 | 109 | PRO |
| 1 | B1 | 116 | THR |
| 1 | B1 | 152 | TRP |
| 1 | B2 | 45 | ASN |
| 1 | B2 | 67 | ASN |
| 1 | B2 | 82 | ARG |
| 1 | B2 | 109 | PRO |
| 1 | B3 | 67 | ASN |
| 1 | B3 | 77 | LEU |
| 1 | B3 | 106 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B3 | 109 | PRO |
| 1 | B3 | 116 | THR |
| 1 | B3 | 129 | THR |
| 1 | B3 | 130 | LYS |
| 1 | B3 | 152 | TRP |
| 1 | B4 | 77 | LEU |
| 1 | B4 | 88 | TYR |
| 1 | B4 | 107 | ASP |
| 1 | B4 | 116 | THR |
| 1 | B4 | 129 | THR |
| 1 | B4 | 149 | SER |
| 1 | B4 | 150 | LYS |
| 1 | B4 | 152 | TRP |
| 1 | CA | 6 | HIS |
| 1 | CA | 21 | PHE |
| 1 | CA | 116 | THR |
| 1 | CA | 147 | HIS |
| 1 | CA | 150 | LYS |
| 1 | CB | 34 | LEU |
| 1 | CB | 43 | GLU |
| 1 | CB | 77 | LEU |
| 1 | CB | 88 | TYR |
| 1 | CB | 103 | SER |
| 1 | CB | 104 | LEU |
| 1 | CB | 106 | THR |
| 1 | CB | 109 | PRO |
| 1 | CB | 116 | THR |
| 1 | CB | 152 | TRP |
| 1 | CC | 45 | ASN |
| 1 | CC | 67 | ASN |
| 1 | CC | 82 | ARG |
| 1 | CC | 109 | PRO |
| 1 | CD | 67 | ASN |
| 1 | CD | 77 | LEU |
| 1 | CD | 106 | THR |
| 1 | CD | 109 | PRO |
| 1 | CD | 116 | THR |
| 1 | CD | 129 | THR |
| 1 | CD | 130 | LYS |
| 1 | CD | 152 | TRP |
| 1 | CE | 77 | LEU |
| 1 | CE | 88 | TYR |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CE | 107 | ASP |
| 1 | CE | 116 | THR |
| 1 | CE | 129 | THR |
| 1 | CE | 149 | SER |
| 1 | CE | 150 | LYS |
| 1 | CE | 152 | TRP |
| 1 | CF | 6 | HIS |
| 1 | CF | 21 | PHE |
| 1 | CF | 116 | THR |
| 1 | CF | 147 | HIS |
| 1 | CF | 150 | LYS |
| 1 | CG | 34 | LEU |
| 1 | CG | 43 | GLU |
| 1 | CG | 77 | LEU |
| 1 | CG | 88 | TYR |
| 1 | CG | 103 | SER |
| 1 | CG | 104 | LEU |
| 1 | CG | 106 | THR |
| 1 | CG | 109 | PRO |
| 1 | CG | 116 | THR |
| 1 | CG | 152 | TRP |
| 1 | CH | 45 | ASN |
| 1 | CH | 67 | ASN |
| 1 | CH | 82 | ARG |
| 1 | CH | 109 | PRO |
| 1 | CI | 67 | ASN |
| 1 | CI | 77 | LEU |
| 1 | CI | 106 | THR |
| 1 | CI | 109 | PRO |
| 1 | CI | 116 | THR |
| 1 | CI | 129 | THR |
| 1 | CI | 130 | LYS |
| 1 | CI | 152 | TRP |
| 1 | CJ | 77 | LEU |
| 1 | CJ | 88 | TYR |
| 1 | CJ | 107 | ASP |
| 1 | CJ | 116 | THR |
| 1 | CJ | 129 | THR |
| 1 | CJ | 149 | SER |
| 1 | CJ | 150 | LYS |
| 1 | CJ | 152 | TRP |
| 1 | CK | 6 | HIS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CK | 21 | PHE |
| 1 | CK | 116 | THR |
| 1 | CK | 147 | HIS |
| 1 | CK | 150 | LYS |
| 1 | CL | 34 | LEU |
| 1 | CL | 43 | GLU |
| 1 | CL | 77 | LEU |
| 1 | CL | 88 | TYR |
| 1 | CL | 103 | SER |
| 1 | CL | 104 | LEU |
| 1 | CL | 106 | THR |
| 1 | CL | 109 | PRO |
| 1 | CL | 116 | THR |
| 1 | CL | 152 | TRP |
| 1 | CM | 45 | ASN |
| 1 | CM | 67 | ASN |
| 1 | CM | 82 | ARG |
| 1 | CM | 109 | PRO |
| 1 | CN | 67 | ASN |
| 1 | CN | 77 | LEU |
| 1 | CN | 106 | THR |
| 1 | CN | 109 | PRO |
| 1 | CN | 116 | THR |
| 1 | CN | 129 | THR |
| 1 | CN | 130 | LYS |
| 1 | CN | 152 | TRP |
| 1 | CO | 77 | LEU |
| 1 | CO | 88 | TYR |
| 1 | CO | 107 | ASP |
| 1 | CO | 116 | THR |
| 1 | CO | 129 | THR |
| 1 | CO | 149 | SER |
| 1 | CO | 150 | LYS |
| 1 | CO | 152 | TRP |
| 1 | CP | 6 | HIS |
| 1 | CP | 21 | PHE |
| 1 | CP | 116 | THR |
| 1 | CP | 147 | HIS |
| 1 | CP | 150 | LYS |
| 1 | CQ | 34 | LEU |
| 1 | CQ | 43 | GLU |
| 1 | CQ | 77 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CQ | 88 | TYR |
| 1 | CQ | 103 | SER |
| 1 | CQ | 104 | LEU |
| 1 | CQ | 106 | THR |
| 1 | CQ | 109 | PRO |
| 1 | CQ | 116 | THR |
| 1 | CQ | 152 | TRP |
| 1 | CR | 45 | ASN |
| 1 | CR | 67 | ASN |
| 1 | CR | 82 | ARG |
| 1 | CR | 109 | PRO |
| 1 | CS | 67 | ASN |
| 1 | CS | 77 | LEU |
| 1 | CS | 106 | THR |
| 1 | CS | 109 | PRO |
| 1 | CS | 116 | THR |
| 1 | CS | 129 | THR |
| 1 | CS | 130 | LYS |
| 1 | CS | 152 | TRP |
| 1 | CT | 77 | LEU |
| 1 | CT | 88 | TYR |
| 1 | CT | 107 | ASP |
| 1 | CT | 116 | THR |
| 1 | CT | 129 | THR |
| 1 | CT | 149 | SER |
| 1 | CT | 150 | LYS |
| 1 | CT | 152 | TRP |
| 1 | CU | 6 | HIS |
| 1 | CU | 21 | PHE |
| 1 | CU | 116 | THR |
| 1 | CU | 147 | HIS |
| 1 | CU | 150 | LYS |
| 1 | CV | 34 | LEU |
| 1 | CV | 43 | GLU |
| 1 | CV | 77 | LEU |
| 1 | CV | 88 | TYR |
| 1 | CV | 103 | SER |
| 1 | CV | 104 | LEU |
| 1 | CV | 106 | THR |
| 1 | CV | 109 | PRO |
| 1 | CV | 116 | THR |
| 1 | CV | 152 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CW | 45 | ASN |
| 1 | CW | 67 | ASN |
| 1 | CW | 82 | ARG |
| 1 | CW | 109 | PRO |
| 1 | CX | 67 | ASN |
| 1 | CX | 77 | LEU |
| 1 | CX | 106 | THR |
| 1 | CX | 109 | PRO |
| 1 | CX | 116 | THR |
| 1 | CX | 129 | THR |
| 1 | CX | 130 | LYS |
| 1 | CX | 152 | TRP |
| 1 | CY | 77 | LEU |
| 1 | CY | 88 | TYR |
| 1 | CY | 107 | ASP |
| 1 | CY | 116 | THR |
| 1 | CY | 129 | THR |
| 1 | CY | 149 | SER |
| 1 | CY | 150 | LYS |
| 1 | CY | 152 | TRP |
| 1 | CZ | 6 | HIS |
| 1 | CZ | 21 | PHE |
| 1 | CZ | 116 | THR |
| 1 | CZ | 147 | HIS |
| 1 | CZ | 150 | LYS |
| 1 | C1 | 34 | LEU |
| 1 | C1 | 43 | GLU |
| 1 | C1 | 77 | LEU |
| 1 | C1 | 88 | TYR |
| 1 | C1 | 103 | SER |
| 1 | C1 | 104 | LEU |
| 1 | C1 | 106 | THR |
| 1 | C1 | 109 | PRO |
| 1 | C1 | 116 | THR |
| 1 | C1 | 152 | TRP |
| 1 | C2 | 45 | ASN |
| 1 | C2 | 67 | ASN |
| 1 | C2 | 82 | ARG |
| 1 | C2 | 109 | PRO |
| 1 | C3 | 67 | ASN |
| 1 | C3 | 77 | LEU |
| 1 | C3 | 106 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C3 | 109 | PRO |
| 1 | C3 | 116 | THR |
| 1 | C3 | 129 | THR |
| 1 | C3 | 130 | LYS |
| 1 | C3 | 152 | TRP |
| 1 | C4 | 77 | LEU |
| 1 | C4 | 88 | TYR |
| 1 | C4 | 107 | ASP |
| 1 | C4 | 116 | THR |
| 1 | C4 | 129 | THR |
| 1 | C4 | 149 | SER |
| 1 | C4 | 150 | LYS |
| 1 | C4 | 152 | TRP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (252) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 45 | ASN |
| 1 | AA | 67 | ASN |
| 1 | AA | 151 | HIS |
| 1 | AB | 45 | ASN |
| 1 | AB | 67 | ASN |
| 1 | AB | 93 | ASN |
| 1 | AC | 6 | HIS |
| 1 | AC | 45 | ASN |
| 1 | AC | 67 | ASN |
| 1 | AC | 93 | ASN |
| 1 | AC | 147 | HIS |
| 1 | AD | 67 | ASN |
| 1 | AD | 93 | ASN |
| 1 | AD | 147 | HIS |
| 1 | AE | 67 | ASN |
| 1 | AF | 45 | ASN |
| 1 | AF | 67 | ASN |
| 1 | AG | 45 | ASN |
| 1 | AG | 67 | ASN |
| 1 | AG | 93 | ASN |
| 1 | AH | 6 | HIS |
| 1 | AH | 45 | ASN |
| 1 | AH | 67 | ASN |
| 1 | AH | 93 | ASN |
| 1 | AH | 147 | HIS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AI | 67 | ASN |
| 1 | AI | 93 | ASN |
| 1 | AI | 147 | HIS |
| 1 | AJ | 67 | ASN |
| 1 | AK | 45 | ASN |
| 1 | AK | 67 | ASN |
| 1 | AK | 151 | HIS |
| 1 | AL | 45 | ASN |
| 1 | AL | 67 | ASN |
| 1 | AL | 93 | ASN |
| 1 | AM | 45 | ASN |
| 1 | AM | 67 | ASN |
| 1 | AM | 93 | ASN |
| 1 | AM | 147 | HIS |
| 1 | AN | 67 | ASN |
| 1 | AN | 93 | ASN |
| 1 | AN | 147 | HIS |
| 1 | AO | 67 | ASN |
| 1 | AP | 45 | ASN |
| 1 | AP | 67 | ASN |
| 1 | AP | 151 | HIS |
| 1 | AQ | 45 | ASN |
| 1 | AQ | 67 | ASN |
| 1 | AQ | 93 | ASN |
| 1 | AR | 6 | HIS |
| 1 | AR | 45 | ASN |
| 1 | AR | 67 | ASN |
| 1 | AR | 93 | ASN |
| 1 | AR | 147 | HIS |
| 1 | AS | 67 | ASN |
| 1 | AS | 93 | ASN |
| 1 | AS | 147 | HIS |
| 1 | AT | 67 | ASN |
| 1 | AU | 45 | ASN |
| 1 | AU | 67 | ASN |
| 1 | AU | 151 | HIS |
| 1 | AV | 45 | ASN |
| 1 | AV | 67 | ASN |
| 1 | AV | 93 | ASN |
| 1 | AW | 45 | ASN |
| 1 | AW | 67 | ASN |
| 1 | AW | 93 | ASN |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AW | 147 | HIS |
| 1 | AX | 67 | ASN |
| 1 | AX | 93 | ASN |
| 1 | AX | 147 | HIS |
| 1 | AY | 67 | ASN |
| 1 | AZ | 45 | ASN |
| 1 | AZ | 67 | ASN |
| 1 | AZ | 151 | HIS |
| 1 | A1 | 45 | ASN |
| 1 | A1 | 67 | ASN |
| 1 | A1 | 93 | ASN |
| 1 | A2 | 6 | HIS |
| 1 | A2 | 45 | ASN |
| 1 | A2 | 67 | ASN |
| 1 | A2 | 93 | ASN |
| 1 | A2 | 147 | HIS |
| 1 | A3 | 67 | ASN |
| 1 | A3 | 93 | ASN |
| 1 | A3 | 147 | HIS |
| 1 | A4 | 67 | ASN |
| 1 | BA | 45 | ASN |
| 1 | BA | 67 | ASN |
| 1 | BB | 45 | ASN |
| 1 | BB | 67 | ASN |
| 1 | BB | 93 | ASN |
| 1 | BC | 45 | ASN |
| 1 | BC | 67 | ASN |
| 1 | BC | 93 | ASN |
| 1 | BC | 147 | HIS |
| 1 | BD | 67 | ASN |
| 1 | BD | 147 | HIS |
| 1 | BE | 67 | ASN |
| 1 | BF | 45 | ASN |
| 1 | BF | 67 | ASN |
| 1 | BF | 151 | HIS |
| 1 | BG | 45 | ASN |
| 1 | BG | 67 | ASN |
| 1 | BG | 93 | ASN |
| 1 | BH | 45 | ASN |
| 1 | BH | 67 | ASN |
| 1 | BH | 93 | ASN |
| 1 | BH | 147 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BI | 67 | ASN |
| 1 | BI | 147 | HIS |
| 1 | BJ | 67 | ASN |
| 1 | BK | 45 | ASN |
| 1 | BK | 67 | ASN |
| 1 | BK | 151 | HIS |
| 1 | BL | 45 | ASN |
| 1 | BL | 67 | ASN |
| 1 | BL | 93 | ASN |
| 1 | BM | 45 | ASN |
| 1 | BM | 67 | ASN |
| 1 | BM | 93 | ASN |
| 1 | BM | 147 | HIS |
| 1 | BN | 67 | ASN |
| 1 | BN | 93 | ASN |
| 1 | BN | 147 | HIS |
| 1 | BO | 67 | ASN |
| 1 | BP | 45 | ASN |
| 1 | BP | 67 | ASN |
| 1 | BP | 151 | HIS |
| 1 | BQ | 45 | ASN |
| 1 | BQ | 67 | ASN |
| 1 | BQ | 93 | ASN |
| 1 | BR | 6 | HIS |
| 1 | BR | 45 | ASN |
| 1 | BR | 67 | ASN |
| 1 | BR | 93 | ASN |
| 1 | BR | 147 | HIS |
| 1 | BS | 67 | ASN |
| 1 | BS | 93 | ASN |
| 1 | BS | 147 | HIS |
| 1 | BT | 67 | ASN |
| 1 | BU | 45 | ASN |
| 1 | BU | 67 | ASN |
| 1 | BU | 151 | HIS |
| 1 | BV | 45 | ASN |
| 1 | BV | 67 | ASN |
| 1 | BV | 93 | ASN |
| 1 | BW | 6 | HIS |
| 1 | BW | 45 | ASN |
| 1 | BW | 67 | ASN |
| 1 | BW | 93 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BW | 147 | HIS |
| 1 | BX | 67 | ASN |
| 1 | BX | 147 | HIS |
| 1 | BY | 67 | ASN |
| 1 | BZ | 45 | ASN |
| 1 | BZ | 67 | ASN |
| 1 | BZ | 151 | HIS |
| 1 | B1 | 45 | ASN |
| 1 | B1 | 67 | ASN |
| 1 | B1 | 93 | ASN |
| 1 | B2 | 45 | ASN |
| 1 | B2 | 67 | ASN |
| 1 | B2 | 93 | ASN |
| 1 | B2 | 147 | HIS |
| 1 | B3 | 67 | ASN |
| 1 | B3 | 147 | HIS |
| 1 | B4 | 67 | ASN |
| 1 | CA | 45 | ASN |
| 1 | CA | 67 | ASN |
| 1 | CA | 151 | HIS |
| 1 | CB | 45 | ASN |
| 1 | CB | 67 | ASN |
| 1 | CB | 93 | ASN |
| 1 | CC | 45 | ASN |
| 1 | CC | 67 | ASN |
| 1 | CC | 93 | ASN |
| 1 | CC | 147 | HIS |
| 1 | CD | 67 | ASN |
| 1 | CD | 147 | HIS |
| 1 | CE | 67 | ASN |
| 1 | CF | 45 | ASN |
| 1 | CF | 67 | ASN |
| 1 | CF | 151 | HIS |
| 1 | CG | 45 | ASN |
| 1 | CG | 67 | ASN |
| 1 | CG | 93 | ASN |
| 1 | CH | 6 | HIS |
| 1 | CH | 45 | ASN |
| 1 | CH | 67 | ASN |
| 1 | CH | 93 | ASN |
| 1 | CH | 147 | HIS |
| 1 | CI | 67 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CI | 93 | ASN |
| 1 | CI | 147 | HIS |
| 1 | CJ | 67 | ASN |
| 1 | CK | 45 | ASN |
| 1 | CK | 67 | ASN |
| 1 | CK | 151 | HIS |
| 1 | CL | 45 | ASN |
| 1 | CL | 67 | ASN |
| 1 | CL | 93 | ASN |
| 1 | CM | 45 | ASN |
| 1 | CM | 67 | ASN |
| 1 | CM | 93 | ASN |
| 1 | CM | 147 | HIS |
| 1 | CN | 67 | ASN |
| 1 | CN | 147 | HIS |
| 1 | CO | 67 | ASN |
| 1 | CP | 45 | ASN |
| 1 | CP | 67 | ASN |
| 1 | CP | 151 | HIS |
| 1 | CQ | 45 | ASN |
| 1 | CQ | 67 | ASN |
| 1 | CQ | 93 | ASN |
| 1 | CR | 45 | ASN |
| 1 | CR | 67 | ASN |
| 1 | CR | 93 | ASN |
| 1 | CR | 147 | HIS |
| 1 | CS | 67 | ASN |
| 1 | CS | 93 | ASN |
| 1 | CS | 147 | HIS |
| 1 | CT | 67 | ASN |
| 1 | CU | 45 | ASN |
| 1 | CU | 67 | ASN |
| 1 | CU | 151 | HIS |
| 1 | CV | 45 | ASN |
| 1 | CV | 67 | ASN |
| 1 | CV | 93 | ASN |
| 1 | CW | 6 | HIS |
| 1 | CW | 45 | ASN |
| 1 | CW | 67 | ASN |
| 1 | CW | 93 | ASN |
| 1 | CW | 147 | HIS |
| 1 | CX | 67 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CX | 93 | ASN |
| 1 | CX | 147 | HIS |
| 1 | CY | 67 | ASN |
| 1 | CZ | 45 | ASN |
| 1 | CZ | 67 | ASN |
| 1 | CZ | 151 | HIS |
| 1 | C1 | 45 | ASN |
| 1 | C1 | 67 | ASN |
| 1 | C1 | 93 | ASN |
| 1 | C2 | 45 | ASN |
| 1 | C2 | 67 | ASN |
| 1 | C2 | 93 | ASN |
| 1 | C2 | 147 | HIS |
| 1 | C3 | 67 | ASN |
| 1 | C3 | 93 | ASN |
| 1 | C3 | 147 | HIS |
| 1 | C4 | 67 | ASN |

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

90 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | PO4 | A1 | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | A2 | 1001 | - | 4,4,4 | 0.40 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | A3 | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | A4 | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AA | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AB | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AC | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AD | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AE | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AF | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AG | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AH | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AI | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AJ | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AK | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AL | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AM | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AN | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AO | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AP | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AQ | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AR | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AS | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AT | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AU | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AV | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AW | 201 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AX | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | AY | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | AZ | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | B1 | 1001 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | B2 | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | B3 | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | B4 | 1001 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BA | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BB | 1001 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BC | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BD | 1001 | - | 4,4,4 | 0.35 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BE | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BF | 1001 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BG | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BH | 1001 | - | 4,4,4 | 0.40 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BI | 1001 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.28 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | PO4 | BJ | 1001 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BK | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BL | 1001 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BM | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BN | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BO | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BP | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BQ | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BR | 1001 | - | 4,4,4 | 0.40 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BS | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BT | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BU | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BV | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BW | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BX | 1001 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | BY | 1001 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | BZ | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | C1 | 1201 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | C2 | 2201 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | C3 | 3201 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | C4 | 4201 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CA | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CB | 1001 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CC | 1001 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CD | 1001 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CE | 1001 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CF | 201 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CG | 1201 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CH | 2201 | - | 4,4,4 | 0.40 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CI | 3201 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CJ | 4201 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CK | 201 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CL | 1201 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CM | 2201 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CN | 3201 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CO | 4201 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CP | 201 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CQ | 1201 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CR | 2201 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CS | 3201 | - | 4,4,4 | 0.36 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CT | 4201 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CU | 201 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CV | 1201 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.28 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | PO4 | CW | 2201 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CX | 3201 | - | 4,4,4 | 0.35 | 0 | 6,6,6 | 0.28 | 0 |
| 2 | PO4 | CY | 4201 | - | 4,4,4 | 0.37 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | PO4 | CZ | 201 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.29 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 2 | PO4 | A1 | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | A2 | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | A3 | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | A4 | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AA | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AB | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AC | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AD | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AE | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AF | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AG | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AH | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AI | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AJ | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AK | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AL | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AM | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AN | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AO | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AP | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AQ | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AR | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AS | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AT | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AU | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AV | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AW | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AX | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AY | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | AZ | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | B1 | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | B2 | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 2 | PO4 | B3 | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | B4 | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BA | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BB | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BC | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BD | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BE | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BF | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BG | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BH | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BI | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BJ | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BK | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BL | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BM | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BN | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BO | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BP | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BQ | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BR | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BS | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BT | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BU | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BV | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BW | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BX | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BY | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | BZ | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | C1 | 1201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | C2 | 2201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | C3 | 3201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | C4 | 4201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CA | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CB | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CC | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CD | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CE | 1001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CF | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CG | 1201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CH | 2201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CI | 3201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CJ | 4201 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 2 | PO4 | CK | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CL | 1201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CM | 2201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CN | 3201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CO | 4201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CP | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CQ | 1201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CR | 2201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CS | 3201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CT | 4201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CU | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CV | 1201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CW | 2201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CX | 3201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CY | 4201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | PO4 | CZ | 201 | - | - | 0/0/0/0 | 0/0/0/0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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 ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1 | A1 | 152/153 (99%) | 0.25 | 3 (1%) 62 30 | 65, 95, 151, 347 | 0 |
| 1 | A2 | 152/153 (99%) | 0.14 | 3 (1%) 62 30 | 56, 97, 184, 226 | 0 |
| 1 | A3 | 152/153 (99%) | 0.13 | 1 (0%) 84 56 | 57, 96, 147, 259 | 0 |
| 1 | A4 | 152/153 (99%) | 0.16 | 3 (1%) 62 30 | 56, 94, 153, 393 | 0 |
| 1 | AA | 152/153 (99%) | 0.09 | 1 (0%) 84 56 | 55, 97, 150, 271 | 0 |
| 1 | AB | 152/153 (99%) | 0.18 | 2 (1%) 74 40 | 65, 95, 151, 347 | 0 |
| 1 | AC | 152/153 (99%) | 0.15 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | AD | 152/153 (99%) | 0.14 | 2 (1%) 74 40 | 57, 96, 147, 259 | 0 |
| 1 | AE | 152/153 (99%) | 0.10 | 2 (1%) 74 40 | 56, 94, 153, 393 | 0 |
| 1 | AF | 152/153 (99%) | 0.18 | 1 (0%) 84 56 | 55, 97, 150, 271 | 0 |
| 1 | AG | 152/153 (99%) | 0.30 | 3 (1%) 62 30 | 65, 95, 151, 347 | 0 |
| 1 | AH | 152/153 (99%) | 0.32 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | AI | 152/153 (99%) | 0.21 | 1 (0%) 84 56 | 57, 96, 147, 259 | 0 |
| 1 | AJ | 152/153 (99%) | 0.27 | 3 (1%) 62 30 | 56, 94, 153, 393 | 0 |
| 1 | AK | 152/153 (99%) | 0.15 | 1 (0%) 84 56 | 55, 97, 150, 271 | 0 |
| 1 | AL | 152/153 (99%) | 0.28 | 2 (1%) 74 40 | 65, 95, 151, 347 | 0 |
| 1 | AM | 152/153 (99%) | 0.18 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | AN | 152/153 (99%) | 0.20 | 2 (1%) 74 40 | 57, 96, 147, 259 | 0 |
| 1 | AO | 152/153 (99%) | 0.19 | 3 (1%) 62 30 | 56, 94, 153, 393 | 0 |
| 1 | AP | 152/153 (99%) | 0.10 | 0 100 100 | 55, 97, 150, 271 | 0 |
| 1 | AQ | 152/153 (99%) | 0.16 | 1 (0%) 84 56 | 65, 95, 151, 347 | 0 |
| 1 | AR | 152/153 (99%) | 0.21 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | AS | 152/153 (99%) | 0.19 | 1 (0%) 84 56 | 57, 96, 147, 259 | 0 |
| 1 | AT | 152/153 (99%) | 0.10 | 1 (0%) 84 56 | 56, 94, 153, 393 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1 | AU | 152/153 (99%) | 0.21 | 1 (0%) 84 56 | 55, 97, 150, 271 | 0 |
| 1 | AV | 152/153 (99%) | 0.28 | 2 (1%) 74 40 | 65, 95, 151, 347 | 0 |
| 1 | AW | 152/153 (99%) | 0.35 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | AX | 152/153 (99%) | 0.24 | 2 (1%) 74 40 | 57, 96, 147, 259 | 0 |
| 1 | AY | 152/153 (99%) | 0.17 | 3 (1%) 62 30 | 56, 94, 153, 393 | 0 |
| 1 | AZ | 152/153 (99%) | 0.14 | 1 (0%) 84 56 | 55, 97, 150, 271 | 0 |
| 1 | B1 | 152/153 (99%) | 0.29 | 3 (1%) 62 30 | 60, 95, 151, 347 | 0 |
| 1 | B2 | 152/153 (99%) | 0.30 | 3 (1%) 62 30 | 56, 97, 184, 226 | 0 |
| 1 | B3 | 152/153 (99%) | 0.32 | 4 (2%) 53 24 | 57, 96, 147, 259 | 0 |
| 1 | B4 | 152/153 (99%) | 0.26 | 2 (1%) 74 40 | 55, 93, 153, 393 | 0 |
| 1 | BA | 152/153 (99%) | 0.22 | 4 (2%) 53 24 | 55, 97, 147, 271 | 0 |
| 1 | BB | 152/153 (99%) | 0.39 | 3 (1%) 62 30 | 60, 95, 151, 347 | 0 |
| 1 | BC | 152/153 (99%) | 0.29 | 4 (2%) 53 24 | 56, 97, 184, 226 | 0 |
| 1 | BD | 152/153 (99%) | 0.19 | 1 (0%) 84 56 | 57, 96, 147, 259 | 0 |
| 1 | BE | 152/153 (99%) | 0.37 | 2 (1%) 74 40 | 55, 93, 153, 393 | 0 |
| 1 | BF | 152/153 (99%) | 0.32 | 3 (1%) 62 30 | 55, 97, 147, 271 | 0 |
| 1 | BG | 152/153 (99%) | 0.25 | 2 (1%) 74 40 | 60, 95, 151, 347 | 0 |
| 1 | BH | 152/153 (99%) | 0.20 | 3 (1%) 62 30 | 56, 97, 184, 226 | 0 |
| 1 | BI | 152/153 (99%) | 0.27 | 3 (1%) 62 30 | 57, 96, 147, 259 | 0 |
| 1 | BJ | 152/153 (99%) | 0.24 | 3 (1%) 62 30 | 55, 93, 153, 393 | 0 |
| 1 | BK | 152/153 (99%) | 0.07 | 1 (0%) 84 56 | 55, 97, 147, 271 | 0 |
| 1 | BL | 152/153 (99%) | 0.31 | 3 (1%) 62 30 | 60, 95, 151, 347 | 0 |
| 1 | BM | 152/153 (99%) | 0.31 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | BN | 152/153 (99%) | 0.14 | 1 (0%) 84 56 | 57, 96, 147, 259 | 0 |
| 1 | BO | 152/153 (99%) | 0.19 | 4 (2%) 53 24 | 55, 93, 153, 393 | 0 |
| 1 | BP | 152/153 (99%) | 0.24 | 2 (1%) 74 40 | 55, 97, 147, 271 | 0 |
| 1 | BQ | 152/153 (99%) | 0.25 | 2 (1%) 74 40 | 60, 95, 151, 347 | 0 |
| 1 | BR | 152/153 (99%) | 0.25 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | BS | 152/153 (99%) | 0.30 | 3 (1%) 62 30 | 57, 96, 147, 259 | 0 |
| 1 | BT | 152/153 (99%) | 0.29 | 3 (1%) 62 30 | 55, 93, 153, 393 | 0 |
| 1 | BU | 152/153 (99%) | 0.27 | 1 (0%) 84 56 | 55, 97, 147, 271 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1 | BV | 152/153 (99%) | 0.39 | 4 (2%) 53 24 | 60, 95, 151, 347 | 0 |
| 1 | BW | 152/153 (99%) | 0.26 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | BX | 152/153 (99%) | 0.19 | 0 100 100 | 57, 96, 147, 259 | 0 |
| 1 | BY | 152/153 (99%) | 0.26 | 3 (1%) 62 30 | 55, 93, 153, 393 | 0 |
| 1 | BZ | 152/153 (99%) | 0.20 | 2 (1%) 74 40 | 55, 97, 147, 271 | 0 |
| 1 | C1 | 152/153 (99%) | 0.96 | 12 (7%) 13 7 | 60, 95, 151, 347 | 0 |
| 1 | C2 | 152/153 (99%) | 0.80 | 9 (5%) 22 9 | 56, 97, 184, 226 | 0 |
| 1 | C3 | 152/153 (99%) | 0.98 | 15 (9%) 8 5 | 57, 96, 147, 259 | 0 |
| 1 | C4 | 152/153 (99%) | 1.05 | 17 (11%) 6 4 | 55, 93, 153, 393 | 0 |
| 1 | CA | 152/153 (99%) | 0.48 | 6 (3%) 37 16 | 55, 97, 147, 271 | 0 |
| 1 | CB | 152/153 (99%) | 0.69 | 10 (6%) 18 8 | 60, 95, 151, 347 | 0 |
| 1 | CC | 152/153 (99%) | 0.75 | 7 (4%) 31 14 | 56, 97, 184, 226 | 0 |
| 1 | CD | 152/153 (99%) | 0.83 | 12 (7%) 13 7 | 57, 96, 147, 259 | 0 |
| 1 | CE | 152/153 (99%) | 0.41 | 5 (3%) 44 20 | 55, 93, 153, 393 | 0 |
| 1 | CF | 152/153 (99%) | 0.86 | 12 (7%) 13 7 | 55, 97, 147, 271 | 0 |
| 1 | CG | 152/153 (99%) | 0.50 | 3 (1%) 62 30 | 60, 95, 151, 347 | 0 |
| 1 | CH | 152/153 (99%) | 0.20 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | CI | 152/153 (99%) | 0.23 | 3 (1%) 62 30 | 57, 96, 147, 259 | 0 |
| 1 | CJ | 152/153 (99%) | 0.62 | 9 (5%) 22 9 | 55, 93, 153, 393 | 0 |
| 1 | CK | 152/153 (99%) | 0.07 | 1 (0%) 84 56 | 55, 97, 147, 271 | 0 |
| 1 | CL | 152/153 (99%) | 0.24 | 2 (1%) 74 40 | 60, 95, 151, 347 | 0 |
| 1 | CM | 152/153 (99%) | 0.15 | 2 (1%) 74 40 | 56, 97, 184, 226 | 0 |
| 1 | CN | 152/153 (99%) | 0.30 | 2 (1%) 74 40 | 57, 96, 147, 259 | 0 |
| 1 | CO | 152/153 (99%) | 0.22 | 4 (2%) 53 24 | 55, 93, 153, 393 | 0 |
| 1 | CP | 152/153 (99%) | 0.88 | 11 (7%) 15 7 | 55, 97, 147, 271 | 0 |
| 1 | CQ | 152/153 (99%) | 1.07 | 16 (10%) 7 5 | 60, 95, 151, 347 | 0 |
| 1 | CR | 152/153 (99%) | 1.18 | 15 (9%) 8 5 | 56, 97, 184, 226 | 0 |
| 1 | CS | 152/153 (99%) | 1.30 | 30 (19%) 2 2 | 57, 96, 147, 259 | 0 |
| 1 | CT | 152/153 (99%) | 1.18 | 18 (11%) 5 4 | 55, 93, 153, 393 | 0 |
| 1 | CU | 152/153 (99%) | 0.42 | 5 (3%) 44 20 | 55, 97, 147, 271 | 0 |
| 1 | CV | 152/153 (99%) | 0.72 | 8 (5%) 25 10 | 60, 95, 151, 347 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 1 | CW | 152/153 (99%) | 0.74 | 11 (7%) 15 7 | 56, 97, 184, 226 | 0 |
| 1 | CX | 152/153 (99%) | 0.46 | 3 (1%) 62 30 | 57, 96, 147, 259 | 0 |
| 1 | CY | 152/153 (99%) | 0.24 | 4 (2%) 53 24 | 55, 93, 153, 393 | 0 |
| 1 | CZ | 152/153 (99%) | 1.17 | 21 (13%) 4 3 | 55, 97, 147, 271 | 0 |
| All | All | 13680/13770 (99%) | 0.37 | 405 (2%) 48 22 | 55, 96, 157, 393 | 0 |

All (405) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | BE | 151 | HIS | 13.0 |
| 1 | AN | 153 | ALA | 11.9 |
| 1 | BM | 153 | ALA | 11.8 |
| 1 | CD | 153 | ALA | 10.7 |
| 1 | AM | 153 | ALA | 10.5 |
| 1 | B3 | 153 | ALA | 10.1 |
| 1 | CW | 153 | ALA | 9.5 |
| 1 | CQ | 153 | ALA | 8.4 |
| 1 | CC | 153 | ALA | 8.3 |
| 1 | AJ | 151 | HIS | 8.2 |
| 1 | CR | 153 | ALA | 7.9 |
| 1 | AS | 153 | ALA | 7.5 |
| 1 | BI | 153 | ALA | 7.5 |
| 1 | CN | 153 | ALA | 7.4 |
| 1 | AL | 153 | ALA | 7.4 |
| 1 | BA | 153 | ALA | 7.4 |
| 1 | AO | 151 | HIS | 7.3 |
| 1 | B4 | 151 | HIS | 7.3 |
| 1 | BW | 153 | ALA | 7.2 |
| 1 | BJ | 151 | HIS | 6.9 |
| 1 | AE | 151 | HIS | 6.7 |
| 1 | AW | 153 | ALA | 6.7 |
| 1 | BP | 153 | ALA | 6.7 |
| 1 | BE | 150 | LYS | 6.5 |
| 1 | A1 | 152 | TRP | 6.4 |
| 1 | AL | 152 | TRP | 6.4 |
| 1 | AR | 153 | ALA | 6.4 |
| 1 | AH | 153 | ALA | 6.3 |
| 1 | CS | 73 | ALA | 6.3 |
| 1 | BH | 153 | ALA | 6.3 |
| 1 | CT | 151 | HIS | 6.2 |
| 1 | AG | 152 | TRP | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | AD | 153 | ALA | 6.0 |
| 1 | CD | 152 | TRP | 5.8 |
| 1 | CM | 153 | ALA | 5.8 |
| 1 | A1 | 153 | ALA | 5.8 |
| 1 | CQ | 152 | TRP | 5.7 |
| 1 | BB | 152 | TRP | 5.7 |
| 1 | AY | 151 | HIS | 5.7 |
| 1 | CH | 153 | ALA | 5.6 |
| 1 | AC | 153 | ALA | 5.5 |
| 1 | AJ | 150 | LYS | 5.5 |
| 1 | AI | 153 | ALA | 5.5 |
| 1 | CV | 153 | ALA | 5.4 |
| 1 | AV | 153 | ALA | 5.4 |
| 1 | B2 | 153 | ALA | 5.3 |
| 1 | AV | 152 | TRP | 5.2 |
| 1 | AU | 153 | ALA | 5.2 |
| 1 | CZ | 73 | ALA | 5.2 |
| 1 | CO | 151 | HIS | 5.1 |
| 1 | AW | 152 | TRP | 5.0 |
| 1 | A2 | 153 | ALA | 5.0 |
| 1 | CU | 153 | ALA | 4.8 |
| 1 | AQ | 152 | TRP | 4.8 |
| 1 | A4 | 151 | HIS | 4.7 |
| 1 | BM | 152 | TRP | 4.7 |
| 1 | CF | 73 | ALA | 4.7 |
| 1 | BV | 153 | ALA | 4.7 |
| 1 | CQ | 9 | GLY | 4.7 |
| 1 | CR | 142 | ALA | 4.6 |
| 1 | BB | 153 | ALA | 4.6 |
| 1 | C1 | 153 | ALA | 4.6 |
| 1 | A2 | 152 | TRP | 4.5 |
| 1 | C2 | 153 | ALA | 4.5 |
| 1 | CG | 152 | TRP | 4.5 |
| 1 | CV | 151 | HIS | 4.4 |
| 1 | BL | 153 | ALA | 4.3 |
| 1 | CI | 153 | ALA | 4.3 |
| 1 | A4 | 150 | LYS | 4.2 |
| 1 | B1 | 153 | ALA | 4.2 |
| 1 | CV | 152 | TRP | 4.1 |
| 1 | B1 | 152 | TRP | 4.1 |
| 1 | AH | 152 | TRP | 4.1 |
| 1 | CE | 150 | LYS | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | C3 | 9 | GLY | 4.1 |
| 1 | C2 | 152 | TRP | 4.1 |
| 1 | C4 | 105 | GLN | 4.1 |
| 1 | CA | 153 | ALA | 4.0 |
| 1 | AO | 150 | LYS | 4.0 |
| 1 | AX | 153 | ALA | 3.9 |
| 1 | CJ | 73 | ALA | 3.9 |
| 1 | CB | 151 | HIS | 3.8 |
| 1 | BV | 152 | TRP | 3.8 |
| 1 | AB | 152 | TRP | 3.7 |
| 1 | CZ | 153 | ALA | 3.7 |
| 1 | C4 | 145 | MET | 3.7 |
| 1 | C1 | 40 | HIS | 3.6 |
| 1 | AT | 151 | HIS | 3.6 |
| 1 | BT | 151 | HIS | 3.6 |
| 1 | B1 | 151 | HIS | 3.6 |
| 1 | C4 | 92 | CYS | 3.6 |
| 1 | CZ | 145 | MET | 3.6 |
| 1 | CQ | 151 | HIS | 3.6 |
| 1 | CJ | 151 | HIS | 3.5 |
| 1 | C2 | 151 | HIS | 3.5 |
| 1 | A3 | 153 | ALA | 3.5 |
| 1 | AM | 152 | TRP | 3.5 |
| 1 | AG | 151 | HIS | 3.5 |
| 1 | CQ | 74 | VAL | 3.5 |
| 1 | CQ | 40 | HIS | 3.5 |
| 1 | BU | 153 | ALA | 3.5 |
| 1 | CS | 109 | PRO | 3.5 |
| 1 | BT | 150 | LYS | 3.5 |
| 1 | CS | 74 | VAL | 3.4 |
| 1 | C1 | 152 | TRP | 3.4 |
| 1 | CZ | 78 | GLY | 3.4 |
| 1 | BI | 152 | TRP | 3.4 |
| 1 | B4 | 150 | LYS | 3.4 |
| 1 | BC | 152 | TRP | 3.4 |
| 1 | CT | 50 | ALA | 3.4 |
| 1 | CV | 44 | GLU | 3.4 |
| 1 | CQ | 73 | ALA | 3.3 |
| 1 | C3 | 153 | ALA | 3.3 |
| 1 | B2 | 152 | TRP | 3.3 |
| 1 | C4 | 37 | LEU | 3.3 |
| 1 | CD | 151 | HIS | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | CZ | 72 | ASP | 3.3 |
| 1 | BD | 153 | ALA | 3.3 |
| 1 | C2 | 145 | MET | 3.3 |
| 1 | C1 | 7 | LEU | 3.3 |
| 1 | CZ | 113 | GLY | 3.3 |
| 1 | AY | 150 | LYS | 3.3 |
| 1 | BS | 153 | ALA | 3.3 |
| 1 | CY | 149 | SER | 3.2 |
| 1 | CD | 8 | VAL | 3.2 |
| 1 | CT | 19 | GLY | 3.2 |
| 1 | CK | 153 | ALA | 3.2 |
| 1 | CS | 72 | ASP | 3.2 |
| 1 | CF | 7 | LEU | 3.2 |
| 1 | AN | 152 | TRP | 3.2 |
| 1 | CT | 16 | VAL | 3.2 |
| 1 | BC | 153 | ALA | 3.2 |
| 1 | CB | 152 | TRP | 3.1 |
| 1 | CV | 6 | HIS | 3.1 |
| 1 | CZ | 8 | VAL | 3.1 |
| 1 | C3 | 152 | TRP | 3.1 |
| 1 | CT | 15 | GLY | 3.1 |
| 1 | CT | 49 | VAL | 3.1 |
| 1 | CA | 14 | VAL | 3.1 |
| 1 | CB | 73 | ALA | 3.1 |
| 1 | CR | 92 | CYS | 3.1 |
| 1 | CE | 151 | HIS | 3.1 |
| 1 | CS | 145 | MET | 3.1 |
| 1 | CX | 153 | ALA | 3.1 |
| 1 | CZ | 65 | MET | 3.1 |
| 1 | CS | 153 | ALA | 3.1 |
| 1 | AD | 152 | TRP | 3.0 |
| 1 | BN | 153 | ALA | 3.0 |
| 1 | BW | 152 | TRP | 3.0 |
| 1 | BO | 151 | HIS | 3.0 |
| 1 | CJ | 149 | SER | 3.0 |
| 1 | CO | 150 | LYS | 3.0 |
| 1 | CH | 152 | TRP | 3.0 |
| 1 | CS | 65 | MET | 3.0 |
| 1 | AA | 153 | ALA | 2.9 |
| 1 | CF | 5 | GLY | 2.9 |
| 1 | CR | 90 | TYR | 2.9 |
| 1 | CP | 37 | LEU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B3 | 70 | LYS | 2.9 |
| 1 | BV | 151 | HIS | 2.9 |
| 1 | CB | 153 | ALA | 2.9 |
| 1 | BQ | 153 | ALA | 2.9 |
| 1 | BY | 151 | HIS | 2.9 |
| 1 | CF | 143 | ILE | 2.9 |
| 1 | CJ | 72 | ASP | 2.9 |
| 1 | CP | 108 | ILE | 2.9 |
| 1 | CS | 76 | THR | 2.9 |
| 1 | AX | 152 | TRP | 2.9 |
| 1 | CS | 15 | GLY | 2.9 |
| 1 | CL | 152 | TRP | 2.8 |
| 1 | C1 | 151 | HIS | 2.8 |
| 1 | CP | 10 | THR | 2.8 |
| 1 | CW | 143 | ILE | 2.8 |
| 1 | CZ | 74 | VAL | 2.8 |
| 1 | C1 | 43 | GLU | 2.8 |
| 1 | BC | 6 | HIS | 2.8 |
| 1 | BA | 43 | GLU | 2.8 |
| 1 | CS | 66 | ALA | 2.8 |
| 1 | C3 | 44 | GLU | 2.8 |
| 1 | CS | 62 | ALA | 2.8 |
| 1 | C4 | 63 | LYS | 2.8 |
| 1 | CW | 15 | GLY | 2.8 |
| 1 | CX | 6 | HIS | 2.8 |
| 1 | BP | 152 | TRP | 2.8 |
| 1 | C2 | 40 | HIS | 2.7 |
| 1 | AB | 153 | ALA | 2.7 |
| 1 | CQ | 41 | GLY | 2.7 |
| 1 | CP | 153 | ALA | 2.7 |
| 1 | CT | 40 | HIS | 2.7 |
| 1 | CO | 12 | LEU | 2.7 |
| 1 | BQ | 152 | TRP | 2.7 |
| 1 | CW | 73 | ALA | 2.7 |
| 1 | CP | 70 | LYS | 2.7 |
| 1 | A4 | 149 | SER | 2.7 |
| 1 | BJ | 150 | LYS | 2.7 |
| 1 | CR | 45 | ASN | 2.7 |
| 1 | CZ | 143 | ILE | 2.7 |
| 1 | CX | 73 | ALA | 2.7 |
| 1 | CS | 108 | ILE | 2.7 |
| 1 | BR | 152 | TRP | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | CV | 142 | ALA | 2.6 |
| 1 | CY | 151 | HIS | 2.6 |
| 1 | CV | 143 | ILE | 2.6 |
| 1 | CT | 72 | ASP | 2.6 |
| 1 | CL | 151 | HIS | 2.6 |
| 1 | CR | 62 | ALA | 2.6 |
| 1 | CA | 73 | ALA | 2.6 |
| 1 | CW | 14 | VAL | 2.6 |
| 1 | AR | 152 | TRP | 2.6 |
| 1 | CM | 152 | TRP | 2.6 |
| 1 | BO | 73 | ALA | 2.6 |
| 1 | CW | 86 | THR | 2.6 |
| 1 | CT | 9 | GLY | 2.6 |
| 1 | CS | 67 | ASN | 2.6 |
| 1 | CT | 36 | GLY | 2.6 |
| 1 | CY | 150 | LYS | 2.6 |
| 1 | C3 | 50 | ALA | 2.6 |
| 1 | CZ | 76 | THR | 2.6 |
| 1 | CI | 152 | TRP | 2.6 |
| 1 | BK | 10 | THR | 2.6 |
| 1 | CJ | 109 | PRO | 2.6 |
| 1 | CP | 12 | LEU | 2.6 |
| 1 | A2 | 151 | HIS | 2.6 |
| 1 | BV | 6 | HIS | 2.6 |
| 1 | CF | 15 | GLY | 2.5 |
| 1 | CR | 37 | LEU | 2.5 |
| 1 | CQ | 148 | LEU | 2.5 |
| 1 | CE | 14 | VAL | 2.5 |
| 1 | C4 | 151 | HIS | 2.5 |
| 1 | CA | 45 | ASN | 2.5 |
| 1 | CR | 145 | MET | 2.5 |
| 1 | BB | 151 | HIS | 2.5 |
| 1 | CZ | 139 | ALA | 2.5 |
| 1 | C3 | 4 | GLU | 2.5 |
| 1 | CE | 90 | TYR | 2.5 |
| 1 | BR | 153 | ALA | 2.5 |
| 1 | C3 | 142 | ALA | 2.5 |
| 1 | C2 | 92 | CYS | 2.5 |
| 1 | C4 | 11 | GLY | 2.5 |
| 1 | CW | 152 | TRP | 2.5 |
| 1 | CG | 151 | HIS | 2.5 |
| 1 | C4 | 153 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | CB | 34 | LEU | 2.5 |
| 1 | CD | 45 | ASN | 2.5 |
| 1 | CZ | 148 | LEU | 2.5 |
| 1 | CC | 152 | TRP | 2.5 |
| 1 | CT | 45 | ASN | 2.5 |
| 1 | BO | 149 | SER | 2.5 |
| 1 | CD | 130 | LYS | 2.5 |
| 1 | CW | 72 | ASP | 2.5 |
| 1 | BF | 153 | ALA | 2.4 |
| 1 | CD | 40 | HIS | 2.4 |
| 1 | CS | 6 | HIS | 2.4 |
| 1 | BL | 151 | HIS | 2.4 |
| 1 | AO | 149 | SER | 2.4 |
| 1 | CG | 10 | THR | 2.4 |
| 1 | CT | 78 | GLY | 2.4 |
| 1 | C4 | 10 | THR | 2.4 |
| 1 | BT | 40 | HIS | 2.4 |
| 1 | AZ | 153 | ALA | 2.4 |
| 1 | BG | 152 | TRP | 2.4 |
| 1 | CS | 79 | THR | 2.4 |
| 1 | CS | 63 | LYS | 2.4 |
| 1 | CZ | 93 | ASN | 2.4 |
| 1 | C3 | 34 | LEU | 2.4 |
| 1 | CS | 141 | ALA | 2.4 |
| 1 | BI | 70 | LYS | 2.4 |
| 1 | CZ | 14 | VAL | 2.4 |
| 1 | BL | 152 | TRP | 2.4 |
| 1 | CT | 10 | THR | 2.4 |
| 1 | BH | 152 | TRP | 2.4 |
| 1 | CP | 65 | MET | 2.4 |
| 1 | CT | 73 | ALA | 2.3 |
| 1 | CU | 146 | ALA | 2.3 |
| 1 | B3 | 151 | HIS | 2.3 |
| 1 | C1 | 44 | GLU | 2.3 |
| 1 | CB | 38 | LYS | 2.3 |
| 1 | CR | 63 | LYS | 2.3 |
| 1 | CS | 126 | ARG | 2.3 |
| 1 | CF | 6 | HIS | 2.3 |
| 1 | CS | 75 | ILE | 2.3 |
| 1 | CS | 78 | GLY | 2.3 |
| 1 | CS | 5 | GLY | 2.3 |
| 1 | CC | 146 | ALA | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | CZ | 50 | ALA | 2.3 |
| 1 | CC | 12 | LEU | 2.3 |
| 1 | C4 | 149 | SER | 2.3 |
| 1 | CT | 43 | GLU | 2.3 |
| 1 | CS | 90 | TYR | 2.3 |
| 1 | CD | 70 | LYS | 2.3 |
| 1 | CJ | 150 | LYS | 2.3 |
| 1 | CU | 152 | TRP | 2.3 |
| 1 | CC | 72 | ASP | 2.3 |
| 1 | BY | 149 | SER | 2.3 |
| 1 | C4 | 69 | GLY | 2.3 |
| 1 | BG | 44 | GLU | 2.3 |
| 1 | CS | 59 | PRO | 2.3 |
| 1 | CJ | 143 | ILE | 2.2 |
| 1 | CC | 68 | SER | 2.2 |
| 1 | CF | 50 | ALA | 2.2 |
| 1 | CT | 142 | ALA | 2.2 |
| 1 | CN | 152 | TRP | 2.2 |
| 1 | CQ | 92 | CYS | 2.2 |
| 1 | AG | 153 | ALA | 2.2 |
| 1 | CF | 38 | LYS | 2.2 |
| 1 | BH | 44 | GLU | 2.2 |
| 1 | CU | 44 | GLU | 2.2 |
| 1 | CF | 14 | VAL | 2.2 |
| 1 | CS | 68 | SER | 2.2 |
| 1 | CB | 72 | ASP | 2.2 |
| 1 | CP | 49 | VAL | 2.2 |
| 1 | CZ | 13 | LYS | 2.2 |
| 1 | C4 | 72 | ASP | 2.2 |
| 1 | C1 | 82 | ARG | 2.2 |
| 1 | CF | 10 | THR | 2.2 |
| 1 | AK | 153 | ALA | 2.2 |
| 1 | CZ | 77 | LEU | 2.2 |
| 1 | CW | 65 | MET | 2.2 |
| 1 | BY | 150 | LYS | 2.2 |
| 1 | AC | 152 | TRP | 2.2 |
| 1 | CR | 11 | GLY | 2.2 |
| 1 | CQ | 8 | VAL | 2.2 |
| 1 | CS | 51 | TRP | 2.2 |
| 1 | CR | 14 | VAL | 2.2 |
| 1 | AF | 153 | ALA | 2.2 |
| 1 | CS | 50 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | CD | 42 | VAL | 2.2 |
| 1 | CB | 15 | GLY | 2.2 |
| 1 | CZ | 146 | ALA | 2.2 |
| 1 | CS | 64 | LYS | 2.2 |
| 1 | CR | 73 | ALA | 2.2 |
| 1 | CQ | 132 | GLY | 2.2 |
| 1 | C3 | 73 | ALA | 2.2 |
| 1 | B2 | 47 | ILE | 2.2 |
| 1 | C1 | 38 | LYS | 2.2 |
| 1 | CW | 67 | ASN | 2.1 |
| 1 | CD | 71 | TYR | 2.1 |
| 1 | CC | 13 | LYS | 2.1 |
| 1 | C4 | 107 | ASP | 2.1 |
| 1 | CQ | 42 | VAL | 2.1 |
| 1 | CU | 45 | ASN | 2.1 |
| 1 | BC | 5 | GLY | 2.1 |
| 1 | CD | 9 | GLY | 2.1 |
| 1 | AY | 149 | SER | 2.1 |
| 1 | C3 | 42 | VAL | 2.1 |
| 1 | C1 | 142 | ALA | 2.1 |
| 1 | AJ | 149 | SER | 2.1 |
| 1 | CE | 107 | ASP | 2.1 |
| 1 | CF | 34 | LEU | 2.1 |
| 1 | CR | 107 | ASP | 2.1 |
| 1 | BZ | 40 | HIS | 2.1 |
| 1 | CS | 40 | HIS | 2.1 |
| 1 | B3 | 72 | ASP | 2.1 |
| 1 | CB | 8 | VAL | 2.1 |
| 1 | C1 | 19 | GLY | 2.1 |
| 1 | C2 | 150 | LYS | 2.1 |
| 1 | CZ | 152 | TRP | 2.1 |
| 1 | CW | 7 | LEU | 2.1 |
| 1 | BJ | 149 | SER | 2.1 |
| 1 | CI | 151 | HIS | 2.1 |
| 1 | CV | 7 | LEU | 2.1 |
| 1 | BA | 152 | TRP | 2.1 |
| 1 | CQ | 44 | GLU | 2.1 |
| 1 | CT | 4 | GLU | 2.1 |
| 1 | CS | 82 | ARG | 2.1 |
| 1 | C4 | 66 | ALA | 2.1 |
| 1 | CD | 7 | LEU | 2.1 |
| 1 | BF | 151 | HIS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C1 | 88 | TYR | 2.1 |
| 1 | C3 | 3 | PHE | 2.1 |
| 1 | CR | 35 | ASP | 2.1 |
| 1 | CA | 47 | ILE | 2.1 |
| 1 | C3 | 40 | HIS | 2.1 |
| 1 | C4 | 65 | MET | 2.1 |
| 1 | CS | 143 | ILE | 2.1 |
| 1 | C3 | 71 | TYR | 2.1 |
| 1 | C2 | 142 | ALA | 2.1 |
| 1 | C3 | 8 | VAL | 2.1 |
| 1 | BS | 152 | TRP | 2.1 |
| 1 | AE | 149 | SER | 2.1 |
| 1 | BF | 43 | GLU | 2.1 |
| 1 | CP | 143 | ILE | 2.1 |
| 1 | C4 | 108 | ILE | 2.1 |
| 1 | CP | 152 | TRP | 2.1 |
| 1 | CQ | 75 | ILE | 2.1 |
| 1 | CJ | 145 | MET | 2.1 |
| 1 | BO | 150 | LYS | 2.1 |
| 1 | BS | 82 | ARG | 2.1 |
| 1 | C4 | 59 | PRO | 2.1 |
| 1 | CY | 13 | LYS | 2.1 |
| 1 | CT | 14 | VAL | 2.0 |
| 1 | C2 | 44 | GLU | 2.0 |
| 1 | CZ | 59 | PRO | 2.0 |
| 1 | BZ | 8 | VAL | 2.0 |
| 1 | CO | 10 | THR | 2.0 |
| 1 | A1 | 44 | GLU | 2.0 |
| 1 | CB | 64 | LYS | 2.0 |
| 1 | CQ | 38 | LYS | 2.0 |
| 1 | BA | 6 | HIS | 2.0 |
| 1 | CP | 6 | HIS | 2.0 |
| 1 | CA | 12 | LEU | 2.0 |
| 1 | CF | 145 | MET | 2.0 |
| 1 | C3 | 19 | GLY | 2.0 |
| 1 | CJ | 13 | LYS | 2.0 |
| 1 | CR | 39 | ARG | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 2 | PO4 | AI | 1001 | 5/5 | 0.31 | 2.04 | 58,65,106,138 | 0 |
| 2 | PO4 | AX | 1001 | 5/5 | 0.31 | 2.03 | 58,65,106,138 | 0 |
| 2 | PO4 | BG | 1001 | 5/5 | 0.27 | 1.47 | 74,78,104,213 | 0 |
| 2 | PO4 | CD | 1001 | 5/5 | 0.32 | 1.04 | 58,65,106,138 | 0 |
| 2 | PO4 | BD | 1001 | 5/5 | 0.23 | 0.39 | 58,65,106,138 | 0 |
| 2 | PO4 | AW | 201 | 5/5 | 0.24 | 0.18 | 34,46,111,116 | 0 |
| 2 | PO4 | CQ | 1201 | 5/5 | 0.32 | 0.13 | 74,78,104,213 | 0 |
| 2 | PO4 | AK | 1001 | 5/5 | 0.23 | 0.09 | 80,81,83,167 | 0 |
| 2 | PO4 | CB | 1001 | 5/5 | 0.35 | 0.08 | 74,78,104,213 | 0 |
| 2 | PO4 | AL | 1001 | 5/5 | 0.24 | 0.06 | 74,78,104,213 | 0 |
| 2 | PO4 | AJ | 1001 | 5/5 | 0.23 | -0.03 | 23,28,53,142 | 0 |
| 2 | PO4 | AG | 1001 | 5/5 | 0.23 | -0.13 | 74,78,104,213 | 0 |
| 2 | PO4 | AY | 1001 | 5/5 | 0.24 | -0.15 | 23,28,53,142 | 0 |
| 2 | PO4 | CZ | 201 | 5/5 | 0.29 | -0.20 | 80,81,83,167 | 0 |
| 2 | PO4 | CY | 4201 | 5/5 | 0.32 | -0.21 | 23,28,53,142 | 0 |
| 2 | PO4 | CJ | 4201 | 5/5 | 0.25 | -0.22 | 23,28,53,142 | 0 |
| 2 | PO4 | BR | 1001 | 5/5 | 0.22 | -0.24 | 34,46,111,116 | 0 |
| 2 | PO4 | AH | 1001 | 5/5 | 0.20 | -0.26 | 34,46,111,116 | 0 |
| 2 | PO4 | BL | 1001 | 5/5 | 0.26 | -0.27 | 74,78,104,213 | 0 |
| 2 | PO4 | CT | 4201 | 5/5 | 0.38 | -0.37 | 23,28,53,142 | 0 |
| 2 | PO4 | BZ | 1001 | 5/5 | 0.20 | -0.39 | 80,81,83,167 | 0 |
| 2 | PO4 | CK | 201 | 5/5 | 0.18 | -0.40 | 80,81,83,167 | 0 |
| 2 | PO4 | CN | 3201 | 5/5 | 0.20 | -0.43 | 58,65,106,138 | 0 |
| 2 | PO4 | AC | 1001 | 5/5 | 0.17 | -0.48 | 34,46,111,116 | 0 |
| 2 | PO4 | CG | 1201 | 5/5 | 0.24 | -0.48 | 74,78,104,213 | 0 |
| 2 | PO4 | BX | 1001 | 5/5 | 0.17 | -0.53 | 58,65,106,138 | 0 |
| 2 | PO4 | BB | 1001 | 5/5 | 0.21 | -0.53 | 74,78,104,213 | 0 |
| 2 | PO4 | B1 | 1001 | 5/5 | 0.20 | -0.57 | 74,78,104,213 | 0 |
| 2 | PO4 | BP | 1001 | 5/5 | 0.17 | -0.70 | 80,81,83,167 | 0 |
| 2 | PO4 | BE | 1001 | 5/5 | 0.22 | -0.71 | 23,28,53,142 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 2 | PO4 | C2 | 2201 | 5/5 | 0.28 | -0.71 | 34,46,111,116 | 0 |
| 2 | PO4 | AM | 1001 | 5/5 | 0.19 | -0.73 | 34,46,111,116 | 0 |
| 2 | PO4 | CW | 2201 | 5/5 | 0.29 | -0.74 | 34,46,111,116 | 0 |
| 2 | PO4 | CH | 2201 | 5/5 | 0.24 | -0.75 | 34,46,111,116 | 0 |
| 2 | PO4 | AV | 1001 | 5/5 | 0.19 | -0.75 | 74,78,104,213 | 0 |
| 2 | PO4 | BK | 1001 | 5/5 | 0.17 | -0.76 | 80,81,83,167 | 0 |
| 2 | PO4 | CX | 3201 | 5/5 | 0.20 | -0.78 | 58,65,106,138 | 0 |
| 2 | PO4 | CL | 1201 | 5/5 | 0.19 | -0.81 | 74,78,104,213 | 0 |
| 2 | PO4 | AS | 1001 | 5/5 | 0.18 | -0.83 | 58,65,106,138 | 0 |
| 2 | PO4 | AB | 1001 | 5/5 | 0.19 | -0.83 | 74,78,104,213 | 0 |
| 2 | PO4 | BA | 1001 | 5/5 | 0.18 | -0.84 | 80,81,83,167 | 0 |
| 2 | PO4 | AZ | 1001 | 5/5 | 0.18 | -0.88 | 80,81,83,167 | 0 |
| 2 | PO4 | BW | 1001 | 5/5 | 0.20 | -0.89 | 34,46,111,116 | 0 |
| 2 | PO4 | CC | 1001 | 5/5 | 0.30 | -0.90 | 34,46,111,116 | 0 |
| 2 | PO4 | BQ | 1001 | 5/5 | 0.17 | -0.90 | 74,78,104,213 | 0 |
| 2 | PO4 | AA | 1001 | 5/5 | 0.15 | -0.98 | 80,81,83,167 | 0 |
| 2 | PO4 | CF | 201 | 5/5 | 0.22 | -0.98 | 80,81,83,167 | 0 |
| 2 | PO4 | BV | 1001 | 5/5 | 0.22 | -1.00 | 74,78,104,213 | 0 |
| 2 | PO4 | A3 | 1001 | 5/5 | 0.17 | -1.04 | 58,65,106,138 | 0 |
| 2 | PO4 | BH | 1001 | 5/5 | 0.16 | -1.07 | 34,46,111,116 | 0 |
| 2 | PO4 | BM | 1001 | 5/5 | 0.16 | -1.07 | 34,46,111,116 | 0 |
| 2 | PO4 | AP | 1001 | 5/5 | 0.17 | -1.08 | 80,81,83,167 | 0 |
| 2 | PO4 | AT | 1001 | 5/5 | 0.19 | -1.12 | 23,28,53,142 | 0 |
| 2 | PO4 | A4 | 1001 | 5/5 | 0.16 | -1.12 | 23,28,53,142 | 0 |
| 2 | PO4 | CE | 1001 | 5/5 | 0.27 | -1.14 | 23,28,53,142 | 0 |
| 2 | PO4 | BF | 1001 | 5/5 | 0.21 | -1.18 | 80,81,83,167 | 0 |
| 2 | PO4 | B3 | 1001 | 5/5 | 0.17 | -1.19 | 58,65,106,138 | 0 |
| 2 | PO4 | CA | 1001 | 5/5 | 0.18 | -1.21 | 80,81,83,167 | 0 |
| 2 | PO4 | BS | 1001 | 5/5 | 0.20 | -1.30 | 58,65,106,138 | 0 |
| 2 | PO4 | A2 | 1001 | 5/5 | 0.16 | -1.32 | 34,46,111,116 | 0 |
| 2 | PO4 | B4 | 1001 | 5/5 | 0.17 | -1.34 | 23,28,53,142 | 0 |
| 2 | PO4 | CV | 1201 | 5/5 | 0.20 | -1.37 | 74,78,104,213 | 0 |
| 2 | PO4 | B2 | 1001 | 5/5 | 0.20 | -1.38 | 34,46,111,116 | 0 |
| 2 | PO4 | CU | 201 | 5/5 | 0.13 | -1.41 | 80,81,83,167 | 0 |
| 2 | PO4 | A1 | 1001 | 5/5 | 0.17 | -1.47 | 74,78,104,213 | 0 |
| 2 | PO4 | AU | 1001 | 5/5 | 0.18 | -1.52 | 80,81,83,167 | 0 |
| 2 | PO4 | BC | 1001 | 5/5 | 0.15 | -1.53 | 34,46,111,116 | 0 |
| 2 | PO4 | CS | 3201 | 5/5 | 0.30 | -1.55 | 58,65,106,138 | 0 |
| 2 | PO4 | AN | 1001 | 5/5 | 0.16 | -1.59 | 58,65,106,138 | 0 |
| 2 | PO4 | BO | 1001 | 5/5 | 0.12 | -1.60 | 23,28,53,142 | 0 |
| 2 | PO4 | CP | 201 | 5/5 | 0.23 | -1.61 | 80,81,83,167 | 0 |
| 2 | PO4 | CM | 2201 | 5/5 | 0.15 | -1.63 | 34,46,111,116 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 2 | PO4 | BT | 1001 | 5/5 | 0.12 | -1.64 | 23,28,53,142 | 0 |
| 2 | PO4 | AD | 1001 | 5/5 | 0.15 | -1.68 | 58,65,106,138 | 0 |
| 2 | PO4 | BJ | 1001 | 5/5 | 0.13 | -1.71 | 23,28,53,142 | 0 |
| 2 | PO4 | C3 | 3201 | 5/5 | 0.22 | -1.76 | 58,65,106,138 | 0 |
| 2 | PO4 | BU | 1001 | 5/5 | 0.12 | -1.79 | 80,81,83,167 | 0 |
| 2 | PO4 | AO | 1001 | 5/5 | 0.17 | -1.82 | 23,28,53,142 | 0 |
| 2 | PO4 | CR | 2201 | 5/5 | 0.26 | -1.90 | 34,46,111,116 | 0 |
| 2 | PO4 | AQ | 1001 | 5/5 | 0.16 | -1.99 | 74,78,104,213 | 0 |
| 2 | PO4 | AF | 1001 | 5/5 | 0.14 | -2.01 | 80,81,83,167 | 0 |
| 2 | PO4 | BY | 1001 | 5/5 | 0.16 | -2.05 | 23,28,53,142 | 0 |
| 2 | PO4 | BN | 1001 | 5/5 | 0.14 | -2.15 | 58,65,106,138 | 0 |
| 2 | PO4 | C1 | 1201 | 5/5 | 0.23 | -2.18 | 74,78,104,213 | 0 |
| 2 | PO4 | BI | 1001 | 5/5 | 0.14 | -2.25 | 58,65,106,138 | 0 |
| 2 | PO4 | CI | 3201 | 5/5 | 0.16 | -2.30 | 58,65,106,138 | 0 |
| 2 | PO4 | AR | 1001 | 5/5 | 0.13 | -2.41 | 34,46,111,116 | 0 |
| 2 | PO4 | CO | 4201 | 5/5 | 0.18 | -2.67 | 23,28,53,142 | 0 |
| 2 | PO4 | AE | 1001 | 5/5 | 0.11 | -3.87 | 23,28,53,142 | 0 |
| 2 | PO4 | C4 | 4201 | 5/5 | 0.25 | -4.53 | 23,28,53,142 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.