



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:19 pm BST

PDB ID : 2W5J
Title : Structure of the c14-rotor ring of the proton translocating chloroplast ATP synthase
Authors : Vollmar, M.; Schlieper, D.; Winn, M.; Buechner, C.; Groth, G.
Deposited on : 2008-12-10
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

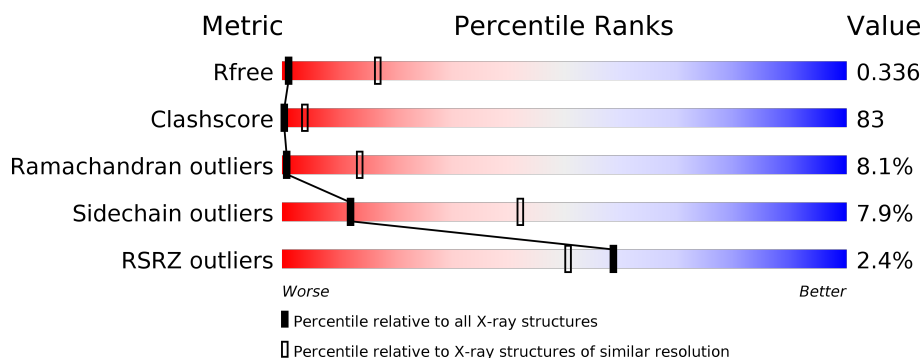
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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} | 130704 | 1212 (4.00-3.60) |
| Clashscore | 141614 | 1288 (4.00-3.60) |
| Ramachandran outliers | 138981 | 1243 (4.00-3.60) |
| Sidechain outliers | 138945 | 1237 (4.00-3.60) |
| RSRZ outliers | 127900 | 1121 (4.00-3.60) |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 78 | <div> <div>%</div> <div> <div></div> <div>32%</div> <div>60%</div> <div>8%</div> </div> </div> |
| 1 | B | 78 | <div> <div>5%</div> <div> <div></div> <div>32%</div> <div>58%</div> <div>10%</div> </div> </div> |
| 1 | C | 78 | <div> <div>%</div> <div> <div></div> <div>28%</div> <div>63%</div> <div>9%</div> </div> </div> |
| 1 | D | 78 | <div> <div>4%</div> <div> <div></div> <div>33%</div> <div>58%</div> <div>9%</div> </div> </div> |
| 1 | E | 78 | <div> <div>4%</div> <div> <div></div> <div>28%</div> <div>62%</div> <div>10%</div> </div> </div> |
| 1 | F | 78 | <div> <div></div> <div> <div></div> <div>32%</div> <div>59%</div> <div>9%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | G | 78 | <div> <div>%</div> <div> <div></div> <div>33%</div> <div>56%</div> <div>10%</div> </div> </div> |
| 1 | H | 78 | <div> <div>%</div> <div> <div></div> <div>33%</div> <div>58%</div> <div>9%</div> </div> </div> |
| 1 | I | 78 | <div> <div>%</div> <div> <div></div> <div>37%</div> <div>55%</div> <div>8%</div> </div> </div> |
| 1 | J | 78 | <div> <div>%</div> <div> <div></div> <div>33%</div> <div>58%</div> <div>9%</div> </div> </div> |
| 1 | K | 78 | <div> <div>4%</div> <div> <div></div> <div>36%</div> <div>54%</div> <div>10%</div> </div> </div> |
| 1 | L | 78 | <div> <div>4%</div> <div> <div></div> <div>33%</div> <div>58%</div> <div>9%</div> </div> </div> |
| 1 | M | 78 | <div> <div>3%</div> <div> <div></div> <div>33%</div> <div>55%</div> <div>12%</div> </div> </div> |
| 1 | V | 78 | <div> <div>3%</div> <div> <div></div> <div>36%</div> <div>54%</div> <div>10%</div> </div> </div> |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6860 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

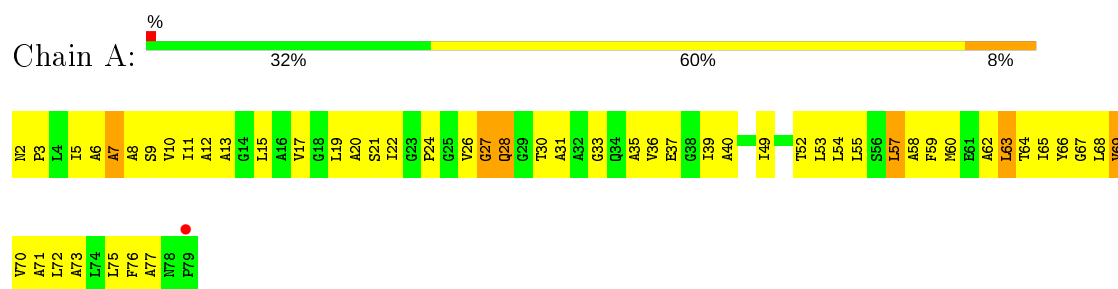
- Molecule 1 is a protein called ATP SYNTHASE C CHAIN, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 1 | A | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | B | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | C | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | D | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | E | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | F | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | G | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | H | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | I | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | J | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | K | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | L | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | M | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |
| 1 | V | 78 | Total | C | N | O | 0 | 0 | 0 |
| | | | 490 | 315 | 85 | 90 | | | |

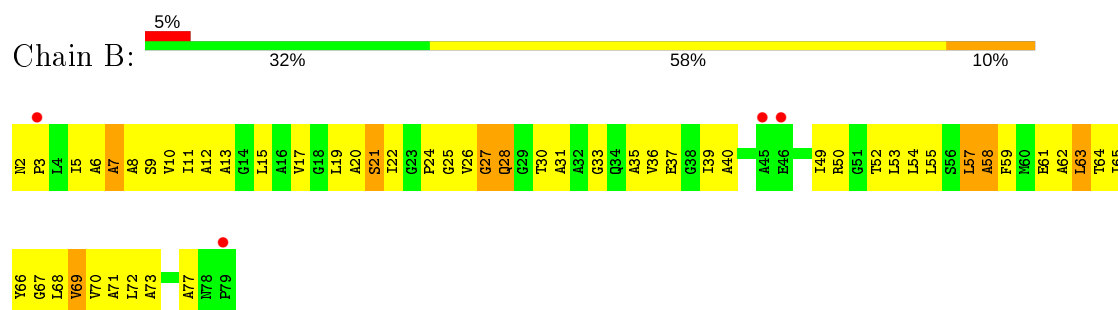
3 Residue-property plots [i](#)

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

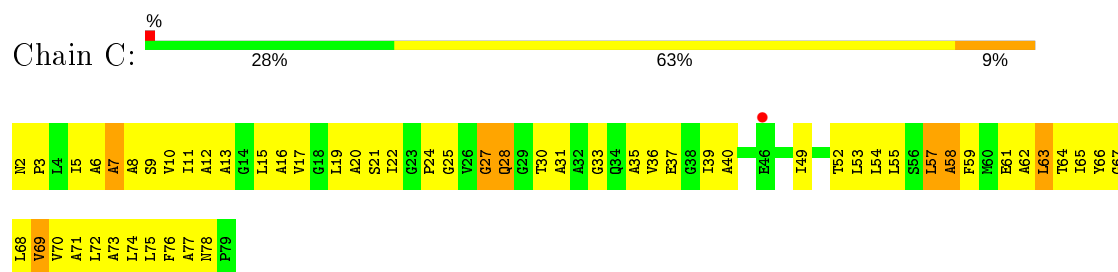
• Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC



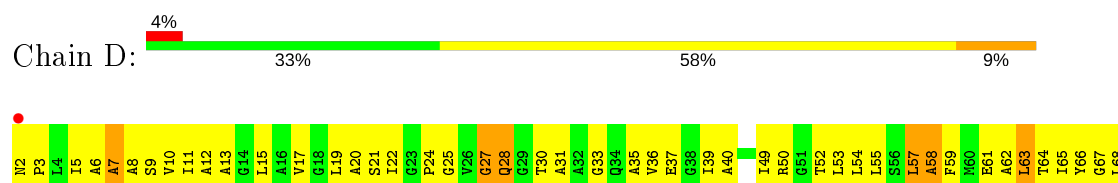
• Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC

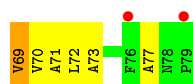


• Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC

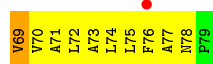


• Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC

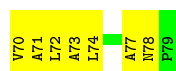




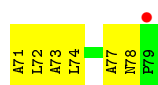
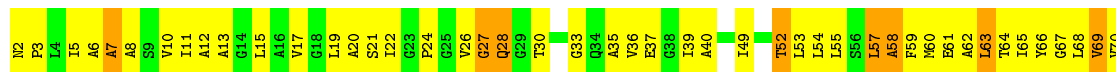
- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC



- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC



- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC

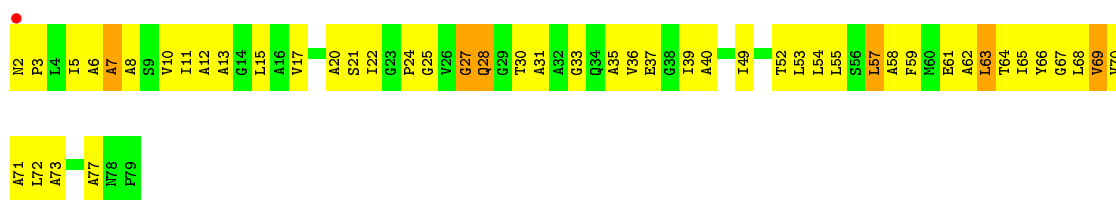


- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC

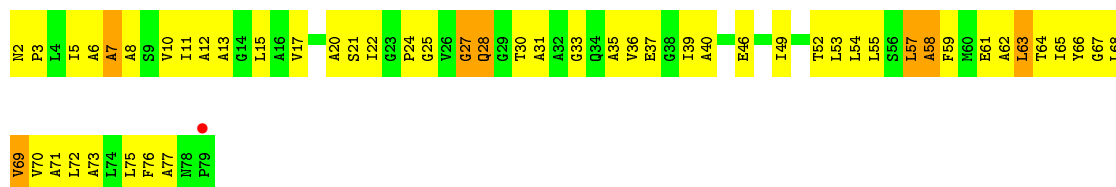


- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC

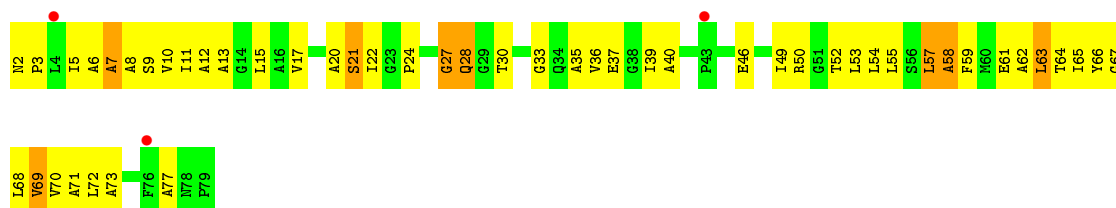




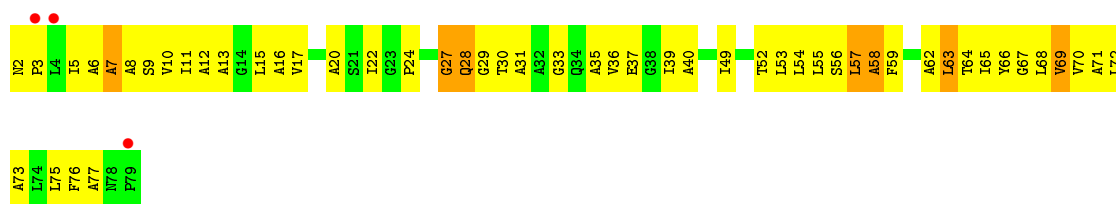
- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC



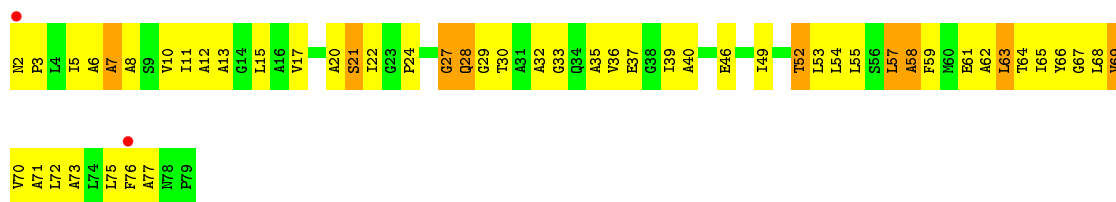
- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC



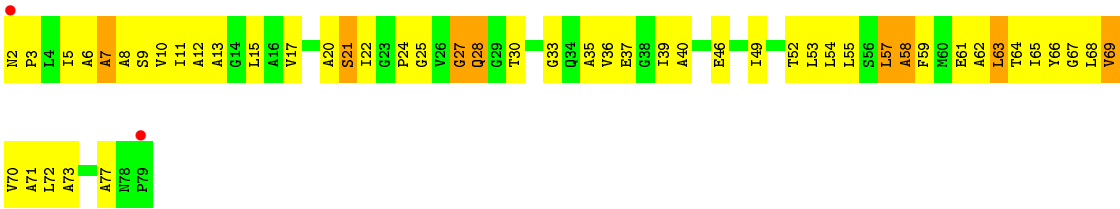
- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC



- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC



- Molecule 1: ATP SYNTHASE C CHAIN, CHLOROPLASTIC



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 128.60Å 90.00Å 124.89Å 90.00° 104.70° 90.00° | Depositor |
| Resolution (Å) | 19.75 – 3.80 19.75 – 3.80 | Depositor EDS |
| % Data completeness (in resolution range) | 92.5 (19.75-3.80) 92.5 (19.75-3.80) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.78 (at 3.82Å) | Xtriage |
| Refinement program | REFMAC 5.5.0063 | Depositor |
| R, R_{free} | 0.317 , 0.335 0.323 , 0.336 | Depositor DCC |
| R_{free} test set | 628 reflections (4.97%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 140.7 | Xtriage |
| Anisotropy | 0.186 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.38 , 211.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.37$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 6860 | wwPDB-VP |
| Average B, all atoms (Å ²) | 69.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.62 | 0/496 | 0.64 | 0/681 |
| 1 | B | 0.68 | 0/496 | 0.66 | 0/681 |
| 1 | C | 0.68 | 0/496 | 0.65 | 0/681 |
| 1 | D | 0.67 | 0/496 | 0.65 | 0/681 |
| 1 | E | 0.69 | 0/496 | 0.65 | 0/681 |
| 1 | F | 0.63 | 0/496 | 0.65 | 0/681 |
| 1 | G | 0.60 | 0/496 | 0.63 | 0/681 |
| 1 | H | 0.57 | 0/496 | 0.63 | 0/681 |
| 1 | I | 0.62 | 0/496 | 0.64 | 0/681 |
| 1 | J | 0.62 | 0/496 | 0.64 | 0/681 |
| 1 | K | 0.63 | 0/496 | 0.64 | 0/681 |
| 1 | L | 0.64 | 0/496 | 0.64 | 0/681 |
| 1 | M | 0.63 | 0/496 | 0.65 | 0/681 |
| 1 | V | 0.63 | 0/496 | 0.65 | 0/681 |
| All | All | 0.64 | 0/6944 | 0.65 | 0/9534 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 490 | 0 | 477 | 123 | 0 |
| 1 | B | 490 | 0 | 477 | 126 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | C | 490 | 0 | 477 | 121 | 0 |
| 1 | D | 490 | 0 | 477 | 129 | 0 |
| 1 | E | 490 | 0 | 477 | 124 | 0 |
| 1 | F | 490 | 0 | 477 | 116 | 0 |
| 1 | G | 490 | 0 | 477 | 101 | 0 |
| 1 | H | 490 | 0 | 477 | 105 | 0 |
| 1 | I | 490 | 0 | 477 | 111 | 0 |
| 1 | J | 490 | 0 | 477 | 122 | 0 |
| 1 | K | 490 | 0 | 477 | 118 | 0 |
| 1 | L | 490 | 0 | 477 | 129 | 0 |
| 1 | M | 490 | 0 | 477 | 127 | 0 |
| 1 | V | 490 | 0 | 477 | 105 | 0 |
| All | All | 6860 | 0 | 6678 | 1122 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 83.

All (1122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:70:VAL:HG22 | 1:E:72:LEU:HD21 | 1.33 | 1.09 |
| 1:A:70:VAL:HG22 | 1:B:72:LEU:HD21 | 1.35 | 1.08 |
| 1:A:5:ILE:HG22 | 1:B:8:ALA:HB2 | 1.34 | 1.07 |
| 1:K:5:ILE:HG22 | 1:L:8:ALA:HB2 | 1.34 | 1.06 |
| 1:K:70:VAL:HG22 | 1:L:72:LEU:HD21 | 1.43 | 1.00 |
| 1:I:39:ILE:HD11 | 1:I:49:ILE:CB | 1.93 | 0.99 |
| 1:B:70:VAL:HG22 | 1:C:72:LEU:HD21 | 1.45 | 0.98 |
| 1:A:5:ILE:HG22 | 1:B:8:ALA:CB | 1.94 | 0.97 |
| 1:V:39:ILE:HD11 | 1:V:49:ILE:CB | 1.94 | 0.97 |
| 1:D:39:ILE:HD11 | 1:D:49:ILE:CB | 1.95 | 0.97 |
| 1:C:70:VAL:HG22 | 1:D:72:LEU:HD21 | 1.46 | 0.96 |
| 1:C:63:LEU:HD22 | 1:D:64:THR:HG21 | 1.45 | 0.96 |
| 1:E:70:VAL:HG22 | 1:F:72:LEU:HD21 | 1.46 | 0.96 |
| 1:J:63:LEU:HD22 | 1:K:64:THR:HG21 | 1.47 | 0.96 |
| 1:H:39:ILE:HD11 | 1:H:49:ILE:CB | 1.96 | 0.96 |
| 1:I:70:VAL:HG22 | 1:J:72:LEU:HD21 | 1.46 | 0.96 |
| 1:K:39:ILE:HD11 | 1:K:49:ILE:CB | 1.96 | 0.96 |
| 1:M:39:ILE:HD11 | 1:M:49:ILE:CB | 1.95 | 0.96 |
| 1:C:39:ILE:HD11 | 1:C:49:ILE:CB | 1.96 | 0.95 |
| 1:L:63:LEU:HD22 | 1:M:64:THR:HG21 | 1.44 | 0.95 |
| 1:E:63:LEU:HD22 | 1:F:64:THR:HG21 | 1.48 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:5:ILE:HG22 | 1:I:8:ALA:HB2 | 1.48 | 0.95 |
| 1:E:39:ILE:HD11 | 1:E:49:ILE:CB | 1.97 | 0.95 |
| 1:L:39:ILE:HD11 | 1:L:49:ILE:CB | 1.95 | 0.95 |
| 1:B:39:ILE:HD11 | 1:B:49:ILE:CB | 1.96 | 0.94 |
| 1:C:55:LEU:HD11 | 1:D:54:LEU:HD21 | 1.49 | 0.94 |
| 1:J:39:ILE:HD11 | 1:J:49:ILE:CB | 1.96 | 0.94 |
| 1:F:39:ILE:HD11 | 1:F:49:ILE:CB | 1.98 | 0.94 |
| 1:I:55:LEU:HD11 | 1:J:54:LEU:HD21 | 1.50 | 0.94 |
| 1:I:55:LEU:HD11 | 1:J:54:LEU:CD2 | 1.99 | 0.93 |
| 1:G:39:ILE:HD11 | 1:G:49:ILE:CB | 1.97 | 0.93 |
| 1:I:63:LEU:HD22 | 1:J:64:THR:HG21 | 1.51 | 0.93 |
| 1:L:55:LEU:HD11 | 1:M:54:LEU:HD21 | 1.49 | 0.93 |
| 1:A:39:ILE:HD11 | 1:A:49:ILE:CB | 1.99 | 0.92 |
| 1:D:5:ILE:HG22 | 1:E:8:ALA:HB2 | 1.50 | 0.92 |
| 1:A:55:LEU:HD11 | 1:B:54:LEU:HD21 | 1.50 | 0.92 |
| 1:L:55:LEU:HD11 | 1:M:54:LEU:CD2 | 2.00 | 0.91 |
| 1:A:63:LEU:HD22 | 1:B:64:THR:HG21 | 1.53 | 0.91 |
| 1:E:13:ALA:HB2 | 1:F:12:ALA:HA | 1.53 | 0.90 |
| 1:J:55:LEU:HD21 | 1:K:54:LEU:HD21 | 1.53 | 0.90 |
| 1:K:5:ILE:HG22 | 1:L:8:ALA:CB | 1.99 | 0.90 |
| 1:J:70:VAL:HG22 | 1:K:72:LEU:HD21 | 1.52 | 0.89 |
| 1:L:70:VAL:HG22 | 1:M:72:LEU:HD21 | 1.52 | 0.89 |
| 1:H:70:VAL:HG22 | 1:I:72:LEU:HD21 | 1.52 | 0.89 |
| 1:C:63:LEU:CD2 | 1:D:64:THR:HG21 | 2.03 | 0.88 |
| 1:L:63:LEU:CD2 | 1:M:64:THR:HG21 | 2.02 | 0.88 |
| 1:C:5:ILE:HG22 | 1:D:8:ALA:HB2 | 1.54 | 0.88 |
| 1:E:55:LEU:HD21 | 1:F:54:LEU:HD21 | 1.55 | 0.86 |
| 1:C:35:ALA:HB2 | 1:D:36:VAL:HG21 | 1.56 | 0.86 |
| 1:C:55:LEU:HD11 | 1:D:54:LEU:CD2 | 2.05 | 0.86 |
| 1:A:72:LEU:HD21 | 1:V:70:VAL:HG22 | 1.56 | 0.86 |
| 1:I:63:LEU:CD2 | 1:J:64:THR:HG21 | 2.06 | 0.85 |
| 1:L:55:LEU:HD21 | 1:M:54:LEU:HD21 | 1.57 | 0.85 |
| 1:M:5:ILE:HG22 | 1:V:8:ALA:HB2 | 1.56 | 0.85 |
| 1:L:35:ALA:HB2 | 1:M:36:VAL:HG21 | 1.58 | 0.85 |
| 1:A:55:LEU:HD11 | 1:B:54:LEU:CD2 | 2.07 | 0.85 |
| 1:L:52:THR:HG21 | 1:M:53:LEU:HD13 | 1.60 | 0.84 |
| 1:G:55:LEU:HD11 | 1:H:54:LEU:HD21 | 1.59 | 0.84 |
| 1:J:63:LEU:CD2 | 1:K:64:THR:HG21 | 2.06 | 0.84 |
| 1:A:20:ALA:O | 1:A:64:THR:HG22 | 1.75 | 0.84 |
| 1:E:35:ALA:HB2 | 1:F:36:VAL:HG21 | 1.60 | 0.84 |
| 1:J:52:THR:HG21 | 1:K:53:LEU:HD13 | 1.60 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:5:ILE:HG22 | 1:F:8:ALA:HB2 | 1.60 | 0.83 |
| 1:M:7:ALA:O | 1:M:10:VAL:HG22 | 1.78 | 0.83 |
| 1:B:63:LEU:HD22 | 1:C:64:THR:HG21 | 1.61 | 0.83 |
| 1:M:63:LEU:HD22 | 1:V:64:THR:HG21 | 1.60 | 0.83 |
| 1:E:63:LEU:CD2 | 1:F:64:THR:HG21 | 2.08 | 0.83 |
| 1:J:55:LEU:HD11 | 1:K:54:LEU:HD21 | 1.58 | 0.83 |
| 1:L:20:ALA:O | 1:L:64:THR:HG22 | 1.78 | 0.83 |
| 1:M:20:ALA:O | 1:M:64:THR:HG22 | 1.78 | 0.83 |
| 1:F:20:ALA:O | 1:F:64:THR:HG22 | 1.79 | 0.82 |
| 1:B:7:ALA:O | 1:B:10:VAL:HG22 | 1.80 | 0.82 |
| 1:L:35:ALA:CB | 1:M:36:VAL:HG21 | 2.10 | 0.82 |
| 1:L:55:LEU:CD1 | 1:M:54:LEU:HD21 | 2.09 | 0.82 |
| 1:E:10:VAL:HA | 1:F:11:ILE:HG21 | 1.62 | 0.82 |
| 1:J:55:LEU:HD11 | 1:K:54:LEU:CD2 | 2.10 | 0.82 |
| 1:C:55:LEU:HD21 | 1:D:54:LEU:HD21 | 1.62 | 0.82 |
| 1:D:55:LEU:HD21 | 1:E:54:LEU:HD21 | 1.61 | 0.82 |
| 1:I:55:LEU:CD1 | 1:J:54:LEU:HD21 | 2.09 | 0.81 |
| 1:G:53:LEU:HD21 | 1:G:57:LEU:HD22 | 1.62 | 0.81 |
| 1:H:53:LEU:CD2 | 1:H:57:LEU:HD22 | 2.09 | 0.81 |
| 1:M:59:PHE:CZ | 1:V:57:LEU:HD23 | 2.15 | 0.81 |
| 1:M:5:ILE:HG22 | 1:V:8:ALA:CB | 2.10 | 0.81 |
| 1:A:8:ALA:HB2 | 1:V:5:ILE:HG22 | 1.62 | 0.81 |
| 1:H:20:ALA:O | 1:H:64:THR:HG22 | 1.80 | 0.81 |
| 1:A:53:LEU:CD2 | 1:A:57:LEU:HD22 | 2.10 | 0.81 |
| 1:C:35:ALA:CB | 1:D:36:VAL:HG21 | 2.10 | 0.81 |
| 1:A:54:LEU:HD21 | 1:V:55:LEU:HD21 | 1.63 | 0.81 |
| 1:J:7:ALA:O | 1:J:10:VAL:HG22 | 1.81 | 0.81 |
| 1:L:5:ILE:HG22 | 1:M:8:ALA:HB2 | 1.61 | 0.81 |
| 1:A:35:ALA:HB2 | 1:B:36:VAL:HG21 | 1.61 | 0.81 |
| 1:L:52:THR:CG2 | 1:M:53:LEU:HD13 | 2.10 | 0.81 |
| 1:A:13:ALA:HB2 | 1:B:12:ALA:HA | 1.60 | 0.80 |
| 1:L:13:ALA:HB2 | 1:M:12:ALA:HA | 1.64 | 0.80 |
| 1:L:7:ALA:O | 1:L:10:VAL:HG22 | 1.82 | 0.80 |
| 1:C:20:ALA:O | 1:C:64:THR:HG22 | 1.82 | 0.80 |
| 1:H:53:LEU:HD21 | 1:H:57:LEU:HD22 | 1.60 | 0.80 |
| 1:F:53:LEU:HD21 | 1:F:57:LEU:HD22 | 1.64 | 0.80 |
| 1:A:7:ALA:O | 1:A:10:VAL:HG22 | 1.81 | 0.80 |
| 1:C:5:ILE:HG22 | 1:D:8:ALA:CB | 2.11 | 0.80 |
| 1:F:7:ALA:O | 1:F:10:VAL:HG22 | 1.81 | 0.80 |
| 1:H:55:LEU:HD21 | 1:I:54:LEU:HD21 | 1.63 | 0.80 |
| 1:I:55:LEU:HD21 | 1:J:54:LEU:HD21 | 1.62 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:13:ALA:O | 1:B:15:LEU:CB | 2.30 | 0.80 |
| 1:D:63:LEU:HD22 | 1:E:64:THR:HG21 | 1.63 | 0.80 |
| 1:H:5:ILE:HG22 | 1:I:8:ALA:CB | 2.11 | 0.80 |
| 1:V:53:LEU:CD2 | 1:V:57:LEU:HD22 | 2.12 | 0.80 |
| 1:H:7:ALA:O | 1:H:10:VAL:HG22 | 1.82 | 0.79 |
| 1:H:63:LEU:HD22 | 1:I:64:THR:HG21 | 1.64 | 0.79 |
| 1:V:53:LEU:HD21 | 1:V:57:LEU:HD22 | 1.63 | 0.79 |
| 1:A:63:LEU:CD2 | 1:B:64:THR:HG21 | 2.11 | 0.79 |
| 1:D:63:LEU:CD2 | 1:E:64:THR:HG21 | 2.12 | 0.79 |
| 1:B:5:ILE:HG22 | 1:C:8:ALA:HB2 | 1.64 | 0.79 |
| 1:I:7:ALA:O | 1:I:10:VAL:HG22 | 1.82 | 0.79 |
| 1:K:53:LEU:CD2 | 1:K:57:LEU:HD22 | 2.12 | 0.79 |
| 1:E:55:LEU:HD11 | 1:F:54:LEU:CD2 | 2.12 | 0.79 |
| 1:E:55:LEU:HD11 | 1:F:54:LEU:HD21 | 1.63 | 0.79 |
| 1:B:55:LEU:HD11 | 1:C:54:LEU:HD21 | 1.65 | 0.79 |
| 1:G:53:LEU:CD2 | 1:G:57:LEU:HD22 | 2.12 | 0.79 |
| 1:E:35:ALA:CB | 1:F:36:VAL:HG21 | 2.13 | 0.79 |
| 1:I:5:ILE:HG22 | 1:J:8:ALA:HB2 | 1.62 | 0.79 |
| 1:F:20:ALA:HB1 | 1:F:64:THR:HA | 1.65 | 0.79 |
| 1:F:53:LEU:CD2 | 1:F:57:LEU:HD22 | 2.12 | 0.79 |
| 1:D:55:LEU:HD11 | 1:E:54:LEU:HD21 | 1.65 | 0.79 |
| 1:D:7:ALA:O | 1:D:10:VAL:HG22 | 1.82 | 0.78 |
| 1:A:53:LEU:HD21 | 1:A:57:LEU:HD22 | 1.63 | 0.78 |
| 1:F:63:LEU:HD22 | 1:G:64:THR:HG21 | 1.62 | 0.78 |
| 1:C:7:ALA:O | 1:C:10:VAL:HG22 | 1.84 | 0.78 |
| 1:M:63:LEU:CD2 | 1:V:64:THR:HG21 | 2.14 | 0.78 |
| 1:K:53:LEU:HD21 | 1:K:57:LEU:HD22 | 1.64 | 0.78 |
| 1:E:5:ILE:HG22 | 1:F:8:ALA:CB | 2.13 | 0.78 |
| 1:G:55:LEU:HD11 | 1:H:54:LEU:CD2 | 2.13 | 0.78 |
| 1:J:55:LEU:HD21 | 1:K:54:LEU:CD2 | 2.12 | 0.78 |
| 1:V:7:ALA:O | 1:V:10:VAL:HG22 | 1.83 | 0.78 |
| 1:A:35:ALA:CB | 1:B:36:VAL:HG21 | 2.14 | 0.77 |
| 1:B:63:LEU:CD2 | 1:C:64:THR:HG21 | 2.14 | 0.77 |
| 1:E:7:ALA:O | 1:E:10:VAL:HG22 | 1.84 | 0.77 |
| 1:J:20:ALA:O | 1:J:64:THR:HG22 | 1.83 | 0.77 |
| 1:B:53:LEU:CD2 | 1:B:57:LEU:HD22 | 2.15 | 0.77 |
| 1:I:52:THR:HG21 | 1:J:53:LEU:HD13 | 1.65 | 0.77 |
| 1:J:55:LEU:CD2 | 1:K:54:LEU:HD21 | 2.15 | 0.77 |
| 1:B:20:ALA:O | 1:B:64:THR:HG22 | 1.85 | 0.77 |
| 1:E:10:VAL:HA | 1:F:11:ILE:CG2 | 2.15 | 0.77 |
| 1:J:35:ALA:HB2 | 1:K:36:VAL:HG21 | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:35:ALA:CB | 1:K:36:VAL:HG21 | 2.15 | 0.76 |
| 1:L:55:LEU:HD21 | 1:M:54:LEU:CD2 | 2.14 | 0.76 |
| 1:B:55:LEU:HD21 | 1:C:54:LEU:HD21 | 1.67 | 0.76 |
| 1:C:55:LEU:CD1 | 1:D:54:LEU:HD21 | 2.14 | 0.76 |
| 1:L:55:LEU:CD2 | 1:M:54:LEU:HD21 | 2.15 | 0.76 |
| 1:K:20:ALA:O | 1:K:64:THR:HG22 | 1.85 | 0.76 |
| 1:K:7:ALA:O | 1:K:10:VAL:HG22 | 1.86 | 0.76 |
| 1:M:70:VAL:HG22 | 1:V:72:LEU:HD21 | 1.66 | 0.76 |
| 1:I:20:ALA:O | 1:I:64:THR:HG22 | 1.86 | 0.76 |
| 1:I:35:ALA:HB2 | 1:J:36:VAL:HG21 | 1.67 | 0.76 |
| 1:J:53:LEU:CD2 | 1:J:57:LEU:HD22 | 2.15 | 0.76 |
| 1:H:55:LEU:HD11 | 1:I:54:LEU:HD21 | 1.67 | 0.76 |
| 1:M:20:ALA:HB1 | 1:M:64:THR:HA | 1.68 | 0.76 |
| 1:A:55:LEU:HD21 | 1:B:54:LEU:HD21 | 1.67 | 0.75 |
| 1:A:55:LEU:CD1 | 1:B:54:LEU:HD21 | 2.15 | 0.75 |
| 1:B:53:LEU:HD21 | 1:B:57:LEU:HD22 | 1.67 | 0.75 |
| 1:E:53:LEU:CD2 | 1:E:57:LEU:HD22 | 2.16 | 0.75 |
| 1:G:70:VAL:HG22 | 1:H:72:LEU:HD21 | 1.68 | 0.75 |
| 1:J:53:LEU:HD21 | 1:J:57:LEU:HD22 | 1.68 | 0.75 |
| 1:C:13:ALA:HB2 | 1:D:12:ALA:HA | 1.67 | 0.75 |
| 1:E:53:LEU:HD21 | 1:E:57:LEU:HD22 | 1.69 | 0.75 |
| 1:F:63:LEU:CD2 | 1:G:64:THR:HG21 | 2.15 | 0.75 |
| 1:H:20:ALA:HB1 | 1:H:64:THR:HA | 1.67 | 0.75 |
| 1:H:63:LEU:CD2 | 1:I:64:THR:HG21 | 2.16 | 0.75 |
| 1:E:55:LEU:HD21 | 1:F:54:LEU:CD2 | 2.16 | 0.75 |
| 1:G:55:LEU:HD21 | 1:H:54:LEU:HD21 | 1.68 | 0.75 |
| 1:I:55:LEU:HD21 | 1:J:54:LEU:CD2 | 2.17 | 0.75 |
| 1:K:67:GLY:O | 1:K:71:ALA:N | 2.20 | 0.75 |
| 1:K:55:LEU:HD11 | 1:L:54:LEU:HD21 | 1.69 | 0.74 |
| 1:F:5:ILE:HG22 | 1:G:8:ALA:HB2 | 1.69 | 0.74 |
| 1:F:13:ALA:HB2 | 1:G:12:ALA:HA | 1.68 | 0.74 |
| 1:L:20:ALA:HB1 | 1:L:64:THR:HA | 1.69 | 0.74 |
| 1:B:55:LEU:HD11 | 1:C:54:LEU:CD2 | 2.17 | 0.74 |
| 1:G:63:LEU:HD22 | 1:H:64:THR:HG21 | 1.69 | 0.74 |
| 1:L:5:ILE:HG22 | 1:M:8:ALA:CB | 2.17 | 0.74 |
| 1:K:20:ALA:HB1 | 1:K:64:THR:HA | 1.70 | 0.74 |
| 1:L:67:GLY:O | 1:L:71:ALA:N | 2.21 | 0.74 |
| 1:M:55:LEU:HD11 | 1:V:54:LEU:HD21 | 1.68 | 0.74 |
| 1:A:10:VAL:HA | 1:B:11:ILE:CG2 | 2.18 | 0.73 |
| 1:B:35:ALA:HB2 | 1:C:36:VAL:HG21 | 1.69 | 0.73 |
| 1:M:53:LEU:CD2 | 1:M:57:LEU:HD22 | 2.16 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:63:LEU:HD22 | 1:L:64:THR:HG21 | 1.69 | 0.73 |
| 1:A:10:VAL:HA | 1:B:11:ILE:HG21 | 1.70 | 0.73 |
| 1:E:55:LEU:CD2 | 1:F:54:LEU:HD21 | 2.17 | 0.73 |
| 1:E:24:PRO:HG2 | 1:E:64:THR:HG22 | 1.70 | 0.73 |
| 1:J:20:ALA:HB1 | 1:J:64:THR:HA | 1.70 | 0.73 |
| 1:D:53:LEU:CD2 | 1:D:57:LEU:HD22 | 2.19 | 0.73 |
| 1:J:5:ILE:HG22 | 1:K:8:ALA:HB2 | 1.70 | 0.73 |
| 1:V:20:ALA:O | 1:V:64:THR:HG22 | 1.88 | 0.73 |
| 1:A:64:THR:HG21 | 1:V:63:LEU:HD22 | 1.70 | 0.73 |
| 1:D:20:ALA:O | 1:D:64:THR:HG22 | 1.88 | 0.73 |
| 1:D:53:LEU:HD21 | 1:D:57:LEU:HD22 | 1.70 | 0.73 |
| 1:J:55:LEU:CD1 | 1:K:54:LEU:HD21 | 2.19 | 0.73 |
| 1:G:63:LEU:CD2 | 1:H:64:THR:HG21 | 2.17 | 0.73 |
| 1:F:24:PRO:HG2 | 1:F:64:THR:HG22 | 1.68 | 0.73 |
| 1:J:52:THR:CG2 | 1:K:53:LEU:HD13 | 2.18 | 0.73 |
| 1:E:20:ALA:O | 1:E:64:THR:HG22 | 1.89 | 0.72 |
| 1:L:53:LEU:CD2 | 1:L:57:LEU:HD22 | 2.18 | 0.72 |
| 1:A:54:LEU:HD21 | 1:V:55:LEU:HD11 | 1.69 | 0.72 |
| 1:G:20:ALA:O | 1:G:64:THR:HG22 | 1.89 | 0.72 |
| 1:J:67:GLY:O | 1:J:71:ALA:N | 2.20 | 0.72 |
| 1:B:24:PRO:HG2 | 1:B:64:THR:HG22 | 1.71 | 0.72 |
| 1:K:55:LEU:HD21 | 1:L:54:LEU:HD21 | 1.71 | 0.72 |
| 1:E:66:TYR:CG | 1:F:68:LEU:HD22 | 2.24 | 0.72 |
| 1:G:7:ALA:O | 1:G:10:VAL:HG22 | 1.88 | 0.72 |
| 1:I:55:LEU:CD2 | 1:J:54:LEU:HD21 | 2.18 | 0.72 |
| 1:D:55:LEU:HD11 | 1:E:54:LEU:CD2 | 2.19 | 0.72 |
| 1:F:70:VAL:HG22 | 1:G:72:LEU:HD21 | 1.71 | 0.72 |
| 1:I:52:THR:CG2 | 1:J:53:LEU:HD13 | 2.20 | 0.71 |
| 1:D:70:VAL:HG22 | 1:E:72:LEU:CD2 | 2.17 | 0.71 |
| 1:F:59:PHE:CZ | 1:G:57:LEU:HD23 | 2.25 | 0.71 |
| 1:M:13:ALA:HB2 | 1:V:12:ALA:HA | 1.72 | 0.71 |
| 1:A:24:PRO:HG2 | 1:A:64:THR:HG22 | 1.72 | 0.71 |
| 1:E:20:ALA:HB1 | 1:E:64:THR:HA | 1.73 | 0.71 |
| 1:I:24:PRO:HG2 | 1:I:64:THR:HG22 | 1.72 | 0.71 |
| 1:V:20:ALA:HB1 | 1:V:64:THR:HA | 1.73 | 0.71 |
| 1:A:10:VAL:N | 1:B:11:ILE:HG21 | 2.05 | 0.71 |
| 1:I:20:ALA:HB1 | 1:I:64:THR:HA | 1.71 | 0.71 |
| 1:A:20:ALA:HB1 | 1:A:64:THR:HA | 1.70 | 0.71 |
| 1:G:20:ALA:HB1 | 1:G:64:THR:HA | 1.73 | 0.71 |
| 1:L:53:LEU:HD21 | 1:L:57:LEU:HD22 | 1.71 | 0.71 |
| 1:M:53:LEU:HD21 | 1:M:57:LEU:HD22 | 1.70 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:52:THR:HG21 | 1:B:53:LEU:HD13 | 1.73 | 0.71 |
| 1:H:59:PHE:CZ | 1:I:57:LEU:HD23 | 2.26 | 0.70 |
| 1:D:5:ILE:HG22 | 1:E:8:ALA:CB | 2.21 | 0.70 |
| 1:B:5:ILE:HG22 | 1:C:8:ALA:CB | 2.20 | 0.70 |
| 1:G:52:THR:HG21 | 1:H:53:LEU:HD13 | 1.74 | 0.70 |
| 1:A:36:VAL:HG21 | 1:V:35:ALA:HB2 | 1.73 | 0.70 |
| 1:I:53:LEU:CD2 | 1:I:57:LEU:HD22 | 2.20 | 0.70 |
| 1:I:53:LEU:HD21 | 1:I:57:LEU:HD22 | 1.71 | 0.70 |
| 1:V:24:PRO:HG2 | 1:V:64:THR:HG22 | 1.73 | 0.70 |
| 1:B:20:ALA:HB1 | 1:B:64:THR:HA | 1.74 | 0.70 |
| 1:I:67:GLY:O | 1:I:71:ALA:N | 2.23 | 0.70 |
| 1:B:59:PHE:CZ | 1:C:57:LEU:HD23 | 2.27 | 0.70 |
| 1:I:5:ILE:HG22 | 1:J:8:ALA:CB | 2.21 | 0.70 |
| 1:M:10:VAL:HA | 1:V:11:ILE:HG21 | 1.74 | 0.70 |
| 1:C:67:GLY:O | 1:C:71:ALA:N | 2.24 | 0.70 |
| 1:L:13:ALA:O | 1:M:15:LEU:CB | 2.38 | 0.70 |
| 1:C:53:LEU:CD2 | 1:C:57:LEU:HD22 | 2.21 | 0.70 |
| 1:I:10:VAL:HA | 1:J:11:ILE:HG21 | 1.74 | 0.69 |
| 1:C:13:ALA:O | 1:D:15:LEU:CB | 2.40 | 0.69 |
| 1:F:5:ILE:HG22 | 1:G:8:ALA:CB | 2.22 | 0.69 |
| 1:G:55:LEU:CD1 | 1:H:54:LEU:HD21 | 2.22 | 0.69 |
| 1:C:59:PHE:CZ | 1:D:57:LEU:HD23 | 2.27 | 0.69 |
| 1:C:24:PRO:HG2 | 1:C:64:THR:HG22 | 1.74 | 0.69 |
| 1:E:55:LEU:CD1 | 1:F:54:LEU:HD21 | 2.23 | 0.69 |
| 1:C:55:LEU:HD21 | 1:D:54:LEU:CD2 | 2.21 | 0.69 |
| 1:C:10:VAL:HA | 1:D:11:ILE:HG21 | 1.74 | 0.69 |
| 1:D:24:PRO:HG2 | 1:D:64:THR:HG22 | 1.74 | 0.69 |
| 1:M:24:PRO:HG2 | 1:M:64:THR:HG22 | 1.74 | 0.69 |
| 1:C:52:THR:HG21 | 1:D:53:LEU:HD13 | 1.72 | 0.69 |
| 1:E:10:VAL:HG12 | 1:F:11:ILE:HG13 | 1.74 | 0.69 |
| 1:C:53:LEU:HD21 | 1:C:57:LEU:HD22 | 1.73 | 0.69 |
| 1:B:67:GLY:O | 1:B:71:ALA:N | 2.26 | 0.69 |
| 1:E:52:THR:HG21 | 1:F:53:LEU:HD13 | 1.73 | 0.68 |
| 1:H:55:LEU:HD11 | 1:I:54:LEU:CD2 | 2.23 | 0.68 |
| 1:I:35:ALA:CB | 1:J:36:VAL:HG21 | 2.22 | 0.68 |
| 1:G:24:PRO:HG2 | 1:G:64:THR:HG22 | 1.74 | 0.68 |
| 1:H:13:ALA:O | 1:I:15:LEU:CB | 2.42 | 0.68 |
| 1:B:13:ALA:HB2 | 1:C:12:ALA:HA | 1.75 | 0.68 |
| 1:F:24:PRO:HG2 | 1:F:64:THR:CG2 | 2.23 | 0.68 |
| 1:H:24:PRO:HG2 | 1:H:64:THR:HG22 | 1.75 | 0.68 |
| 1:C:55:LEU:CD2 | 1:D:54:LEU:HD21 | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:10:VAL:HA | 1:I:11:ILE:HG21 | 1.76 | 0.68 |
| 1:D:20:ALA:HB1 | 1:D:64:THR:HA | 1.73 | 0.68 |
| 1:H:10:VAL:HG12 | 1:I:11:ILE:CD1 | 2.23 | 0.68 |
| 1:L:10:VAL:HA | 1:M:11:ILE:HG21 | 1.76 | 0.68 |
| 1:F:55:LEU:HD21 | 1:G:54:LEU:HD21 | 1.76 | 0.68 |
| 1:L:59:PHE:CZ | 1:M:57:LEU:HD23 | 2.29 | 0.67 |
| 1:K:59:PHE:CZ | 1:L:57:LEU:HD23 | 2.28 | 0.67 |
| 1:C:20:ALA:HB1 | 1:C:64:THR:HA | 1.76 | 0.67 |
| 1:F:10:VAL:HA | 1:G:11:ILE:HG21 | 1.77 | 0.67 |
| 1:A:66:TYR:CE2 | 1:B:65:ILE:HG22 | 2.30 | 0.67 |
| 1:M:55:LEU:HD11 | 1:V:54:LEU:CD2 | 2.24 | 0.67 |
| 1:D:66:TYR:CG | 1:E:68:LEU:HD22 | 2.29 | 0.67 |
| 1:I:13:ALA:HB2 | 1:J:12:ALA:HA | 1.77 | 0.67 |
| 1:J:13:ALA:HB2 | 1:K:12:ALA:HA | 1.77 | 0.67 |
| 1:D:59:PHE:CZ | 1:E:57:LEU:HD23 | 2.30 | 0.67 |
| 1:A:67:GLY:O | 1:A:71:ALA:N | 2.27 | 0.67 |
| 1:C:10:VAL:HA | 1:D:11:ILE:CG2 | 2.25 | 0.67 |
| 1:A:10:VAL:HG12 | 1:B:11:ILE:CD1 | 2.24 | 0.67 |
| 1:D:55:LEU:HD21 | 1:E:54:LEU:CD2 | 2.25 | 0.67 |
| 1:E:13:ALA:O | 1:F:15:LEU:CB | 2.42 | 0.67 |
| 1:F:55:LEU:HD11 | 1:G:54:LEU:HD21 | 1.75 | 0.66 |
| 1:J:24:PRO:HG2 | 1:J:64:THR:HG22 | 1.76 | 0.66 |
| 1:A:59:PHE:CZ | 1:B:57:LEU:HD23 | 2.30 | 0.66 |
| 1:F:62:ALA:O | 1:F:65:ILE:HG12 | 1.94 | 0.66 |
| 1:E:10:VAL:CA | 1:F:11:ILE:HG21 | 2.24 | 0.66 |
| 1:H:35:ALA:HB2 | 1:I:36:VAL:HG21 | 1.75 | 0.66 |
| 1:A:54:LEU:CD2 | 1:V:55:LEU:HD11 | 2.25 | 0.66 |
| 1:L:10:VAL:HA | 1:M:11:ILE:CG2 | 2.26 | 0.66 |
| 1:A:66:TYR:CG | 1:B:68:LEU:HD22 | 2.30 | 0.66 |
| 1:D:69:VAL:HG12 | 1:D:70:VAL:N | 2.10 | 0.66 |
| 1:G:67:GLY:O | 1:G:71:ALA:N | 2.24 | 0.65 |
| 1:L:66:TYR:CG | 1:M:68:LEU:HD22 | 2.31 | 0.65 |
| 1:D:55:LEU:CD2 | 1:E:54:LEU:HD21 | 2.27 | 0.65 |
| 1:I:66:TYR:CG | 1:J:68:LEU:HD22 | 2.31 | 0.65 |
| 1:G:52:THR:CG2 | 1:H:53:LEU:HD13 | 2.27 | 0.65 |
| 1:A:64:THR:HG21 | 1:V:63:LEU:CD2 | 2.26 | 0.65 |
| 1:A:55:LEU:CD2 | 1:B:54:LEU:HD21 | 2.27 | 0.65 |
| 1:D:62:ALA:O | 1:D:65:ILE:HG12 | 1.96 | 0.65 |
| 1:A:24:PRO:HG2 | 1:A:64:THR:CG2 | 2.26 | 0.65 |
| 1:A:10:VAL:CA | 1:B:11:ILE:HG21 | 2.26 | 0.65 |
| 1:B:62:ALA:O | 1:B:65:ILE:HG12 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:L:24:PRO:HG2 | 1:L:64:THR:HG22 | 1.78 | 0.65 |
| 1:A:52:THR:CG2 | 1:B:53:LEU:HD13 | 2.26 | 0.65 |
| 1:B:35:ALA:CB | 1:C:36:VAL:HG21 | 2.26 | 0.65 |
| 1:G:55:LEU:HD21 | 1:H:54:LEU:CD2 | 2.27 | 0.65 |
| 1:I:10:VAL:HA | 1:J:11:ILE:CG2 | 2.27 | 0.65 |
| 1:H:13:ALA:HB2 | 1:I:12:ALA:HA | 1.77 | 0.64 |
| 1:M:62:ALA:O | 1:M:65:ILE:HG12 | 1.97 | 0.64 |
| 1:M:67:GLY:O | 1:M:71:ALA:N | 2.26 | 0.64 |
| 1:A:55:LEU:HD21 | 1:B:54:LEU:CD2 | 2.27 | 0.64 |
| 1:G:35:ALA:HB2 | 1:H:36:VAL:HG21 | 1.78 | 0.64 |
| 1:H:24:PRO:HG2 | 1:H:64:THR:CG2 | 2.27 | 0.64 |
| 1:K:24:PRO:HG2 | 1:K:64:THR:HG22 | 1.78 | 0.64 |
| 1:A:8:ALA:CB | 1:V:5:ILE:HG22 | 2.27 | 0.64 |
| 1:I:59:PHE:CZ | 1:J:57:LEU:HD23 | 2.32 | 0.64 |
| 1:J:66:TYR:CG | 1:K:68:LEU:HD22 | 2.33 | 0.64 |
| 1:M:10:VAL:HA | 1:V:11:ILE:CG2 | 2.27 | 0.64 |
| 1:A:59:PHE:CE1 | 1:B:57:LEU:HB3 | 2.33 | 0.64 |
| 1:B:10:VAL:HA | 1:C:11:ILE:HG21 | 1.79 | 0.64 |
| 1:I:69:VAL:HG12 | 1:I:70:VAL:N | 2.12 | 0.64 |
| 1:B:55:LEU:CD1 | 1:C:54:LEU:HD21 | 2.27 | 0.64 |
| 1:C:52:THR:CG2 | 1:D:53:LEU:HD13 | 2.27 | 0.64 |
| 1:K:63:LEU:CD2 | 1:L:64:THR:HG21 | 2.27 | 0.64 |
| 1:V:67:GLY:O | 1:V:71:ALA:N | 2.27 | 0.64 |
| 1:L:59:PHE:CE1 | 1:M:57:LEU:HB3 | 2.32 | 0.64 |
| 1:M:24:PRO:HG2 | 1:M:64:THR:CG2 | 2.27 | 0.64 |
| 1:H:67:GLY:O | 1:H:71:ALA:N | 2.26 | 0.64 |
| 1:K:13:ALA:O | 1:L:15:LEU:CB | 2.46 | 0.64 |
| 1:B:24:PRO:HG2 | 1:B:64:THR:CG2 | 2.28 | 0.63 |
| 1:A:70:VAL:HG22 | 1:B:72:LEU:CD2 | 2.21 | 0.63 |
| 1:G:59:PHE:CZ | 1:H:57:LEU:HD23 | 2.33 | 0.63 |
| 1:L:33:GLY:O | 1:L:36:VAL:HG12 | 1.99 | 0.63 |
| 1:B:55:LEU:HD21 | 1:C:54:LEU:CD2 | 2.28 | 0.63 |
| 1:B:52:THR:HG21 | 1:C:53:LEU:HD13 | 1.80 | 0.63 |
| 1:D:10:VAL:HA | 1:E:11:ILE:HG21 | 1.81 | 0.63 |
| 1:H:10:VAL:HA | 1:I:11:ILE:CG2 | 2.29 | 0.63 |
| 1:J:69:VAL:HG12 | 1:J:70:VAL:N | 2.13 | 0.63 |
| 1:L:53:LEU:HD23 | 1:L:54:LEU:N | 2.14 | 0.63 |
| 1:D:33:GLY:O | 1:D:36:VAL:HG12 | 1.97 | 0.63 |
| 1:F:67:GLY:O | 1:F:71:ALA:N | 2.27 | 0.63 |
| 1:M:13:ALA:O | 1:V:15:LEU:CB | 2.46 | 0.63 |
| 1:E:10:VAL:N | 1:F:11:ILE:HG21 | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:69:VAL:HG12 | 1:M:70:VAL:N | 2.14 | 0.62 |
| 1:A:54:LEU:CD2 | 1:V:55:LEU:HD21 | 2.29 | 0.62 |
| 1:B:70:VAL:HG22 | 1:C:72:LEU:CD2 | 2.27 | 0.62 |
| 1:L:69:VAL:HG12 | 1:L:70:VAL:N | 2.12 | 0.62 |
| 1:B:55:LEU:CD2 | 1:C:54:LEU:HD21 | 2.29 | 0.62 |
| 1:D:13:ALA:HB3 | 1:E:11:ILE:CG2 | 2.30 | 0.62 |
| 1:E:67:GLY:O | 1:E:71:ALA:N | 2.27 | 0.62 |
| 1:B:33:GLY:O | 1:B:36:VAL:HG12 | 1.99 | 0.62 |
| 1:A:5:ILE:CG2 | 1:B:8:ALA:CB | 2.75 | 0.62 |
| 1:C:62:ALA:O | 1:C:65:ILE:HG12 | 1.99 | 0.62 |
| 1:C:66:TYR:CG | 1:D:68:LEU:HD22 | 2.34 | 0.62 |
| 1:D:70:VAL:CG2 | 1:E:72:LEU:HD21 | 2.21 | 0.62 |
| 1:J:33:GLY:O | 1:J:36:VAL:HG12 | 1.98 | 0.62 |
| 1:E:52:THR:CG2 | 1:F:53:LEU:HD13 | 2.30 | 0.62 |
| 1:I:62:ALA:O | 1:I:65:ILE:HG12 | 1.99 | 0.62 |
| 1:C:69:VAL:HG12 | 1:C:70:VAL:N | 2.14 | 0.62 |
| 1:E:59:PHE:CZ | 1:F:57:LEU:HD23 | 2.34 | 0.62 |
| 1:A:62:ALA:HB3 | 1:B:61:GLU:OE2 | 1.99 | 0.62 |
| 1:E:13:ALA:CB | 1:F:12:ALA:HA | 2.28 | 0.62 |
| 1:F:10:VAL:HA | 1:G:11:ILE:CG2 | 2.30 | 0.62 |
| 1:C:10:VAL:HG12 | 1:D:11:ILE:CD1 | 2.30 | 0.62 |
| 1:F:69:VAL:HG12 | 1:F:70:VAL:N | 2.14 | 0.62 |
| 1:H:55:LEU:HD21 | 1:I:54:LEU:CD2 | 2.29 | 0.62 |
| 1:I:24:PRO:HG2 | 1:I:64:THR:CG2 | 2.29 | 0.62 |
| 1:B:10:VAL:HA | 1:C:11:ILE:CG2 | 2.30 | 0.61 |
| 1:G:62:ALA:O | 1:G:65:ILE:HG12 | 2.00 | 0.61 |
| 1:G:55:LEU:CD2 | 1:H:54:LEU:HD21 | 2.29 | 0.61 |
| 1:L:62:ALA:O | 1:L:65:ILE:HG12 | 2.00 | 0.61 |
| 1:C:24:PRO:HG2 | 1:C:64:THR:CG2 | 2.30 | 0.61 |
| 1:D:13:ALA:HB2 | 1:E:12:ALA:HA | 1.83 | 0.61 |
| 1:B:69:VAL:HG12 | 1:B:70:VAL:N | 2.15 | 0.61 |
| 1:D:35:ALA:HB2 | 1:E:36:VAL:HG21 | 1.82 | 0.61 |
| 1:K:33:GLY:O | 1:K:36:VAL:HG12 | 2.00 | 0.61 |
| 1:V:62:ALA:O | 1:V:65:ILE:HG12 | 2.01 | 0.61 |
| 1:A:62:ALA:O | 1:A:65:ILE:HG12 | 2.01 | 0.61 |
| 1:H:55:LEU:CD2 | 1:I:54:LEU:HD21 | 2.30 | 0.61 |
| 1:L:24:PRO:HG2 | 1:L:64:THR:CG2 | 2.31 | 0.61 |
| 1:K:69:VAL:HG12 | 1:K:70:VAL:N | 2.15 | 0.61 |
| 1:I:53:LEU:HD23 | 1:I:54:LEU:N | 2.16 | 0.61 |
| 1:K:5:ILE:CG2 | 1:L:8:ALA:CB | 2.77 | 0.61 |
| 1:G:69:VAL:HG12 | 1:G:70:VAL:N | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:5:ILE:HG22 | 1:H:8:ALA:HB2 | 1.83 | 0.61 |
| 1:I:59:PHE:CZ | 1:J:57:LEU:HB3 | 2.36 | 0.61 |
| 1:J:24:PRO:HG2 | 1:J:64:THR:CG2 | 2.30 | 0.61 |
| 1:M:17:VAL:O | 1:M:17:VAL:HG12 | 2.01 | 0.61 |
| 1:M:35:ALA:HB2 | 1:V:36:VAL:HG21 | 1.83 | 0.61 |
| 1:A:69:VAL:HG12 | 1:A:70:VAL:N | 2.16 | 0.61 |
| 1:I:10:VAL:HG12 | 1:J:11:ILE:CD1 | 2.31 | 0.61 |
| 1:L:62:ALA:HB3 | 1:M:61:GLU:OE2 | 2.00 | 0.61 |
| 1:D:67:GLY:O | 1:D:71:ALA:N | 2.28 | 0.60 |
| 1:C:59:PHE:CE1 | 1:D:57:LEU:HB3 | 2.36 | 0.60 |
| 1:E:33:GLY:O | 1:E:36:VAL:HG12 | 2.00 | 0.60 |
| 1:V:24:PRO:HG2 | 1:V:64:THR:CG2 | 2.31 | 0.60 |
| 1:B:66:TYR:CG | 1:C:68:LEU:HD22 | 2.36 | 0.60 |
| 1:K:35:ALA:HB2 | 1:L:36:VAL:HG21 | 1.82 | 0.60 |
| 1:E:62:ALA:O | 1:E:65:ILE:HG12 | 2.02 | 0.60 |
| 1:E:69:VAL:HG12 | 1:E:70:VAL:N | 2.15 | 0.60 |
| 1:G:35:ALA:CB | 1:H:36:VAL:HG21 | 2.32 | 0.60 |
| 1:G:24:PRO:HG2 | 1:G:64:THR:CG2 | 2.31 | 0.60 |
| 1:H:52:THR:HG21 | 1:I:53:LEU:HD13 | 1.82 | 0.60 |
| 1:D:55:LEU:CD1 | 1:E:54:LEU:HD21 | 2.29 | 0.60 |
| 1:I:70:VAL:HG22 | 1:J:72:LEU:CD2 | 2.27 | 0.60 |
| 1:K:5:ILE:CG2 | 1:L:8:ALA:HB2 | 2.22 | 0.60 |
| 1:A:36:VAL:HG21 | 1:V:35:ALA:CB | 2.30 | 0.60 |
| 1:G:53:LEU:HD23 | 1:G:54:LEU:N | 2.15 | 0.60 |
| 1:K:10:VAL:N | 1:L:11:ILE:HG21 | 2.15 | 0.60 |
| 1:A:54:LEU:HD21 | 1:V:55:LEU:CD2 | 2.30 | 0.60 |
| 1:H:62:ALA:O | 1:H:65:ILE:HG12 | 2.02 | 0.60 |
| 1:J:62:ALA:O | 1:J:65:ILE:HG12 | 2.01 | 0.60 |
| 1:L:59:PHE:CZ | 1:M:57:LEU:HB3 | 2.37 | 0.60 |
| 1:M:55:LEU:HD21 | 1:V:54:LEU:HD21 | 1.83 | 0.60 |
| 1:C:10:VAL:N | 1:D:11:ILE:HG21 | 2.17 | 0.60 |
| 1:I:62:ALA:HB3 | 1:J:61:GLU:OE2 | 2.00 | 0.60 |
| 1:J:53:LEU:HD23 | 1:J:54:LEU:N | 2.17 | 0.60 |
| 1:K:66:TYR:CG | 1:L:68:LEU:HD22 | 2.37 | 0.60 |
| 1:A:57:LEU:HD23 | 1:V:59:PHE:CZ | 2.37 | 0.60 |
| 1:I:66:TYR:CE2 | 1:J:65:ILE:HG22 | 2.37 | 0.60 |
| 1:K:55:LEU:HD11 | 1:L:54:LEU:CD2 | 2.31 | 0.60 |
| 1:A:10:VAL:HG12 | 1:B:11:ILE:HG13 | 1.84 | 0.59 |
| 1:H:69:VAL:HG12 | 1:H:70:VAL:N | 2.17 | 0.59 |
| 1:I:59:PHE:CE1 | 1:J:57:LEU:HB3 | 2.37 | 0.59 |
| 1:M:3:PRO:O | 1:M:7:ALA:HB3 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:6:ALA:O | 1:M:10:VAL:HG13 | 2.02 | 0.59 |
| 1:E:24:PRO:HG2 | 1:E:64:THR:CG2 | 2.31 | 0.59 |
| 1:E:70:VAL:HG22 | 1:F:72:LEU:CD2 | 2.27 | 0.59 |
| 1:F:55:LEU:HD11 | 1:G:54:LEU:CD2 | 2.31 | 0.59 |
| 1:I:13:ALA:O | 1:J:15:LEU:CB | 2.50 | 0.59 |
| 1:K:53:LEU:HD23 | 1:K:54:LEU:N | 2.17 | 0.59 |
| 1:L:10:VAL:N | 1:M:11:ILE:HG21 | 2.16 | 0.59 |
| 1:E:66:TYR:CE2 | 1:F:65:ILE:HG22 | 2.37 | 0.59 |
| 1:D:24:PRO:HG2 | 1:D:64:THR:CG2 | 2.32 | 0.59 |
| 1:H:55:LEU:CD1 | 1:I:54:LEU:HD21 | 2.33 | 0.59 |
| 1:E:6:ALA:O | 1:E:10:VAL:HG13 | 2.02 | 0.59 |
| 1:V:69:VAL:HG12 | 1:V:70:VAL:N | 2.17 | 0.59 |
| 1:H:3:PRO:O | 1:H:7:ALA:HB3 | 2.03 | 0.59 |
| 1:F:35:ALA:HB2 | 1:G:36:VAL:HG21 | 1.85 | 0.59 |
| 1:E:62:ALA:HB3 | 1:F:61:GLU:OE2 | 2.03 | 0.59 |
| 1:H:53:LEU:HD23 | 1:H:54:LEU:N | 2.17 | 0.59 |
| 1:K:62:ALA:O | 1:K:65:ILE:HG12 | 2.02 | 0.59 |
| 1:A:53:LEU:HD13 | 1:V:52:THR:HG21 | 1.85 | 0.58 |
| 1:C:33:GLY:O | 1:C:36:VAL:HG12 | 2.03 | 0.58 |
| 1:F:52:THR:HG21 | 1:G:53:LEU:HD13 | 1.83 | 0.58 |
| 1:C:53:LEU:HD23 | 1:C:54:LEU:N | 2.18 | 0.58 |
| 1:K:24:PRO:HG2 | 1:K:64:THR:CG2 | 2.33 | 0.58 |
| 1:V:53:LEU:HD23 | 1:V:54:LEU:N | 2.19 | 0.58 |
| 1:A:33:GLY:O | 1:A:36:VAL:HG12 | 2.04 | 0.58 |
| 1:E:53:LEU:HD23 | 1:E:54:LEU:N | 2.17 | 0.58 |
| 1:H:66:TYR:CG | 1:I:68:LEU:HD22 | 2.39 | 0.58 |
| 1:L:52:THR:CG2 | 1:M:53:LEU:CD1 | 2.81 | 0.58 |
| 1:E:10:VAL:HG12 | 1:F:11:ILE:CD1 | 2.33 | 0.58 |
| 1:H:35:ALA:CB | 1:I:36:VAL:HG21 | 2.33 | 0.58 |
| 1:V:33:GLY:O | 1:V:36:VAL:HG12 | 2.03 | 0.58 |
| 1:A:68:LEU:HD22 | 1:V:66:TYR:CG | 2.39 | 0.58 |
| 1:B:17:VAL:HG12 | 1:B:17:VAL:O | 2.04 | 0.58 |
| 1:F:53:LEU:HD23 | 1:F:54:LEU:N | 2.19 | 0.58 |
| 1:B:53:LEU:HD23 | 1:B:54:LEU:N | 2.18 | 0.58 |
| 1:D:52:THR:HG21 | 1:E:53:LEU:HD13 | 1.85 | 0.57 |
| 1:F:17:VAL:HG12 | 1:F:17:VAL:O | 2.04 | 0.57 |
| 1:K:6:ALA:O | 1:K:10:VAL:HG13 | 2.04 | 0.57 |
| 1:J:6:ALA:O | 1:J:10:VAL:HG13 | 2.04 | 0.57 |
| 1:A:3:PRO:O | 1:A:7:ALA:HB3 | 2.04 | 0.57 |
| 1:A:54:LEU:HD21 | 1:V:55:LEU:CD1 | 2.34 | 0.57 |
| 1:C:17:VAL:O | 1:C:17:VAL:HG12 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:17:VAL:O | 1:D:17:VAL:HG12 | 2.03 | 0.57 |
| 1:K:10:VAL:HG12 | 1:L:11:ILE:CD1 | 2.34 | 0.57 |
| 1:K:13:ALA:HB2 | 1:L:12:ALA:HA | 1.85 | 0.57 |
| 1:L:66:TYR:CE2 | 1:M:65:ILE:HG22 | 2.40 | 0.57 |
| 1:M:53:LEU:HD23 | 1:M:54:LEU:N | 2.19 | 0.57 |
| 1:G:66:TYR:CG | 1:H:68:LEU:HD22 | 2.40 | 0.57 |
| 1:L:10:VAL:CA | 1:M:11:ILE:HG21 | 2.34 | 0.57 |
| 1:V:37:GLU:O | 1:V:40:ALA:HB3 | 2.05 | 0.57 |
| 1:C:10:VAL:CA | 1:D:11:ILE:HG21 | 2.34 | 0.57 |
| 1:G:3:PRO:O | 1:G:7:ALA:HB3 | 2.05 | 0.57 |
| 1:H:33:GLY:O | 1:H:36:VAL:HG12 | 2.05 | 0.57 |
| 1:H:10:VAL:N | 1:I:11:ILE:HG21 | 2.20 | 0.57 |
| 1:A:37:GLU:O | 1:A:40:ALA:HB3 | 2.05 | 0.56 |
| 1:K:13:ALA:HB3 | 1:L:11:ILE:CG2 | 2.35 | 0.56 |
| 1:D:53:LEU:HD23 | 1:D:54:LEU:N | 2.19 | 0.56 |
| 1:E:59:PHE:CE1 | 1:F:57:LEU:HB3 | 2.40 | 0.56 |
| 1:L:6:ALA:O | 1:L:10:VAL:HG13 | 2.05 | 0.56 |
| 1:M:10:VAL:CA | 1:V:11:ILE:HG21 | 2.35 | 0.56 |
| 1:J:10:VAL:HA | 1:K:11:ILE:HG21 | 1.88 | 0.56 |
| 1:I:10:VAL:CA | 1:J:11:ILE:HG21 | 2.36 | 0.56 |
| 1:V:3:PRO:O | 1:V:7:ALA:HB3 | 2.05 | 0.56 |
| 1:A:53:LEU:HD23 | 1:A:54:LEU:N | 2.21 | 0.56 |
| 1:G:17:VAL:O | 1:G:17:VAL:HG12 | 2.06 | 0.56 |
| 1:M:33:GLY:O | 1:M:36:VAL:HG12 | 2.05 | 0.56 |
| 1:A:6:ALA:O | 1:A:10:VAL:HG13 | 2.05 | 0.56 |
| 1:I:6:ALA:O | 1:I:10:VAL:HG13 | 2.05 | 0.56 |
| 1:M:52:THR:CG2 | 1:V:53:LEU:HD13 | 2.35 | 0.56 |
| 1:M:52:THR:HG21 | 1:V:53:LEU:HD13 | 1.87 | 0.56 |
| 1:D:10:VAL:HA | 1:E:11:ILE:CG2 | 2.35 | 0.56 |
| 1:F:52:THR:CG2 | 1:G:53:LEU:HD13 | 2.36 | 0.56 |
| 1:I:17:VAL:O | 1:I:17:VAL:HG12 | 2.05 | 0.56 |
| 1:D:13:ALA:O | 1:E:15:LEU:CB | 2.54 | 0.56 |
| 1:H:2:ASN:O | 1:H:6:ALA:N | 2.39 | 0.56 |
| 1:K:37:GLU:O | 1:K:40:ALA:HB3 | 2.06 | 0.56 |
| 1:M:10:VAL:HG12 | 1:V:11:ILE:CD1 | 2.35 | 0.56 |
| 1:L:10:VAL:HG12 | 1:M:11:ILE:CD1 | 2.35 | 0.56 |
| 1:A:13:ALA:HB3 | 1:B:11:ILE:CG2 | 2.36 | 0.55 |
| 1:E:17:VAL:O | 1:E:17:VAL:HG12 | 2.06 | 0.55 |
| 1:I:3:PRO:O | 1:I:7:ALA:HB3 | 2.06 | 0.55 |
| 1:M:10:VAL:N | 1:V:11:ILE:HG21 | 2.20 | 0.55 |
| 1:B:15:LEU:C | 1:B:17:VAL:H | 2.10 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:10:VAL:HG12 | 1:J:11:ILE:HG13 | 1.88 | 0.55 |
| 1:J:13:ALA:O | 1:K:15:LEU:CB | 2.55 | 0.55 |
| 1:J:5:ILE:HG22 | 1:K:8:ALA:CB | 2.35 | 0.55 |
| 1:L:2:ASN:O | 1:L:6:ALA:N | 2.39 | 0.55 |
| 1:I:55:LEU:HD21 | 1:J:53:LEU:CD2 | 2.37 | 0.55 |
| 1:J:59:PHE:CZ | 1:K:57:LEU:HD23 | 2.42 | 0.55 |
| 1:B:13:ALA:O | 1:C:15:LEU:CB | 2.55 | 0.55 |
| 1:D:35:ALA:CB | 1:E:36:VAL:HG21 | 2.36 | 0.55 |
| 1:L:15:LEU:C | 1:L:17:VAL:H | 2.10 | 0.55 |
| 1:E:3:PRO:O | 1:E:7:ALA:HB3 | 2.06 | 0.55 |
| 1:M:2:ASN:O | 1:M:6:ALA:N | 2.38 | 0.55 |
| 1:E:59:PHE:CZ | 1:F:57:LEU:HB3 | 2.42 | 0.55 |
| 1:G:33:GLY:O | 1:G:36:VAL:HG12 | 2.07 | 0.55 |
| 1:H:10:VAL:CA | 1:I:11:ILE:HG21 | 2.36 | 0.55 |
| 1:L:3:PRO:O | 1:L:7:ALA:HB3 | 2.07 | 0.55 |
| 1:A:59:PHE:CZ | 1:B:57:LEU:HB3 | 2.42 | 0.55 |
| 1:D:6:ALA:O | 1:D:10:VAL:HG13 | 2.06 | 0.55 |
| 1:B:52:THR:CG2 | 1:C:53:LEU:HD13 | 2.37 | 0.54 |
| 1:F:6:ALA:O | 1:F:10:VAL:HG13 | 2.07 | 0.54 |
| 1:G:37:GLU:O | 1:G:40:ALA:HB3 | 2.07 | 0.54 |
| 1:A:2:ASN:O | 1:A:6:ALA:N | 2.41 | 0.54 |
| 1:B:6:ALA:O | 1:B:10:VAL:HG13 | 2.07 | 0.54 |
| 1:C:15:LEU:C | 1:C:17:VAL:H | 2.11 | 0.54 |
| 1:C:66:TYR:CE2 | 1:D:65:ILE:HG22 | 2.42 | 0.54 |
| 1:E:2:ASN:O | 1:E:6:ALA:N | 2.40 | 0.54 |
| 1:I:10:VAL:N | 1:J:11:ILE:HG21 | 2.22 | 0.54 |
| 1:K:17:VAL:O | 1:K:17:VAL:HG12 | 2.07 | 0.54 |
| 1:J:15:LEU:C | 1:J:17:VAL:H | 2.11 | 0.54 |
| 1:K:10:VAL:HA | 1:L:11:ILE:HG21 | 1.88 | 0.54 |
| 1:L:37:GLU:O | 1:L:40:ALA:HB3 | 2.06 | 0.54 |
| 1:G:6:ALA:O | 1:G:10:VAL:HG13 | 2.07 | 0.54 |
| 1:K:3:PRO:O | 1:K:7:ALA:HB3 | 2.08 | 0.54 |
| 1:E:10:VAL:HG12 | 1:F:11:ILE:CG1 | 2.37 | 0.54 |
| 1:F:13:ALA:O | 1:G:15:LEU:CB | 2.55 | 0.54 |
| 1:H:17:VAL:HG12 | 1:H:17:VAL:O | 2.06 | 0.54 |
| 1:H:52:THR:CG2 | 1:I:53:LEU:HD13 | 2.38 | 0.54 |
| 1:K:10:VAL:HA | 1:L:11:ILE:CG2 | 2.37 | 0.54 |
| 1:M:59:PHE:HZ | 1:V:57:LEU:HD23 | 1.72 | 0.54 |
| 1:A:9:SER:C | 1:B:11:ILE:HG21 | 2.28 | 0.54 |
| 1:I:2:ASN:O | 1:I:6:ALA:N | 2.41 | 0.54 |
| 1:D:15:LEU:C | 1:D:17:VAL:H | 2.10 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:2:ASN:O | 1:F:6:ALA:N | 2.41 | 0.54 |
| 1:B:2:ASN:O | 1:B:6:ALA:N | 2.41 | 0.54 |
| 1:B:10:VAL:N | 1:C:11:ILE:HG21 | 2.23 | 0.54 |
| 1:H:24:PRO:HG3 | 1:H:63:LEU:CD1 | 2.38 | 0.54 |
| 1:J:24:PRO:HG3 | 1:J:63:LEU:CD1 | 2.38 | 0.54 |
| 1:A:17:VAL:O | 1:A:17:VAL:HG12 | 2.08 | 0.53 |
| 1:M:55:LEU:CD1 | 1:V:54:LEU:HD21 | 2.35 | 0.53 |
| 1:J:52:THR:CG2 | 1:K:53:LEU:CD1 | 2.87 | 0.53 |
| 1:A:20:ALA:HA | 1:B:21:SER:CB | 2.38 | 0.53 |
| 1:F:33:GLY:O | 1:F:36:VAL:HG12 | 2.09 | 0.53 |
| 1:K:9:SER:OG | 1:L:11:ILE:CG2 | 2.57 | 0.53 |
| 1:D:10:VAL:N | 1:E:11:ILE:HG21 | 2.24 | 0.53 |
| 1:M:59:PHE:CE1 | 1:V:57:LEU:HB3 | 2.43 | 0.53 |
| 1:C:6:ALA:O | 1:C:10:VAL:HG13 | 2.09 | 0.53 |
| 1:L:27:GLY:O | 1:L:28:GLN:C | 2.47 | 0.53 |
| 1:M:27:GLY:O | 1:M:30:THR:N | 2.33 | 0.53 |
| 1:G:59:PHE:CZ | 1:H:57:LEU:HB3 | 2.43 | 0.53 |
| 1:B:52:THR:HG23 | 1:B:55:LEU:HD23 | 1.91 | 0.53 |
| 1:E:15:LEU:C | 1:E:17:VAL:H | 2.11 | 0.53 |
| 1:J:37:GLU:O | 1:J:40:ALA:HB3 | 2.09 | 0.53 |
| 1:A:27:GLY:O | 1:A:30:THR:N | 2.35 | 0.52 |
| 1:D:13:ALA:CB | 1:E:11:ILE:HG22 | 2.39 | 0.52 |
| 1:E:37:GLU:O | 1:E:40:ALA:HB3 | 2.09 | 0.52 |
| 1:H:24:PRO:HG3 | 1:H:63:LEU:HD11 | 1.90 | 0.52 |
| 1:H:53:LEU:HG | 1:H:57:LEU:HD13 | 1.92 | 0.52 |
| 1:V:17:VAL:O | 1:V:17:VAL:HG12 | 2.09 | 0.52 |
| 1:D:37:GLU:O | 1:D:40:ALA:HB3 | 2.10 | 0.52 |
| 1:F:15:LEU:C | 1:F:17:VAL:H | 2.12 | 0.52 |
| 1:M:53:LEU:O | 1:M:57:LEU:N | 2.41 | 0.52 |
| 1:V:6:ALA:O | 1:V:10:VAL:HG13 | 2.08 | 0.52 |
| 1:F:55:LEU:HD21 | 1:G:54:LEU:CD2 | 2.40 | 0.52 |
| 1:J:66:TYR:CE2 | 1:K:65:ILE:HG22 | 2.44 | 0.52 |
| 1:V:15:LEU:C | 1:V:17:VAL:H | 2.12 | 0.52 |
| 1:C:52:THR:OG1 | 1:D:50:ARG:NE | 2.37 | 0.52 |
| 1:L:35:ALA:HB2 | 1:M:36:VAL:HG11 | 1.92 | 0.52 |
| 1:M:24:PRO:HG3 | 1:M:63:LEU:CD1 | 2.40 | 0.52 |
| 1:A:52:THR:HG23 | 1:A:55:LEU:HD23 | 1.91 | 0.52 |
| 1:C:62:ALA:HB3 | 1:D:61:GLU:OE2 | 2.09 | 0.52 |
| 1:F:35:ALA:CB | 1:G:36:VAL:HG21 | 2.39 | 0.52 |
| 1:H:6:ALA:O | 1:H:10:VAL:HG13 | 2.09 | 0.52 |
| 1:H:59:PHE:CE1 | 1:I:57:LEU:HB3 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:62:ALA:HB3 | 1:V:61:GLU:OE2 | 2.09 | 0.52 |
| 1:E:17:VAL:HG11 | 1:E:67:GLY:CA | 2.39 | 0.52 |
| 1:F:24:PRO:HG3 | 1:F:63:LEU:CD1 | 2.40 | 0.52 |
| 1:F:10:VAL:CA | 1:G:11:ILE:HG21 | 2.39 | 0.52 |
| 1:M:3:PRO:O | 1:M:7:ALA:CB | 2.58 | 0.52 |
| 1:A:10:VAL:HG12 | 1:B:11:ILE:CG1 | 2.40 | 0.52 |
| 1:B:24:PRO:HG3 | 1:B:63:LEU:CD1 | 2.40 | 0.52 |
| 1:F:37:GLU:O | 1:F:40:ALA:HB3 | 2.10 | 0.52 |
| 1:L:31:ALA:HA | 1:M:33:GLY:CA | 2.40 | 0.52 |
| 1:D:3:PRO:O | 1:D:7:ALA:HB3 | 2.10 | 0.51 |
| 1:H:15:LEU:C | 1:H:17:VAL:H | 2.13 | 0.51 |
| 1:J:3:PRO:O | 1:J:7:ALA:HB3 | 2.09 | 0.51 |
| 1:G:53:LEU:HG | 1:G:57:LEU:HD13 | 1.92 | 0.51 |
| 1:C:70:VAL:HG22 | 1:D:72:LEU:CD2 | 2.30 | 0.51 |
| 1:D:52:THR:HG23 | 1:D:55:LEU:HD23 | 1.92 | 0.51 |
| 1:G:5:ILE:HD12 | 1:G:5:ILE:H | 1.75 | 0.51 |
| 1:H:52:THR:HG23 | 1:H:55:LEU:HD23 | 1.93 | 0.51 |
| 1:A:13:ALA:HB2 | 1:B:12:ALA:CA | 2.36 | 0.51 |
| 1:F:10:VAL:HG12 | 1:G:11:ILE:CD1 | 2.41 | 0.51 |
| 1:C:52:THR:HG23 | 1:C:55:LEU:HD23 | 1.93 | 0.51 |
| 1:C:59:PHE:CZ | 1:D:57:LEU:HB3 | 2.46 | 0.51 |
| 1:E:17:VAL:CG1 | 1:E:67:GLY:HA3 | 2.40 | 0.51 |
| 1:H:3:PRO:O | 1:H:7:ALA:CB | 2.59 | 0.51 |
| 1:I:52:THR:CG2 | 1:J:53:LEU:CD1 | 2.88 | 0.51 |
| 1:L:55:LEU:HD21 | 1:M:53:LEU:CD2 | 2.40 | 0.51 |
| 1:K:15:LEU:C | 1:K:17:VAL:H | 2.14 | 0.51 |
| 1:B:10:VAL:CA | 1:C:11:ILE:HG21 | 2.39 | 0.51 |
| 1:D:10:VAL:HG12 | 1:E:11:ILE:CD1 | 2.41 | 0.51 |
| 1:F:3:PRO:O | 1:F:7:ALA:HB3 | 2.10 | 0.51 |
| 1:G:15:LEU:C | 1:G:17:VAL:H | 2.14 | 0.51 |
| 1:G:3:PRO:O | 1:G:7:ALA:CB | 2.59 | 0.51 |
| 1:I:15:LEU:C | 1:I:17:VAL:H | 2.14 | 0.51 |
| 1:I:52:THR:HG23 | 1:I:55:LEU:HD23 | 1.93 | 0.51 |
| 1:K:53:LEU:O | 1:K:57:LEU:N | 2.43 | 0.51 |
| 1:B:37:GLU:O | 1:B:40:ALA:HB3 | 2.11 | 0.51 |
| 1:C:73:ALA:O | 1:C:77:ALA:HB3 | 2.11 | 0.51 |
| 1:J:59:PHE:CE1 | 1:K:57:LEU:HB3 | 2.45 | 0.51 |
| 1:M:15:LEU:C | 1:M:17:VAL:H | 2.14 | 0.51 |
| 1:M:53:LEU:O | 1:M:57:LEU:HB2 | 2.11 | 0.51 |
| 1:B:10:VAL:HG12 | 1:C:11:ILE:CD1 | 2.41 | 0.51 |
| 1:H:53:LEU:O | 1:H:57:LEU:N | 2.39 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:55:LEU:HD21 | 1:L:54:LEU:CD2 | 2.40 | 0.50 |
| 1:A:24:PRO:HG3 | 1:A:63:LEU:CD1 | 2.41 | 0.50 |
| 1:G:13:ALA:HB2 | 1:H:12:ALA:HA | 1.93 | 0.50 |
| 1:A:10:VAL:HA | 1:B:11:ILE:HG23 | 1.91 | 0.50 |
| 1:J:52:THR:HG23 | 1:J:55:LEU:HD23 | 1.93 | 0.50 |
| 1:K:5:ILE:HD12 | 1:K:5:ILE:H | 1.76 | 0.50 |
| 1:L:17:VAL:HG12 | 1:L:17:VAL:O | 2.10 | 0.50 |
| 1:K:35:ALA:CB | 1:L:36:VAL:HG21 | 2.41 | 0.50 |
| 1:L:31:ALA:HA | 1:M:33:GLY:HA2 | 1.94 | 0.50 |
| 1:A:15:LEU:C | 1:A:17:VAL:H | 2.14 | 0.50 |
| 1:B:59:PHE:CE1 | 1:C:57:LEU:HB3 | 2.46 | 0.50 |
| 1:E:13:ALA:HB2 | 1:F:12:ALA:CA | 2.34 | 0.50 |
| 1:F:53:LEU:HG | 1:F:57:LEU:HD13 | 1.92 | 0.50 |
| 1:I:24:PRO:HG3 | 1:I:63:LEU:CD1 | 2.41 | 0.50 |
| 1:J:13:ALA:HB3 | 1:K:11:ILE:CG2 | 2.41 | 0.50 |
| 1:J:62:ALA:HB3 | 1:K:61:GLU:OE2 | 2.11 | 0.50 |
| 1:M:73:ALA:O | 1:M:77:ALA:HB3 | 2.11 | 0.50 |
| 1:B:3:PRO:O | 1:B:7:ALA:HB3 | 2.12 | 0.50 |
| 1:C:2:ASN:O | 1:C:6:ALA:N | 2.44 | 0.50 |
| 1:G:59:PHE:CE1 | 1:H:57:LEU:HB3 | 2.46 | 0.50 |
| 1:K:2:ASN:O | 1:K:6:ALA:N | 2.43 | 0.50 |
| 1:M:10:VAL:HG12 | 1:V:11:ILE:HG13 | 1.92 | 0.50 |
| 1:C:10:VAL:HG12 | 1:D:11:ILE:HG13 | 1.94 | 0.50 |
| 1:B:10:VAL:HG12 | 1:C:11:ILE:HG13 | 1.93 | 0.50 |
| 1:K:52:THR:HG23 | 1:K:55:LEU:HD23 | 1.94 | 0.50 |
| 1:K:55:LEU:CD2 | 1:L:54:LEU:HD21 | 2.41 | 0.50 |
| 1:L:24:PRO:HG3 | 1:L:63:LEU:CD1 | 2.41 | 0.50 |
| 1:D:13:ALA:HB3 | 1:E:11:ILE:HG23 | 1.93 | 0.50 |
| 1:I:37:GLU:O | 1:I:40:ALA:HB3 | 2.12 | 0.50 |
| 1:H:66:TYR:CE2 | 1:I:65:ILE:HG22 | 2.47 | 0.50 |
| 1:V:3:PRO:O | 1:V:7:ALA:CB | 2.60 | 0.50 |
| 1:D:10:VAL:CA | 1:E:11:ILE:HG21 | 2.42 | 0.50 |
| 1:K:53:LEU:HG | 1:K:57:LEU:HD13 | 1.94 | 0.50 |
| 1:K:55:LEU:CD1 | 1:L:54:LEU:HD21 | 2.40 | 0.50 |
| 1:K:73:ALA:O | 1:K:77:ALA:HB3 | 2.12 | 0.50 |
| 1:L:5:ILE:H | 1:L:5:ILE:HD12 | 1.77 | 0.50 |
| 1:L:20:ALA:HA | 1:M:21:SER:CB | 2.42 | 0.50 |
| 1:K:27:GLY:O | 1:K:28:GLN:C | 2.50 | 0.49 |
| 1:K:9:SER:C | 1:L:11:ILE:HG21 | 2.32 | 0.49 |
| 1:V:5:ILE:H | 1:V:5:ILE:HD12 | 1.77 | 0.49 |
| 1:D:66:TYR:CE2 | 1:E:65:ILE:HG22 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:55:LEU:CD1 | 1:G:54:LEU:HD21 | 2.42 | 0.49 |
| 1:H:27:GLY:O | 1:H:28:GLN:C | 2.50 | 0.49 |
| 1:V:2:ASN:O | 1:V:6:ALA:N | 2.44 | 0.49 |
| 1:D:2:ASN:O | 1:D:6:ALA:N | 2.45 | 0.49 |
| 1:H:13:ALA:HB3 | 1:I:11:ILE:CG2 | 2.42 | 0.49 |
| 1:A:3:PRO:O | 1:A:7:ALA:CB | 2.60 | 0.49 |
| 1:G:2:ASN:O | 1:G:6:ALA:N | 2.43 | 0.49 |
| 1:G:10:VAL:HA | 1:H:11:ILE:HG21 | 1.94 | 0.49 |
| 1:J:17:VAL:O | 1:J:17:VAL:HG12 | 2.12 | 0.49 |
| 1:I:63:LEU:HD23 | 1:J:64:THR:HG21 | 1.92 | 0.49 |
| 1:G:5:ILE:HG22 | 1:H:8:ALA:CB | 2.43 | 0.49 |
| 1:L:70:VAL:HG22 | 1:M:72:LEU:CD2 | 2.35 | 0.49 |
| 1:M:35:ALA:CB | 1:V:36:VAL:HG21 | 2.42 | 0.49 |
| 1:A:53:LEU:HD13 | 1:V:52:THR:CG2 | 2.43 | 0.49 |
| 1:F:53:LEU:O | 1:F:57:LEU:N | 2.42 | 0.49 |
| 1:I:33:GLY:O | 1:I:36:VAL:HG12 | 2.12 | 0.49 |
| 1:M:37:GLU:O | 1:M:40:ALA:HB3 | 2.12 | 0.49 |
| 1:A:65:ILE:HG22 | 1:V:66:TYR:CE2 | 2.48 | 0.49 |
| 1:C:37:GLU:O | 1:C:40:ALA:HB3 | 2.12 | 0.49 |
| 1:G:62:ALA:HB3 | 1:H:61:GLU:OE2 | 2.13 | 0.49 |
| 1:I:52:THR:HA | 1:I:55:LEU:HB3 | 1.95 | 0.49 |
| 1:L:24:PRO:HG3 | 1:L:63:LEU:HD11 | 1.95 | 0.49 |
| 1:D:24:PRO:HG3 | 1:D:63:LEU:HD11 | 1.94 | 0.49 |
| 1:J:53:LEU:O | 1:J:57:LEU:N | 2.44 | 0.49 |
| 1:D:24:PRO:HG3 | 1:D:63:LEU:CD1 | 2.43 | 0.49 |
| 1:A:11:ILE:HG21 | 1:V:10:VAL:HA | 1.94 | 0.49 |
| 1:V:27:GLY:O | 1:V:30:THR:N | 2.34 | 0.49 |
| 1:V:53:LEU:O | 1:V:57:LEU:N | 2.45 | 0.49 |
| 1:B:24:PRO:HG3 | 1:B:63:LEU:HD11 | 1.94 | 0.48 |
| 1:E:24:PRO:HG3 | 1:E:63:LEU:CD1 | 2.43 | 0.48 |
| 1:C:17:VAL:HG11 | 1:C:67:GLY:CA | 2.43 | 0.48 |
| 1:F:35:ALA:HB2 | 1:G:36:VAL:HG11 | 1.95 | 0.48 |
| 1:J:59:PHE:CZ | 1:K:57:LEU:HB3 | 2.48 | 0.48 |
| 1:A:27:GLY:O | 1:A:28:GLN:C | 2.51 | 0.48 |
| 1:C:5:ILE:H | 1:C:5:ILE:HD12 | 1.78 | 0.48 |
| 1:C:17:VAL:CG1 | 1:C:67:GLY:HA3 | 2.43 | 0.48 |
| 1:J:10:VAL:HA | 1:K:11:ILE:CG2 | 2.43 | 0.48 |
| 1:L:10:VAL:HG12 | 1:M:11:ILE:HG13 | 1.94 | 0.48 |
| 1:M:5:ILE:HD12 | 1:M:5:ILE:H | 1.77 | 0.48 |
| 1:A:59:PHE:HE1 | 1:B:57:LEU:HB3 | 1.77 | 0.48 |
| 1:K:10:VAL:CA | 1:L:11:ILE:HG21 | 2.42 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:17:VAL:HG11 | 1:M:67:GLY:CA | 2.43 | 0.48 |
| 1:M:59:PHE:CZ | 1:V:57:LEU:HB3 | 2.48 | 0.48 |
| 1:L:73:ALA:O | 1:L:77:ALA:HB3 | 2.13 | 0.48 |
| 1:A:53:LEU:HG | 1:A:57:LEU:HD13 | 1.95 | 0.48 |
| 1:G:63:LEU:HD23 | 1:H:64:THR:HG21 | 1.94 | 0.48 |
| 1:B:11:ILE:HG22 | 1:B:12:ALA:N | 2.29 | 0.48 |
| 1:G:53:LEU:O | 1:G:57:LEU:N | 2.43 | 0.48 |
| 1:J:2:ASN:O | 1:J:6:ALA:N | 2.46 | 0.48 |
| 1:K:53:LEU:O | 1:K:57:LEU:HB2 | 2.14 | 0.48 |
| 1:I:24:PRO:HG3 | 1:I:63:LEU:HD11 | 1.95 | 0.48 |
| 1:I:27:GLY:O | 1:I:30:THR:HG23 | 2.14 | 0.48 |
| 1:J:52:THR:HA | 1:J:55:LEU:HB3 | 1.96 | 0.48 |
| 1:K:17:VAL:HG11 | 1:K:67:GLY:CA | 2.43 | 0.48 |
| 1:J:3:PRO:O | 1:J:7:ALA:CB | 2.62 | 0.48 |
| 1:J:24:PRO:HG3 | 1:J:63:LEU:HD11 | 1.96 | 0.48 |
| 1:L:35:ALA:CB | 1:M:36:VAL:CG2 | 2.87 | 0.48 |
| 1:V:52:THR:HG23 | 1:V:55:LEU:HD23 | 1.96 | 0.48 |
| 1:E:9:SER:HB2 | 1:F:8:ALA:HB1 | 1.95 | 0.47 |
| 1:H:53:LEU:O | 1:H:57:LEU:HB2 | 2.13 | 0.47 |
| 1:H:17:VAL:CG1 | 1:H:67:GLY:HA3 | 2.44 | 0.47 |
| 1:J:5:ILE:HD12 | 1:J:5:ILE:H | 1.79 | 0.47 |
| 1:K:66:TYR:CE2 | 1:L:65:ILE:HG22 | 2.49 | 0.47 |
| 1:L:52:THR:HG22 | 1:M:53:LEU:CD1 | 2.44 | 0.47 |
| 1:L:35:ALA:HB1 | 1:M:36:VAL:HG21 | 1.93 | 0.47 |
| 1:M:17:VAL:CG1 | 1:M:67:GLY:HA3 | 2.44 | 0.47 |
| 1:A:9:SER:OG | 1:B:11:ILE:CG2 | 2.63 | 0.47 |
| 1:D:17:VAL:HG11 | 1:D:67:GLY:CA | 2.44 | 0.47 |
| 1:G:17:VAL:CG1 | 1:G:67:GLY:HA3 | 2.44 | 0.47 |
| 1:M:52:THR:HG23 | 1:M:55:LEU:HD23 | 1.97 | 0.47 |
| 1:F:63:LEU:HD23 | 1:G:64:THR:HG21 | 1.96 | 0.47 |
| 1:H:17:VAL:HG11 | 1:H:67:GLY:CA | 2.45 | 0.47 |
| 1:I:3:PRO:O | 1:I:7:ALA:CB | 2.61 | 0.47 |
| 1:L:27:GLY:O | 1:L:30:THR:N | 2.34 | 0.47 |
| 1:F:10:VAL:N | 1:G:11:ILE:HG21 | 2.28 | 0.47 |
| 1:J:70:VAL:HG22 | 1:K:72:LEU:CD2 | 2.35 | 0.47 |
| 1:A:24:PRO:HG3 | 1:A:63:LEU:HD11 | 1.96 | 0.47 |
| 1:D:63:LEU:HD23 | 1:E:64:THR:HG21 | 1.93 | 0.47 |
| 1:G:17:VAL:HG11 | 1:G:67:GLY:CA | 2.44 | 0.47 |
| 1:G:27:GLY:O | 1:G:28:GLN:C | 2.52 | 0.47 |
| 1:J:17:VAL:CG1 | 1:J:67:GLY:HA3 | 2.44 | 0.47 |
| 1:K:17:VAL:CG1 | 1:K:67:GLY:HA3 | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:V:17:VAL:CG1 | 1:V:67:GLY:HA3 | 2.44 | 0.47 |
| 1:D:17:VAL:CG1 | 1:D:67:GLY:HA3 | 2.45 | 0.47 |
| 1:E:52:THR:HG23 | 1:E:55:LEU:HD23 | 1.96 | 0.47 |
| 1:F:27:GLY:O | 1:F:30:THR:N | 2.37 | 0.47 |
| 1:F:52:THR:HG23 | 1:F:55:LEU:HD23 | 1.96 | 0.47 |
| 1:M:24:PRO:HG3 | 1:M:63:LEU:HD11 | 1.97 | 0.47 |
| 1:A:17:VAL:HG11 | 1:A:67:GLY:CA | 2.44 | 0.47 |
| 1:A:53:LEU:O | 1:A:57:LEU:N | 2.43 | 0.47 |
| 1:A:9:SER:HB2 | 1:B:8:ALA:HB1 | 1.96 | 0.47 |
| 1:F:10:VAL:HG12 | 1:G:11:ILE:HG13 | 1.96 | 0.47 |
| 1:F:17:VAL:HG11 | 1:F:67:GLY:CA | 2.44 | 0.47 |
| 1:F:55:LEU:CD2 | 1:G:54:LEU:HD21 | 2.43 | 0.47 |
| 1:I:5:ILE:HD12 | 1:I:5:ILE:H | 1.78 | 0.47 |
| 1:F:13:ALA:CB | 1:G:12:ALA:HA | 2.42 | 0.47 |
| 1:H:52:THR:HA | 1:H:55:LEU:HB3 | 1.96 | 0.47 |
| 1:I:53:LEU:O | 1:I:57:LEU:N | 2.44 | 0.47 |
| 1:V:17:VAL:HG11 | 1:V:67:GLY:CA | 2.45 | 0.47 |
| 1:M:66:TYR:CG | 1:V:68:LEU:HD22 | 2.49 | 0.47 |
| 1:D:10:VAL:HG12 | 1:E:11:ILE:HG13 | 1.97 | 0.47 |
| 1:J:17:VAL:HG11 | 1:J:67:GLY:CA | 2.44 | 0.47 |
| 1:K:52:THR:HA | 1:K:55:LEU:HB3 | 1.97 | 0.47 |
| 1:K:70:VAL:CG2 | 1:L:72:LEU:HD21 | 2.31 | 0.47 |
| 1:M:27:GLY:O | 1:M:28:GLN:C | 2.52 | 0.47 |
| 1:M:55:LEU:HD21 | 1:V:54:LEU:CD2 | 2.44 | 0.47 |
| 1:V:73:ALA:O | 1:V:77:ALA:HB3 | 2.15 | 0.47 |
| 1:A:17:VAL:CG1 | 1:A:67:GLY:HA3 | 2.45 | 0.47 |
| 1:D:27:GLY:O | 1:D:30:THR:N | 2.37 | 0.47 |
| 1:E:24:PRO:HG3 | 1:E:63:LEU:HD11 | 1.97 | 0.47 |
| 1:H:10:VAL:HG12 | 1:I:11:ILE:HG13 | 1.96 | 0.47 |
| 1:L:55:LEU:O | 1:L:58:ALA:HB3 | 2.15 | 0.47 |
| 1:B:27:GLY:O | 1:B:30:THR:N | 2.35 | 0.46 |
| 1:C:9:SER:OG | 1:D:11:ILE:CG2 | 2.63 | 0.46 |
| 1:C:63:LEU:HD23 | 1:D:64:THR:HG21 | 1.93 | 0.46 |
| 1:E:27:GLY:O | 1:E:30:THR:N | 2.34 | 0.46 |
| 1:I:17:VAL:CG1 | 1:I:67:GLY:HA3 | 2.45 | 0.46 |
| 1:J:53:LEU:HG | 1:J:57:LEU:HD13 | 1.97 | 0.46 |
| 1:K:24:PRO:HG3 | 1:K:63:LEU:CD1 | 2.45 | 0.46 |
| 1:E:3:PRO:O | 1:E:7:ALA:CB | 2.62 | 0.46 |
| 1:K:13:ALA:CB | 1:L:11:ILE:HG22 | 2.45 | 0.46 |
| 1:A:11:ILE:CG2 | 1:V:13:ALA:HB3 | 2.44 | 0.46 |
| 1:B:59:PHE:CZ | 1:C:57:LEU:HB3 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:53:LEU:O | 1:C:57:LEU:N | 2.47 | 0.46 |
| 1:H:37:GLU:O | 1:H:40:ALA:HB3 | 2.14 | 0.46 |
| 1:J:75:LEU:CD2 | 1:J:76:PHE:CE2 | 2.99 | 0.46 |
| 1:K:3:PRO:O | 1:K:7:ALA:CB | 2.62 | 0.46 |
| 1:L:17:VAL:HG11 | 1:L:67:GLY:CA | 2.46 | 0.46 |
| 1:L:3:PRO:O | 1:L:7:ALA:CB | 2.63 | 0.46 |
| 1:B:24:PRO:O | 1:B:25:GLY:C | 2.53 | 0.46 |
| 1:C:20:ALA:HA | 1:D:21:SER:CB | 2.46 | 0.46 |
| 1:H:11:ILE:HG22 | 1:H:12:ALA:N | 2.30 | 0.46 |
| 1:A:52:THR:HA | 1:A:55:LEU:HB3 | 1.98 | 0.46 |
| 1:B:17:VAL:HG11 | 1:B:67:GLY:CA | 2.45 | 0.46 |
| 1:C:24:PRO:HG3 | 1:C:63:LEU:CD1 | 2.46 | 0.46 |
| 1:C:27:GLY:O | 1:C:28:GLN:C | 2.53 | 0.46 |
| 1:J:27:GLY:O | 1:J:28:GLN:C | 2.54 | 0.46 |
| 1:L:13:ALA:CB | 1:M:12:ALA:HA | 2.41 | 0.46 |
| 1:A:20:ALA:O | 1:A:64:THR:CG2 | 2.55 | 0.46 |
| 1:A:53:LEU:O | 1:A:57:LEU:HB2 | 2.16 | 0.46 |
| 1:D:52:THR:CG2 | 1:E:53:LEU:HD13 | 2.45 | 0.46 |
| 1:G:24:PRO:HG3 | 1:G:63:LEU:CD1 | 2.45 | 0.46 |
| 1:J:35:ALA:HB1 | 1:K:36:VAL:HG21 | 1.97 | 0.46 |
| 1:C:35:ALA:HB1 | 1:D:36:VAL:HG21 | 1.95 | 0.46 |
| 1:D:52:THR:HA | 1:D:55:LEU:HB3 | 1.97 | 0.46 |
| 1:E:13:ALA:HB3 | 1:F:11:ILE:CG2 | 2.45 | 0.46 |
| 1:I:13:ALA:HB3 | 1:J:11:ILE:CG2 | 2.46 | 0.46 |
| 1:J:73:ALA:O | 1:J:77:ALA:HB3 | 2.16 | 0.46 |
| 1:C:3:PRO:O | 1:C:7:ALA:HB3 | 2.15 | 0.46 |
| 1:F:73:ALA:O | 1:F:77:ALA:HB3 | 2.15 | 0.46 |
| 1:G:52:THR:HA | 1:G:55:LEU:HB3 | 1.98 | 0.46 |
| 1:V:11:ILE:HG22 | 1:V:12:ALA:N | 2.31 | 0.46 |
| 1:V:24:PRO:HG3 | 1:V:63:LEU:CD1 | 2.45 | 0.46 |
| 1:B:66:TYR:CE2 | 1:C:65:ILE:HG22 | 2.51 | 0.46 |
| 1:B:17:VAL:CG1 | 1:B:67:GLY:HA3 | 2.46 | 0.46 |
| 1:D:62:ALA:HB3 | 1:E:61:GLU:OE2 | 2.15 | 0.46 |
| 1:F:17:VAL:CG1 | 1:F:67:GLY:HA3 | 2.45 | 0.46 |
| 1:K:59:PHE:CE1 | 1:L:57:LEU:HB3 | 2.51 | 0.46 |
| 1:L:52:THR:HG23 | 1:L:55:LEU:HD23 | 1.97 | 0.46 |
| 1:B:73:ALA:O | 1:B:77:ALA:HB3 | 2.16 | 0.46 |
| 1:E:53:LEU:O | 1:E:57:LEU:HB2 | 2.16 | 0.46 |
| 1:F:27:GLY:O | 1:F:28:GLN:C | 2.54 | 0.46 |
| 1:I:17:VAL:HG11 | 1:I:67:GLY:CA | 2.45 | 0.46 |
| 1:K:9:SER:OG | 1:L:11:ILE:HG21 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:V:24:PRO:O | 1:V:25:GLY:C | 2.55 | 0.46 |
| 1:V:52:THR:HA | 1:V:55:LEU:HB3 | 1.98 | 0.46 |
| 1:C:35:ALA:CB | 1:D:36:VAL:CG2 | 2.88 | 0.45 |
| 1:F:11:ILE:HG22 | 1:F:12:ALA:N | 2.31 | 0.45 |
| 1:F:20:ALA:O | 1:F:64:THR:CG2 | 2.58 | 0.45 |
| 1:F:59:PHE:CE1 | 1:G:57:LEU:HB3 | 2.50 | 0.45 |
| 1:K:13:ALA:HB3 | 1:L:11:ILE:HG23 | 1.96 | 0.45 |
| 1:A:5:ILE:HD12 | 1:A:5:ILE:H | 1.81 | 0.45 |
| 1:B:70:VAL:CG2 | 1:C:72:LEU:HD21 | 2.31 | 0.45 |
| 1:H:62:ALA:HB3 | 1:I:61:GLU:OE2 | 2.16 | 0.45 |
| 1:L:63:LEU:HD23 | 1:M:64:THR:HG21 | 1.92 | 0.45 |
| 1:M:55:LEU:CD2 | 1:V:54:LEU:HD21 | 2.46 | 0.45 |
| 1:F:62:ALA:O | 1:F:65:ILE:CG1 | 2.62 | 0.45 |
| 1:M:55:LEU:O | 1:M:58:ALA:HB3 | 2.17 | 0.45 |
| 1:B:62:ALA:HB3 | 1:C:61:GLU:OE2 | 2.16 | 0.45 |
| 1:D:17:VAL:HG23 | 1:E:15:LEU:CB | 2.46 | 0.45 |
| 1:D:24:PRO:O | 1:D:25:GLY:C | 2.55 | 0.45 |
| 1:D:27:GLY:O | 1:D:28:GLN:C | 2.55 | 0.45 |
| 1:H:20:ALA:O | 1:H:64:THR:CG2 | 2.59 | 0.45 |
| 1:J:13:ALA:CB | 1:K:11:ILE:HG22 | 2.46 | 0.45 |
| 1:L:17:VAL:CG1 | 1:L:67:GLY:HA3 | 2.46 | 0.45 |
| 1:A:19:LEU:HD12 | 1:B:19:LEU:HD23 | 1.98 | 0.45 |
| 1:B:27:GLY:O | 1:B:28:GLN:C | 2.54 | 0.45 |
| 1:C:59:PHE:HE1 | 1:D:57:LEU:HB3 | 1.79 | 0.45 |
| 1:E:27:GLY:O | 1:E:28:GLN:C | 2.54 | 0.45 |
| 1:F:3:PRO:O | 1:F:7:ALA:CB | 2.64 | 0.45 |
| 1:M:52:THR:HA | 1:M:55:LEU:HB3 | 1.99 | 0.45 |
| 1:M:63:LEU:HD23 | 1:V:64:THR:HG21 | 1.95 | 0.45 |
| 1:C:52:THR:HA | 1:C:55:LEU:HB3 | 1.97 | 0.45 |
| 1:D:5:ILE:H | 1:D:5:ILE:HD12 | 1.82 | 0.45 |
| 1:E:53:LEU:HG | 1:E:57:LEU:HD13 | 1.98 | 0.45 |
| 1:F:52:THR:HA | 1:F:55:LEU:HB3 | 1.99 | 0.45 |
| 1:J:53:LEU:O | 1:J:57:LEU:HB2 | 2.17 | 0.45 |
| 1:A:15:LEU:CB | 1:V:13:ALA:O | 2.65 | 0.45 |
| 1:B:20:ALA:O | 1:B:64:THR:CG2 | 2.62 | 0.45 |
| 1:D:11:ILE:HG22 | 1:D:12:ALA:N | 2.31 | 0.45 |
| 1:C:31:ALA:HA | 1:D:33:GLY:HA2 | 1.98 | 0.45 |
| 1:D:9:SER:C | 1:E:11:ILE:HG21 | 2.37 | 0.45 |
| 1:E:10:VAL:HA | 1:F:11:ILE:HG23 | 1.94 | 0.45 |
| 1:I:73:ALA:O | 1:I:77:ALA:HB3 | 2.17 | 0.45 |
| 1:B:52:THR:HA | 1:B:55:LEU:HB3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:55:LEU:O | 1:D:58:ALA:HB3 | 2.15 | 0.45 |
| 1:F:53:LEU:O | 1:F:57:LEU:HB2 | 2.16 | 0.45 |
| 1:H:5:ILE:H | 1:H:5:ILE:HD12 | 1.81 | 0.45 |
| 1:I:10:VAL:HG12 | 1:J:11:ILE:CG1 | 2.46 | 0.45 |
| 1:I:27:GLY:O | 1:I:28:GLN:C | 2.55 | 0.45 |
| 1:I:53:LEU:HG | 1:I:57:LEU:HD13 | 1.99 | 0.45 |
| 1:L:53:LEU:O | 1:L:57:LEU:N | 2.45 | 0.45 |
| 1:V:24:PRO:HG3 | 1:V:63:LEU:HD11 | 1.99 | 0.45 |
| 1:B:3:PRO:O | 1:B:7:ALA:CB | 2.65 | 0.45 |
| 1:F:5:ILE:H | 1:F:5:ILE:HD12 | 1.82 | 0.45 |
| 1:M:20:ALA:O | 1:M:64:THR:CG2 | 2.58 | 0.45 |
| 1:A:12:ALA:HA | 1:V:13:ALA:HB2 | 1.98 | 0.45 |
| 1:E:52:THR:OG1 | 1:F:50:ARG:NE | 2.45 | 0.45 |
| 1:F:20:ALA:HB1 | 1:F:64:THR:CA | 2.44 | 0.45 |
| 1:E:20:ALA:HA | 1:F:21:SER:CB | 2.46 | 0.45 |
| 1:J:75:LEU:HD23 | 1:J:76:PHE:CE2 | 2.52 | 0.45 |
| 1:J:66:TYR:CD2 | 1:K:68:LEU:HD22 | 2.52 | 0.45 |
| 1:J:70:VAL:CG2 | 1:K:72:LEU:HD21 | 2.37 | 0.45 |
| 1:L:53:LEU:O | 1:L:57:LEU:HB2 | 2.17 | 0.45 |
| 1:V:27:GLY:O | 1:V:28:GLN:C | 2.55 | 0.45 |
| 1:H:10:VAL:HG12 | 1:I:11:ILE:HD12 | 1.97 | 0.44 |
| 1:K:11:ILE:O | 1:K:12:ALA:C | 2.56 | 0.44 |
| 1:K:66:TYR:CD2 | 1:L:68:LEU:HD22 | 2.52 | 0.44 |
| 1:L:52:THR:HA | 1:L:55:LEU:HB3 | 1.98 | 0.44 |
| 1:A:17:VAL:HG23 | 1:B:15:LEU:CB | 2.47 | 0.44 |
| 1:A:73:ALA:O | 1:A:77:ALA:HB3 | 2.17 | 0.44 |
| 1:B:5:ILE:HD12 | 1:B:5:ILE:H | 1.81 | 0.44 |
| 1:D:73:ALA:O | 1:D:77:ALA:HB3 | 2.18 | 0.44 |
| 1:M:5:ILE:HD12 | 1:M:5:ILE:N | 2.32 | 0.44 |
| 1:A:26:VAL:HG11 | 1:B:26:VAL:HG22 | 2.00 | 0.44 |
| 1:H:13:ALA:CB | 1:I:11:ILE:HG22 | 2.48 | 0.44 |
| 1:I:55:LEU:CD2 | 1:J:53:LEU:CD2 | 2.95 | 0.44 |
| 1:K:73:ALA:HA | 1:K:77:ALA:HB3 | 2.00 | 0.44 |
| 1:L:59:PHE:HE1 | 1:M:57:LEU:HB3 | 1.79 | 0.44 |
| 1:A:57:LEU:HB3 | 1:V:59:PHE:CE1 | 2.52 | 0.44 |
| 1:B:27:GLY:O | 1:B:30:THR:HG23 | 2.17 | 0.44 |
| 1:C:31:ALA:HA | 1:D:33:GLY:CA | 2.48 | 0.44 |
| 1:D:3:PRO:O | 1:D:7:ALA:CB | 2.65 | 0.44 |
| 1:H:24:PRO:O | 1:H:25:GLY:C | 2.55 | 0.44 |
| 1:H:59:PHE:CZ | 1:I:57:LEU:HB3 | 2.52 | 0.44 |
| 1:L:9:SER:OG | 1:M:11:ILE:CG2 | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:24:PRO:O | 1:C:25:GLY:C | 2.56 | 0.44 |
| 1:C:73:ALA:HA | 1:C:77:ALA:HB3 | 1.99 | 0.44 |
| 1:E:5:ILE:H | 1:E:5:ILE:HD12 | 1.81 | 0.44 |
| 1:G:66:TYR:CE2 | 1:H:65:ILE:HG22 | 2.53 | 0.44 |
| 1:J:52:THR:OG1 | 1:K:50:ARG:NE | 2.46 | 0.44 |
| 1:M:62:ALA:O | 1:M:65:ILE:CG1 | 2.65 | 0.44 |
| 1:V:53:LEU:HG | 1:V:57:LEU:HD13 | 1.98 | 0.44 |
| 1:A:13:ALA:CB | 1:B:11:ILE:HG22 | 2.48 | 0.44 |
| 1:E:11:ILE:HG22 | 1:E:12:ALA:N | 2.33 | 0.44 |
| 1:E:17:VAL:HG23 | 1:F:15:LEU:CB | 2.47 | 0.44 |
| 1:E:10:VAL:CG1 | 1:F:11:ILE:HG13 | 2.45 | 0.44 |
| 1:F:24:PRO:HG3 | 1:F:63:LEU:HD11 | 1.98 | 0.44 |
| 1:D:66:TYR:CD2 | 1:E:68:LEU:HD22 | 2.52 | 0.44 |
| 1:G:52:THR:HG23 | 1:G:55:LEU:HD23 | 2.00 | 0.44 |
| 1:G:73:ALA:O | 1:G:77:ALA:HB3 | 2.16 | 0.44 |
| 1:A:13:ALA:HB3 | 1:B:11:ILE:HG22 | 2.00 | 0.44 |
| 1:E:52:THR:HA | 1:E:55:LEU:HB3 | 2.00 | 0.44 |
| 1:G:5:ILE:N | 1:G:5:ILE:HD12 | 2.32 | 0.44 |
| 1:J:24:PRO:O | 1:J:27:GLY:N | 2.50 | 0.44 |
| 1:K:9:SER:OG | 1:L:11:ILE:HB | 2.18 | 0.44 |
| 1:A:9:SER:OG | 1:B:11:ILE:HB | 2.18 | 0.43 |
| 1:D:59:PHE:CE1 | 1:E:57:LEU:HB3 | 2.53 | 0.43 |
| 1:F:62:ALA:HB3 | 1:G:61:GLU:OE2 | 2.17 | 0.43 |
| 1:C:53:LEU:O | 1:C:57:LEU:HB2 | 2.17 | 0.43 |
| 1:F:66:TYR:CG | 1:G:68:LEU:HD22 | 2.53 | 0.43 |
| 1:I:24:PRO:O | 1:I:25:GLY:C | 2.56 | 0.43 |
| 1:H:5:ILE:CG2 | 1:I:8:ALA:CB | 2.89 | 0.43 |
| 1:K:5:ILE:HD12 | 1:K:5:ILE:N | 2.32 | 0.43 |
| 1:L:10:VAL:HA | 1:M:11:ILE:HG23 | 2.00 | 0.43 |
| 1:B:53:LEU:O | 1:B:57:LEU:HB2 | 2.17 | 0.43 |
| 1:C:75:LEU:CD2 | 1:C:76:PHE:CE2 | 3.02 | 0.43 |
| 1:G:52:THR:CG2 | 1:H:53:LEU:CD1 | 2.95 | 0.43 |
| 1:H:74:LEU:O | 1:H:78:ASN:CB | 2.66 | 0.43 |
| 1:L:56:SER:HB3 | 1:M:32:ALA:HB2 | 2.00 | 0.43 |
| 1:A:11:ILE:CG2 | 1:V:10:VAL:HA | 2.48 | 0.43 |
| 1:A:13:ALA:HB3 | 1:B:11:ILE:HG23 | 2.00 | 0.43 |
| 1:D:9:SER:OG | 1:E:11:ILE:CG2 | 2.66 | 0.43 |
| 1:M:55:LEU:HD21 | 1:V:53:LEU:CD2 | 2.48 | 0.43 |
| 1:E:53:LEU:O | 1:E:57:LEU:N | 2.46 | 0.43 |
| 1:C:13:ALA:HB3 | 1:D:11:ILE:CG2 | 2.49 | 0.43 |
| 1:C:27:GLY:O | 1:C:30:THR:HG23 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:53:LEU:O | 1:G:57:LEU:HB2 | 2.18 | 0.43 |
| 1:H:30:THR:OG1 | 1:H:31:ALA:N | 2.50 | 0.43 |
| 1:H:73:ALA:O | 1:H:77:ALA:HB3 | 2.18 | 0.43 |
| 1:A:2:ASN:N | 1:A:5:ILE:CD1 | 2.82 | 0.43 |
| 1:C:5:ILE:CG2 | 1:D:8:ALA:CB | 2.91 | 0.43 |
| 1:G:60:MET:O | 1:G:63:LEU:HD12 | 2.19 | 0.43 |
| 1:G:11:ILE:HG22 | 1:G:12:ALA:N | 2.34 | 0.43 |
| 1:H:10:VAL:HG12 | 1:I:11:ILE:CG1 | 2.49 | 0.43 |
| 1:J:55:LEU:O | 1:J:58:ALA:HB3 | 2.19 | 0.43 |
| 1:L:53:LEU:HG | 1:L:57:LEU:HD13 | 2.00 | 0.43 |
| 1:V:5:ILE:HD12 | 1:V:5:ILE:N | 2.33 | 0.43 |
| 1:E:75:LEU:CD2 | 1:E:76:PHE:CE2 | 3.02 | 0.43 |
| 1:F:24:PRO:O | 1:F:25:GLY:C | 2.55 | 0.43 |
| 1:F:59:PHE:HZ | 1:G:57:LEU:HD23 | 1.82 | 0.43 |
| 1:B:55:LEU:O | 1:B:58:ALA:HB3 | 2.18 | 0.43 |
| 1:E:27:GLY:O | 1:E:30:THR:HG23 | 2.18 | 0.43 |
| 1:I:27:GLY:O | 1:I:30:THR:N | 2.36 | 0.43 |
| 1:A:52:THR:CG2 | 1:B:53:LEU:CD1 | 2.97 | 0.42 |
| 1:F:74:LEU:O | 1:F:78:ASN:CB | 2.67 | 0.42 |
| 1:I:11:ILE:HG22 | 1:I:12:ALA:N | 2.34 | 0.42 |
| 1:C:30:THR:OG1 | 1:C:31:ALA:N | 2.52 | 0.42 |
| 1:D:62:ALA:O | 1:D:65:ILE:CG1 | 2.65 | 0.42 |
| 1:L:11:ILE:HG22 | 1:L:12:ALA:N | 2.34 | 0.42 |
| 1:M:27:GLY:O | 1:M:30:THR:HG23 | 2.20 | 0.42 |
| 1:L:55:LEU:CG | 1:M:54:LEU:HD21 | 2.48 | 0.42 |
| 1:G:2:ASN:N | 1:G:5:ILE:CD1 | 2.82 | 0.42 |
| 1:L:5:ILE:N | 1:L:5:ILE:HD12 | 2.33 | 0.42 |
| 1:V:53:LEU:O | 1:V:57:LEU:HB2 | 2.18 | 0.42 |
| 1:C:74:LEU:O | 1:C:78:ASN:CB | 2.67 | 0.42 |
| 1:D:53:LEU:O | 1:D:57:LEU:N | 2.47 | 0.42 |
| 1:A:10:VAL:CG1 | 1:B:11:ILE:HG13 | 2.47 | 0.42 |
| 1:J:39:ILE:HD12 | 1:J:46:GLU:HA | 2.02 | 0.42 |
| 1:L:55:LEU:CD2 | 1:M:53:LEU:CD2 | 2.96 | 0.42 |
| 1:D:53:LEU:HG | 1:D:57:LEU:HD13 | 2.02 | 0.42 |
| 1:F:55:LEU:O | 1:F:58:ALA:HB3 | 2.19 | 0.42 |
| 1:G:73:ALA:HA | 1:G:77:ALA:HB3 | 2.02 | 0.42 |
| 1:I:5:ILE:N | 1:I:5:ILE:HD12 | 2.35 | 0.42 |
| 1:J:24:PRO:O | 1:J:25:GLY:C | 2.57 | 0.42 |
| 1:A:30:THR:OG1 | 1:A:31:ALA:N | 2.52 | 0.42 |
| 1:E:30:THR:OG1 | 1:E:31:ALA:N | 2.53 | 0.42 |
| 1:E:55:LEU:O | 1:E:58:ALA:HB3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:73:ALA:O | 1:E:77:ALA:HB3 | 2.19 | 0.42 |
| 1:G:74:LEU:O | 1:G:78:ASN:CB | 2.67 | 0.42 |
| 1:K:39:ILE:HD12 | 1:K:46:GLU:HA | 2.02 | 0.42 |
| 1:M:5:ILE:CG2 | 1:V:8:ALA:CB | 2.91 | 0.42 |
| 1:B:9:SER:OG | 1:C:11:ILE:CG2 | 2.67 | 0.42 |
| 1:I:30:THR:OG1 | 1:I:31:ALA:N | 2.53 | 0.42 |
| 1:L:11:ILE:HA | 1:L:11:ILE:HD13 | 1.94 | 0.42 |
| 1:M:11:ILE:HG22 | 1:M:12:ALA:N | 2.35 | 0.42 |
| 1:V:24:PRO:O | 1:V:27:GLY:N | 2.52 | 0.42 |
| 1:V:39:ILE:HD12 | 1:V:46:GLU:HA | 2.02 | 0.42 |
| 1:A:2:ASN:N | 1:A:5:ILE:HD13 | 2.35 | 0.42 |
| 1:C:10:VAL:HG12 | 1:D:11:ILE:CG1 | 2.49 | 0.42 |
| 1:D:11:ILE:HA | 1:D:11:ILE:HD13 | 1.95 | 0.42 |
| 1:E:19:LEU:HD23 | 1:E:19:LEU:N | 2.35 | 0.42 |
| 1:G:24:PRO:HG3 | 1:G:63:LEU:HD11 | 2.02 | 0.42 |
| 1:G:55:LEU:O | 1:G:58:ALA:HB3 | 2.20 | 0.42 |
| 1:J:35:ALA:HB2 | 1:K:36:VAL:HG11 | 2.00 | 0.42 |
| 1:G:13:ALA:O | 1:H:15:LEU:CB | 2.67 | 0.42 |
| 1:J:13:ALA:HB3 | 1:K:11:ILE:HG22 | 2.02 | 0.42 |
| 1:L:55:LEU:HD21 | 1:M:53:LEU:HD22 | 2.02 | 0.42 |
| 1:M:13:ALA:HB3 | 1:V:11:ILE:CG2 | 2.49 | 0.42 |
| 1:E:13:ALA:HB3 | 1:F:11:ILE:HG22 | 2.02 | 0.41 |
| 1:A:11:ILE:CG2 | 1:V:9:SER:OG | 2.68 | 0.41 |
| 1:A:13:ALA:CB | 1:B:12:ALA:HA | 2.41 | 0.41 |
| 1:D:30:THR:OG1 | 1:D:31:ALA:N | 2.53 | 0.41 |
| 1:F:20:ALA:HA | 1:G:21:SER:CB | 2.50 | 0.41 |
| 1:G:27:GLY:O | 1:G:30:THR:N | 2.38 | 0.41 |
| 1:J:10:VAL:N | 1:K:11:ILE:HG21 | 2.35 | 0.41 |
| 1:K:24:PRO:HG3 | 1:K:63:LEU:HD11 | 2.02 | 0.41 |
| 1:M:39:ILE:HD12 | 1:M:46:GLU:HA | 2.03 | 0.41 |
| 1:V:55:LEU:O | 1:V:58:ALA:HB3 | 2.19 | 0.41 |
| 1:L:27:GLY:O | 1:L:29:GLY:N | 2.53 | 0.41 |
| 1:L:75:LEU:CD2 | 1:L:76:PHE:CE2 | 3.03 | 0.41 |
| 1:M:10:VAL:HG12 | 1:V:11:ILE:CG1 | 2.50 | 0.41 |
| 1:V:70:VAL:HA | 1:V:73:ALA:HB3 | 2.02 | 0.41 |
| 1:A:68:LEU:HD22 | 1:V:66:TYR:CD2 | 2.54 | 0.41 |
| 1:C:52:THR:O | 1:C:55:LEU:HB3 | 2.20 | 0.41 |
| 1:C:5:ILE:N | 1:C:5:ILE:HD12 | 2.35 | 0.41 |
| 1:K:52:THR:HG21 | 1:L:53:LEU:HD13 | 2.01 | 0.41 |
| 1:A:60:MET:O | 1:A:63:LEU:HD12 | 2.20 | 0.41 |
| 1:C:10:VAL:HG12 | 1:D:11:ILE:HD12 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:53:LEU:O | 1:D:57:LEU:HB2 | 2.20 | 0.41 |
| 1:F:19:LEU:HD12 | 1:G:19:LEU:HD23 | 2.02 | 0.41 |
| 1:J:10:VAL:CA | 1:K:11:ILE:HG21 | 2.50 | 0.41 |
| 1:B:62:ALA:O | 1:B:65:ILE:CG1 | 2.66 | 0.41 |
| 1:D:27:GLY:O | 1:D:30:THR:HG23 | 2.21 | 0.41 |
| 1:C:35:ALA:HB2 | 1:D:36:VAL:HG11 | 2.02 | 0.41 |
| 1:F:11:ILE:HA | 1:F:11:ILE:HD13 | 1.95 | 0.41 |
| 1:H:27:GLY:O | 1:H:30:THR:N | 2.36 | 0.41 |
| 1:H:70:VAL:HA | 1:H:73:ALA:HB3 | 2.03 | 0.41 |
| 1:J:11:ILE:HG22 | 1:J:12:ALA:N | 2.35 | 0.41 |
| 1:K:62:ALA:O | 1:K:65:ILE:CG1 | 2.69 | 0.41 |
| 1:A:52:THR:OG1 | 1:B:50:ARG:NE | 2.45 | 0.41 |
| 1:C:19:LEU:HD12 | 1:D:19:LEU:HD23 | 2.01 | 0.41 |
| 1:H:5:ILE:N | 1:H:5:ILE:HD12 | 2.36 | 0.41 |
| 1:K:7:ALA:O | 1:K:8:ALA:C | 2.59 | 0.41 |
| 1:M:53:LEU:HG | 1:M:57:LEU:HD13 | 2.02 | 0.41 |
| 1:B:24:PRO:O | 1:B:27:GLY:N | 2.54 | 0.41 |
| 1:C:53:LEU:HG | 1:C:57:LEU:HD13 | 2.01 | 0.41 |
| 1:C:55:LEU:O | 1:C:58:ALA:HB3 | 2.21 | 0.41 |
| 1:D:24:PRO:O | 1:D:27:GLY:N | 2.53 | 0.41 |
| 1:E:27:GLY:O | 1:E:29:GLY:N | 2.54 | 0.41 |
| 1:H:20:ALA:HB1 | 1:H:64:THR:CA | 2.45 | 0.41 |
| 1:I:53:LEU:O | 1:I:57:LEU:HB2 | 2.20 | 0.41 |
| 1:I:55:LEU:HD21 | 1:J:53:LEU:HD22 | 2.03 | 0.41 |
| 1:L:55:LEU:CD2 | 1:M:53:LEU:HD22 | 2.50 | 0.41 |
| 1:E:75:LEU:HD23 | 1:E:76:PHE:CE2 | 2.56 | 0.41 |
| 1:J:20:ALA:HA | 1:K:21:SER:CB | 2.51 | 0.41 |
| 1:K:55:LEU:O | 1:K:58:ALA:HB3 | 2.20 | 0.41 |
| 1:J:63:LEU:HD23 | 1:K:64:THR:HG21 | 1.96 | 0.41 |
| 1:K:70:VAL:HG22 | 1:L:72:LEU:CD2 | 2.31 | 0.41 |
| 1:L:62:ALA:O | 1:L:65:ILE:CG1 | 2.68 | 0.41 |
| 1:L:13:ALA:HB3 | 1:M:11:ILE:CG2 | 2.51 | 0.41 |
| 1:A:11:ILE:HA | 1:A:11:ILE:HD13 | 1.95 | 0.41 |
| 1:B:55:LEU:HD21 | 1:C:53:LEU:CD2 | 2.51 | 0.41 |
| 1:F:26:VAL:HG11 | 1:G:26:VAL:HG22 | 2.03 | 0.41 |
| 1:G:24:PRO:O | 1:G:27:GLY:N | 2.54 | 0.41 |
| 1:H:27:GLY:O | 1:H:29:GLY:N | 2.53 | 0.41 |
| 1:H:55:LEU:O | 1:H:58:ALA:HB3 | 2.21 | 0.41 |
| 1:H:7:ALA:O | 1:H:8:ALA:C | 2.59 | 0.41 |
| 1:M:75:LEU:CD2 | 1:M:76:PHE:CE2 | 3.04 | 0.41 |
| 1:B:30:THR:OG1 | 1:B:31:ALA:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:69:VAL:CG1 | 1:B:70:VAL:N | 2.83 | 0.41 |
| 1:B:73:ALA:HA | 1:B:77:ALA:HB3 | 2.03 | 0.41 |
| 1:C:3:PRO:O | 1:C:7:ALA:CB | 2.69 | 0.41 |
| 1:D:59:PHE:CZ | 1:E:57:LEU:HB3 | 2.56 | 0.41 |
| 1:C:52:THR:CG2 | 1:D:53:LEU:CD1 | 2.97 | 0.40 |
| 1:I:7:ALA:O | 1:I:8:ALA:C | 2.58 | 0.40 |
| 1:J:30:THR:OG1 | 1:J:31:ALA:N | 2.53 | 0.40 |
| 1:J:5:ILE:HD12 | 1:J:5:ILE:N | 2.36 | 0.40 |
| 1:J:62:ALA:O | 1:J:65:ILE:CG1 | 2.68 | 0.40 |
| 1:A:11:ILE:HG21 | 1:V:9:SER:OG | 2.21 | 0.40 |
| 1:B:53:LEU:HG | 1:B:57:LEU:HD13 | 2.02 | 0.40 |
| 1:C:35:ALA:HB2 | 1:D:36:VAL:CG2 | 2.39 | 0.40 |
| 1:E:74:LEU:O | 1:E:78:ASN:CB | 2.69 | 0.40 |
| 1:K:27:GLY:O | 1:K:30:THR:N | 2.38 | 0.40 |
| 1:J:55:LEU:HD21 | 1:K:53:LEU:CD2 | 2.51 | 0.40 |
| 1:L:15:LEU:C | 1:L:17:VAL:N | 2.74 | 0.40 |
| 1:A:11:ILE:HG22 | 1:V:13:ALA:CB | 2.51 | 0.40 |
| 1:A:70:VAL:HA | 1:A:73:ALA:HB3 | 2.03 | 0.40 |
| 1:A:75:LEU:CD2 | 1:A:76:PHE:CE2 | 3.05 | 0.40 |
| 1:C:10:VAL:HA | 1:D:11:ILE:HG23 | 2.00 | 0.40 |
| 1:E:39:ILE:HD12 | 1:E:46:GLU:HA | 2.03 | 0.40 |
| 1:I:62:ALA:O | 1:I:65:ILE:CG1 | 2.66 | 0.40 |
| 1:J:27:GLY:O | 1:J:30:THR:N | 2.39 | 0.40 |
| 1:M:27:GLY:O | 1:M:29:GLY:N | 2.55 | 0.40 |
| 1:A:11:ILE:HG21 | 1:V:10:VAL:N | 2.36 | 0.40 |
| 1:A:65:ILE:O | 1:A:66:TYR:C | 2.60 | 0.40 |
| 1:D:10:VAL:HG23 | 1:D:11:ILE:N | 2.37 | 0.40 |
| 1:E:5:ILE:HD12 | 1:E:5:ILE:N | 2.37 | 0.40 |
| 1:H:11:ILE:HD13 | 1:H:11:ILE:HA | 1.95 | 0.40 |
| 1:J:15:LEU:C | 1:J:17:VAL:N | 2.75 | 0.40 |
| 1:A:5:ILE:HD12 | 1:A:5:ILE:N | 2.37 | 0.40 |
| 1:J:31:ALA:HA | 1:K:33:GLY:CA | 2.52 | 0.40 |
| 1:L:27:GLY:O | 1:L:30:THR:HG23 | 2.22 | 0.40 |
| 1:M:20:ALA:HA | 1:V:21:SER:CB | 2.50 | 0.40 |
| 1:V:11:ILE:O | 1:V:12:ALA:C | 2.60 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 1 | A | 76/78 (97%) | 53 (70%) | 17 (22%) | 6 (8%) | 1 | 14 |
| 1 | B | 76/78 (97%) | 51 (67%) | 19 (25%) | 6 (8%) | 1 | 14 |
| 1 | C | 76/78 (97%) | 51 (67%) | 18 (24%) | 7 (9%) | 1 | 12 |
| 1 | D | 76/78 (97%) | 52 (68%) | 18 (24%) | 6 (8%) | 1 | 14 |
| 1 | E | 76/78 (97%) | 51 (67%) | 19 (25%) | 6 (8%) | 1 | 14 |
| 1 | F | 76/78 (97%) | 51 (67%) | 19 (25%) | 6 (8%) | 1 | 14 |
| 1 | G | 76/78 (97%) | 53 (70%) | 17 (22%) | 6 (8%) | 1 | 14 |
| 1 | H | 76/78 (97%) | 51 (67%) | 19 (25%) | 6 (8%) | 1 | 14 |
| 1 | I | 76/78 (97%) | 53 (70%) | 17 (22%) | 6 (8%) | 1 | 14 |
| 1 | J | 76/78 (97%) | 50 (66%) | 20 (26%) | 6 (8%) | 1 | 14 |
| 1 | K | 76/78 (97%) | 52 (68%) | 18 (24%) | 6 (8%) | 1 | 14 |
| 1 | L | 76/78 (97%) | 51 (67%) | 18 (24%) | 7 (9%) | 1 | 12 |
| 1 | M | 76/78 (97%) | 52 (68%) | 18 (24%) | 6 (8%) | 1 | 14 |
| 1 | V | 76/78 (97%) | 51 (67%) | 19 (25%) | 6 (8%) | 1 | 14 |
| All | All | 1064/1092 (97%) | 722 (68%) | 256 (24%) | 86 (8%) | 1 | 14 |

All (86) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 22 | ILE |
| 1 | E | 22 | ILE |
| 1 | G | 22 | ILE |
| 1 | I | 22 | ILE |
| 1 | J | 22 | ILE |
| 1 | L | 22 | ILE |
| 1 | V | 22 | ILE |
| 1 | A | 22 | ILE |
| 1 | A | 27 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 28 | GLN |
| 1 | A | 57 | LEU |
| 1 | B | 22 | ILE |
| 1 | B | 27 | GLY |
| 1 | B | 28 | GLN |
| 1 | B | 57 | LEU |
| 1 | C | 27 | GLY |
| 1 | C | 28 | GLN |
| 1 | C | 57 | LEU |
| 1 | D | 22 | ILE |
| 1 | D | 27 | GLY |
| 1 | D | 28 | GLN |
| 1 | D | 57 | LEU |
| 1 | E | 27 | GLY |
| 1 | E | 28 | GLN |
| 1 | E | 57 | LEU |
| 1 | F | 22 | ILE |
| 1 | F | 27 | GLY |
| 1 | F | 28 | GLN |
| 1 | F | 57 | LEU |
| 1 | G | 27 | GLY |
| 1 | G | 28 | GLN |
| 1 | G | 57 | LEU |
| 1 | H | 22 | ILE |
| 1 | H | 27 | GLY |
| 1 | H | 28 | GLN |
| 1 | H | 57 | LEU |
| 1 | I | 27 | GLY |
| 1 | I | 28 | GLN |
| 1 | I | 57 | LEU |
| 1 | J | 27 | GLY |
| 1 | J | 57 | LEU |
| 1 | K | 22 | ILE |
| 1 | K | 27 | GLY |
| 1 | K | 28 | GLN |
| 1 | K | 57 | LEU |
| 1 | L | 27 | GLY |
| 1 | L | 28 | GLN |
| 1 | L | 57 | LEU |
| 1 | M | 22 | ILE |
| 1 | M | 27 | GLY |
| 1 | M | 28 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 57 | LEU |
| 1 | V | 27 | GLY |
| 1 | V | 28 | GLN |
| 1 | V | 57 | LEU |
| 1 | C | 58 | ALA |
| 1 | D | 58 | ALA |
| 1 | F | 58 | ALA |
| 1 | G | 58 | ALA |
| 1 | H | 58 | ALA |
| 1 | I | 58 | ALA |
| 1 | J | 28 | GLN |
| 1 | J | 58 | ALA |
| 1 | K | 58 | ALA |
| 1 | L | 58 | ALA |
| 1 | M | 58 | ALA |
| 1 | V | 58 | ALA |
| 1 | A | 58 | ALA |
| 1 | B | 58 | ALA |
| 1 | E | 58 | ALA |
| 1 | F | 7 | ALA |
| 1 | G | 7 | ALA |
| 1 | H | 7 | ALA |
| 1 | V | 7 | ALA |
| 1 | A | 7 | ALA |
| 1 | D | 7 | ALA |
| 1 | I | 7 | ALA |
| 1 | J | 7 | ALA |
| 1 | K | 7 | ALA |
| 1 | L | 16 | ALA |
| 1 | M | 7 | ALA |
| 1 | B | 7 | ALA |
| 1 | C | 7 | ALA |
| 1 | C | 16 | ALA |
| 1 | E | 7 | ALA |
| 1 | L | 7 | ALA |

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| 1 | B | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| 1 | C | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| 1 | D | 37/50 (74%) | 35 (95%) | 2 (5%) | 22 | 53 |
| 1 | E | 37/50 (74%) | 33 (89%) | 4 (11%) | 6 | 30 |
| 1 | F | 37/50 (74%) | 35 (95%) | 2 (5%) | 22 | 53 |
| 1 | G | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| 1 | H | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| 1 | I | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| 1 | J | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| 1 | K | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| 1 | L | 37/50 (74%) | 35 (95%) | 2 (5%) | 22 | 53 |
| 1 | M | 37/50 (74%) | 33 (89%) | 4 (11%) | 6 | 30 |
| 1 | V | 37/50 (74%) | 34 (92%) | 3 (8%) | 11 | 41 |
| All | All | 518/700 (74%) | 477 (92%) | 41 (8%) | 12 | 42 |

All (41) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 21 | SER |
| 1 | A | 63 | LEU |
| 1 | A | 69 | VAL |
| 1 | B | 21 | SER |
| 1 | B | 63 | LEU |
| 1 | B | 69 | VAL |
| 1 | C | 21 | SER |
| 1 | C | 63 | LEU |
| 1 | C | 69 | VAL |
| 1 | D | 63 | LEU |
| 1 | D | 69 | VAL |
| 1 | E | 21 | SER |
| 1 | E | 52 | THR |
| 1 | E | 63 | LEU |
| 1 | E | 69 | VAL |
| 1 | F | 63 | LEU |
| 1 | F | 69 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 52 | THR |
| 1 | G | 63 | LEU |
| 1 | G | 69 | VAL |
| 1 | H | 21 | SER |
| 1 | H | 63 | LEU |
| 1 | H | 69 | VAL |
| 1 | I | 21 | SER |
| 1 | I | 63 | LEU |
| 1 | I | 69 | VAL |
| 1 | J | 21 | SER |
| 1 | J | 63 | LEU |
| 1 | J | 69 | VAL |
| 1 | K | 21 | SER |
| 1 | K | 63 | LEU |
| 1 | K | 69 | VAL |
| 1 | L | 63 | LEU |
| 1 | L | 69 | VAL |
| 1 | M | 21 | SER |
| 1 | M | 52 | THR |
| 1 | M | 63 | LEU |
| 1 | M | 69 | VAL |
| 1 | V | 21 | SER |
| 1 | V | 63 | LEU |
| 1 | V | 69 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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 | A | 78/78 (100%) | -0.36 | 1 (1%) 77 70 | 65, 69, 72, 72 | 0 |
| 1 | B | 78/78 (100%) | -0.25 | 4 (5%) 28 24 | 65, 69, 72, 72 | 0 |
| 1 | C | 78/78 (100%) | -0.36 | 1 (1%) 77 70 | 65, 69, 72, 72 | 0 |
| 1 | D | 78/78 (100%) | -0.40 | 3 (3%) 40 33 | 65, 69, 72, 72 | 0 |
| 1 | E | 78/78 (100%) | -0.33 | 3 (3%) 40 33 | 65, 69, 72, 72 | 0 |
| 1 | F | 78/78 (100%) | -0.43 | 0 100 100 | 65, 69, 72, 72 | 0 |
| 1 | G | 78/78 (100%) | -0.35 | 1 (1%) 77 70 | 65, 69, 72, 72 | 0 |
| 1 | H | 78/78 (100%) | -0.41 | 1 (1%) 77 70 | 65, 69, 72, 72 | 0 |
| 1 | I | 78/78 (100%) | -0.27 | 1 (1%) 77 70 | 65, 69, 72, 72 | 0 |
| 1 | J | 78/78 (100%) | -0.28 | 1 (1%) 77 70 | 65, 69, 72, 72 | 0 |
| 1 | K | 78/78 (100%) | -0.18 | 3 (3%) 40 33 | 65, 69, 72, 72 | 0 |
| 1 | L | 78/78 (100%) | -0.26 | 3 (3%) 40 33 | 65, 69, 72, 72 | 0 |
| 1 | M | 78/78 (100%) | -0.36 | 2 (2%) 56 47 | 65, 69, 72, 72 | 0 |
| 1 | V | 78/78 (100%) | -0.30 | 2 (2%) 56 47 | 65, 69, 72, 72 | 0 |
| All | All | 1092/1092 (100%) | -0.32 | 26 (2%) 59 50 | 65, 69, 72, 72 | 0 |

All (26) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | K | 43 | PRO | 3.6 |
| 1 | D | 76 | PHE | 3.5 |
| 1 | V | 79 | PRO | 2.8 |
| 1 | I | 2 | ASN | 2.7 |
| 1 | C | 46 | GLU | 2.6 |
| 1 | H | 79 | PRO | 2.6 |
| 1 | K | 76 | PHE | 2.6 |
| 1 | M | 76 | PHE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | M | 2 | ASN | 2.5 |
| 1 | D | 79 | PRO | 2.5 |
| 1 | B | 45 | ALA | 2.5 |
| 1 | J | 79 | PRO | 2.5 |
| 1 | B | 79 | PRO | 2.4 |
| 1 | K | 4 | LEU | 2.4 |
| 1 | G | 79 | PRO | 2.4 |
| 1 | V | 2 | ASN | 2.4 |
| 1 | L | 79 | PRO | 2.3 |
| 1 | B | 3 | PRO | 2.3 |
| 1 | A | 79 | PRO | 2.3 |
| 1 | E | 46 | GLU | 2.2 |
| 1 | B | 46 | GLU | 2.1 |
| 1 | E | 76 | PHE | 2.1 |
| 1 | E | 2 | ASN | 2.1 |
| 1 | L | 3 | PRO | 2.1 |
| 1 | L | 4 | LEU | 2.1 |
| 1 | D | 2 | ASN | 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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.