



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

PDB ID : 3K19
Title : OmpF porin
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Center for Structures of Membrane Proteins (CSMP)
Deposited on : 2009-09-26
Resolution : 3.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

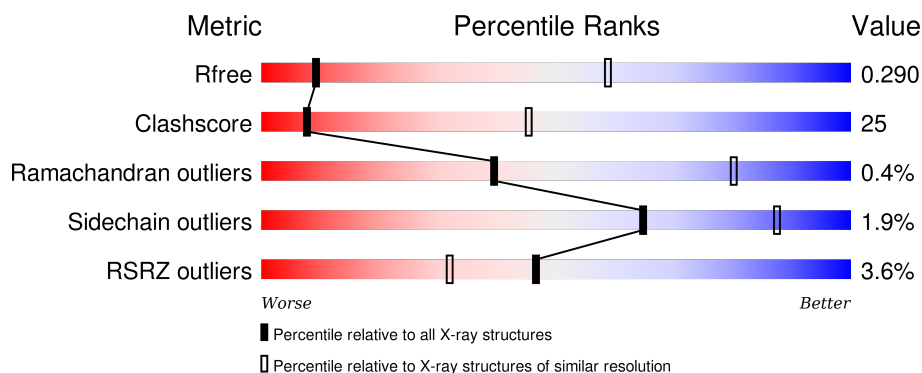
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1317 (4.10-3.50) |
| Clashscore | 102246 | 1458 (4.10-3.50) |
| Ramachandran outliers | 100387 | 1397 (4.10-3.50) |
| Sidechain outliers | 100360 | 1392 (4.10-3.50) |
| RSRZ outliers | 91569 | 1325 (4.10-3.50) |

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. 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 | 340 | <div> <div>4%</div> <div>64%</div> <div>34%</div> <div>.</div> </div> |
| 1 | B | 340 | <div> <div>%</div> <div>64%</div> <div>35%</div> <div>.</div> </div> |
| 1 | C | 340 | <div> <div>2%</div> <div>65%</div> <div>34%</div> <div>.</div> </div> |
| 1 | D | 340 | <div> <div>%</div> <div>64%</div> <div>35%</div> <div>.</div> </div> |
| 1 | E | 340 | <div> <div>%</div> <div>64%</div> <div>35%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | F | 340 | <div> <div>%</div> <div> <div></div> <div>63%</div> <div>35%</div> <div></div> </div> </div> |
| 1 | G | 340 | <div> <div>6%</div> <div> <div></div> <div>64%</div> <div>35%</div> <div></div> </div> </div> |
| 1 | H | 340 | <div> <div>5%</div> <div> <div></div> <div>64%</div> <div>35%</div> <div></div> </div> </div> |
| 1 | I | 340 | <div> <div>6%</div> <div> <div></div> <div>62%</div> <div>36%</div> <div></div> </div> </div> |
| 1 | J | 340 | <div> <div>4%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div></div> </div> </div> |
| 1 | K | 340 | <div> <div>4%</div> <div> <div></div> <div>64%</div> <div>35%</div> <div></div> </div> </div> |
| 1 | L | 340 | <div> <div>8%</div> <div> <div></div> <div>63%</div> <div>36%</div> <div></div> </div> </div> |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31524 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.

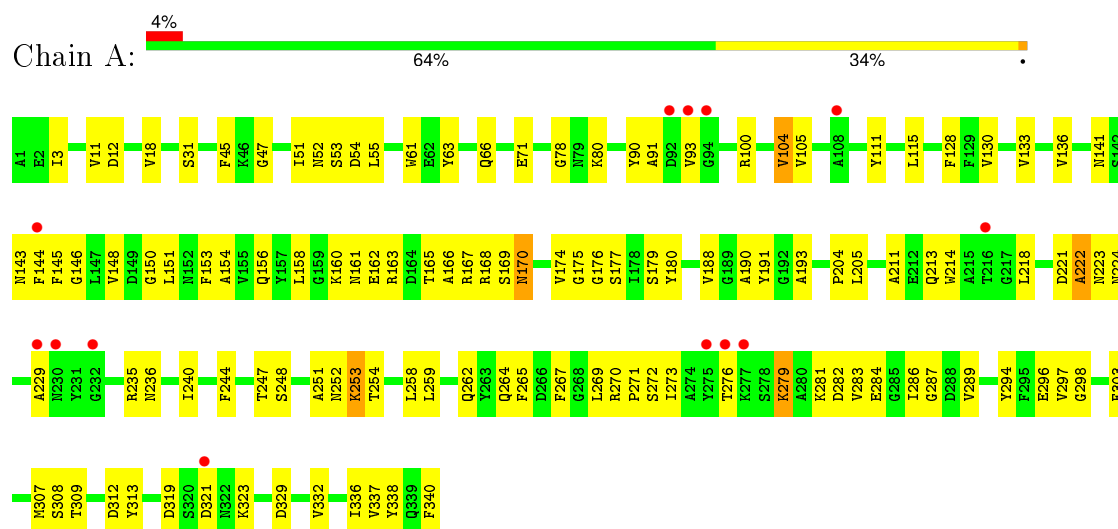
- Molecule 1 is a protein called Outer membrane protein F.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 340 | Total | C | N | O | S | 8 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | B | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | C | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | D | 340 | Total | C | N | O | S | 8 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | E | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | F | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | G | 340 | Total | C | N | O | S | 8 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | H | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | I | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | J | 340 | Total | C | N | O | S | 8 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | K | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |
| 1 | L | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2627 | 1654 | 438 | 532 | 3 | | | |

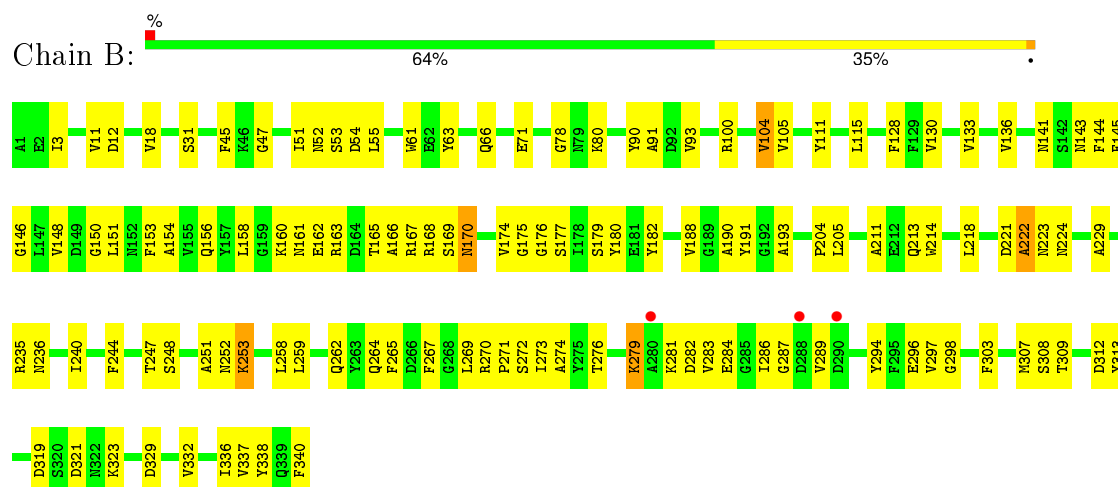
3 Residue-property plots

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: Outer membrane protein F

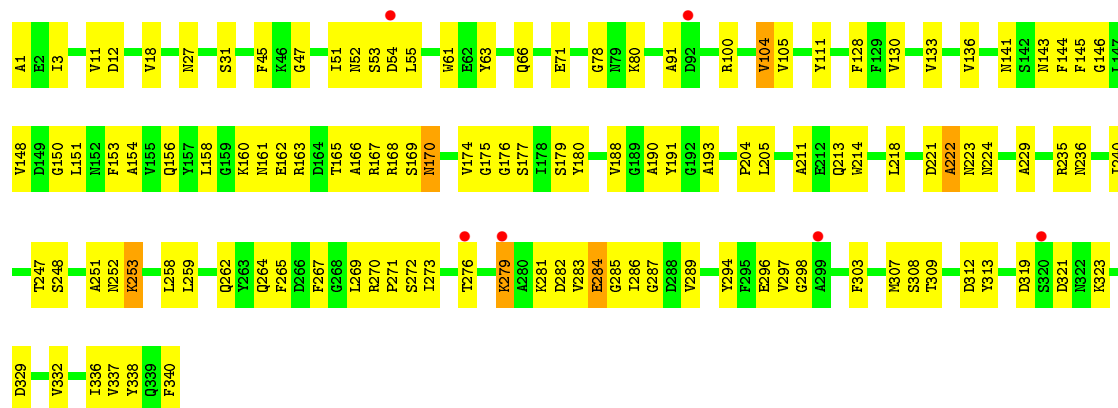


• Molecule 1: Outer membrane protein F

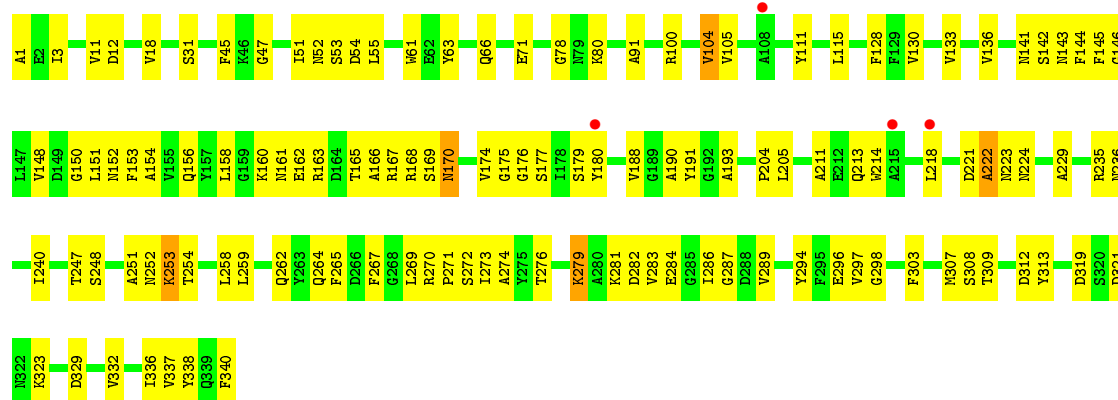


• Molecule 1: Outer membrane protein F

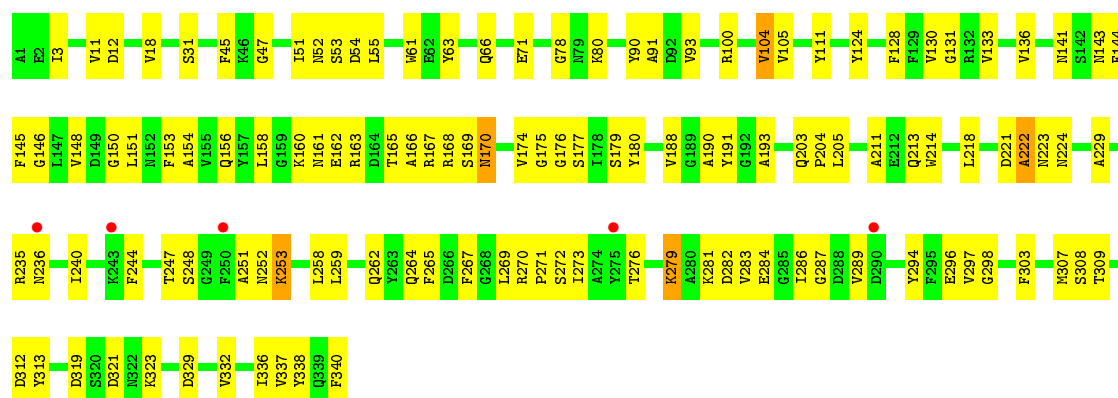




• Molecule 1: Outer membrane protein F

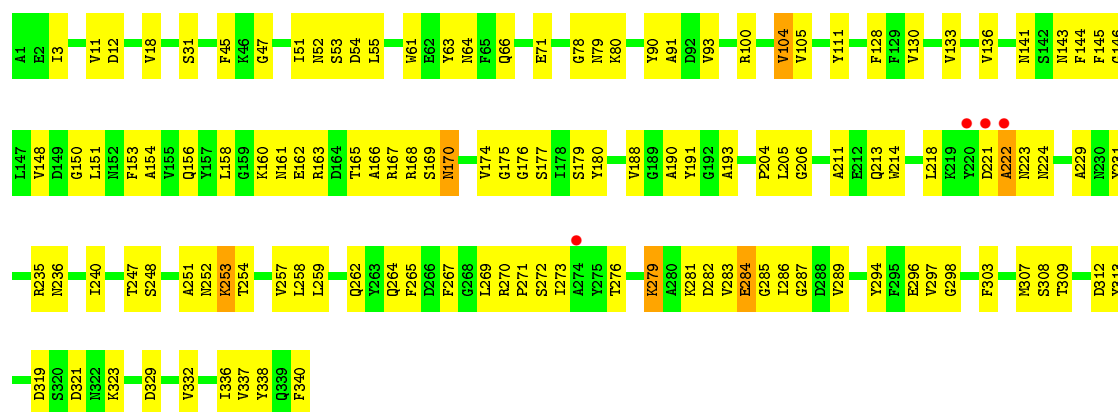


• Molecule 1: Outer membrane protein F

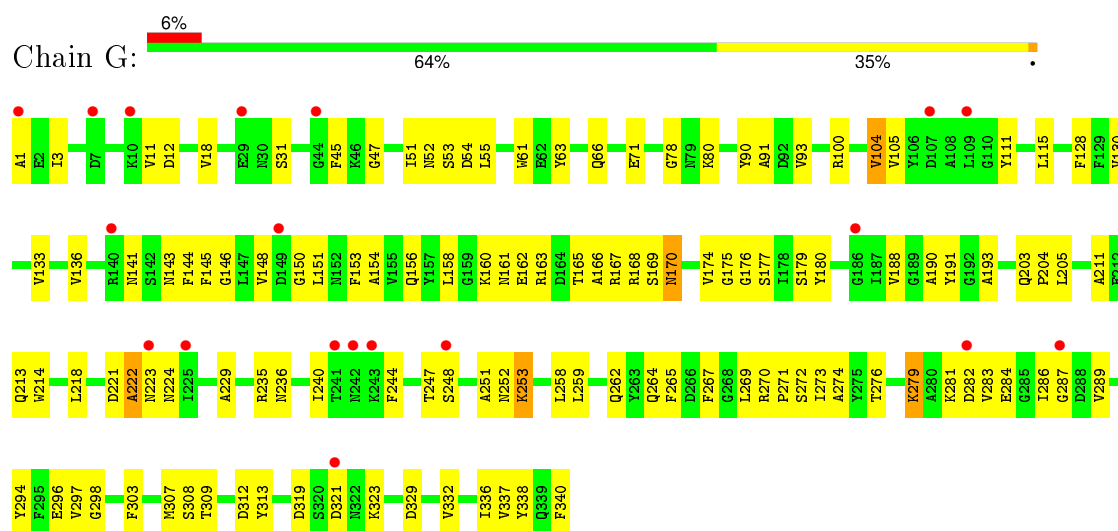


• Molecule 1: Outer membrane protein F

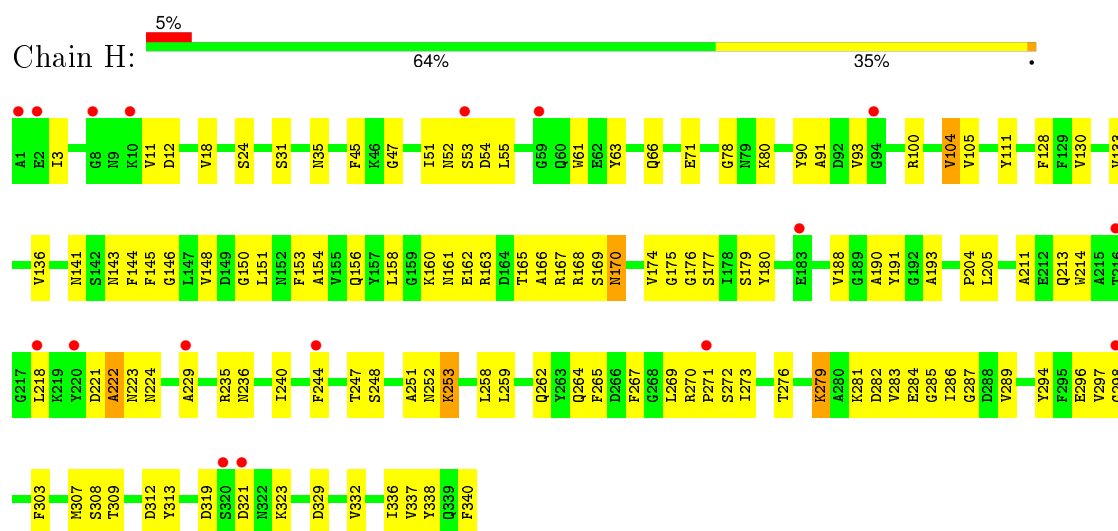




• Molecule 1: Outer membrane protein F

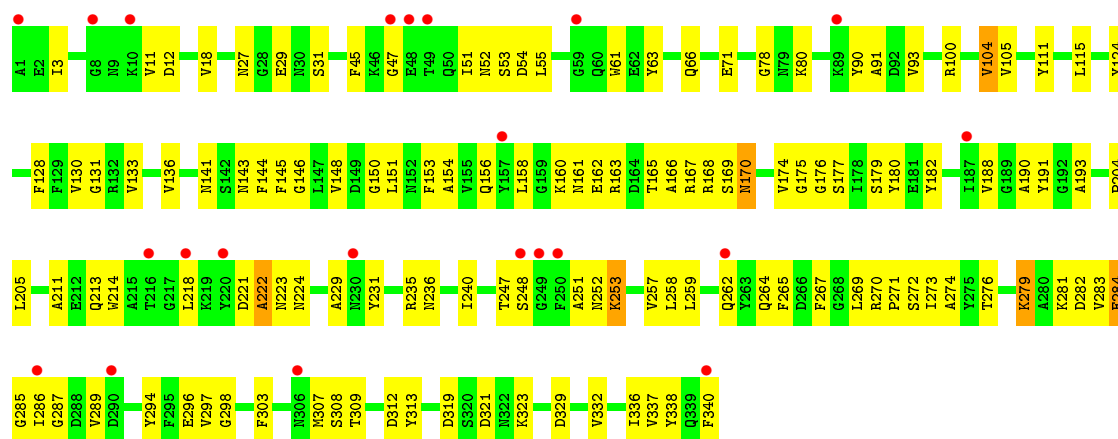


• Molecule 1: Outer membrane protein F

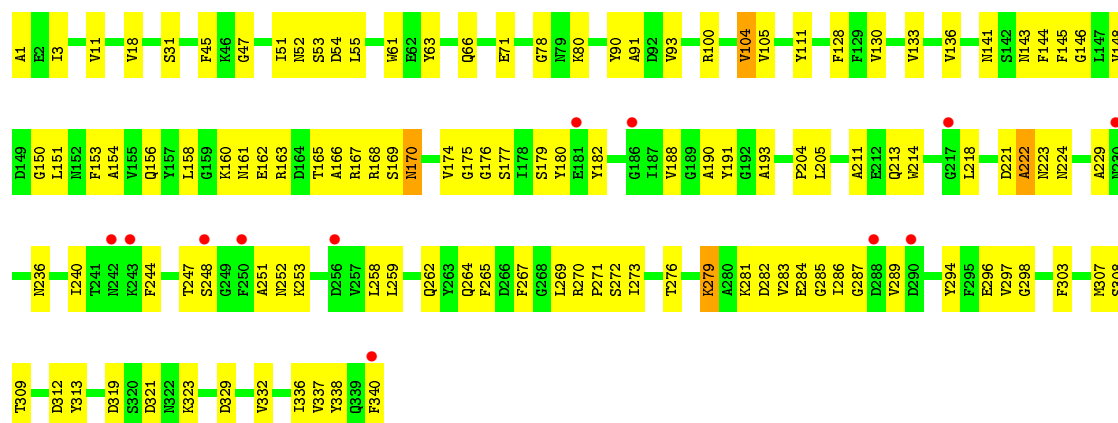


• Molecule 1: Outer membrane protein F

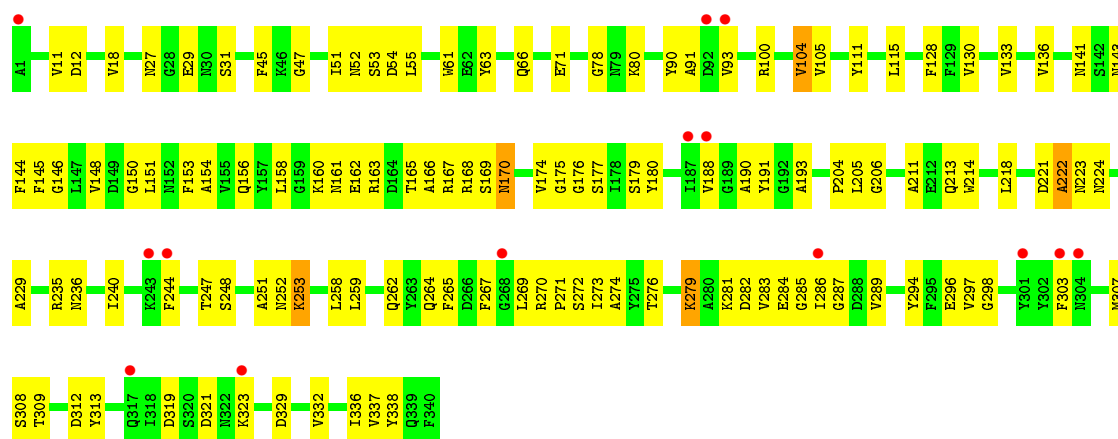




• Molecule 1: Outer membrane protein F

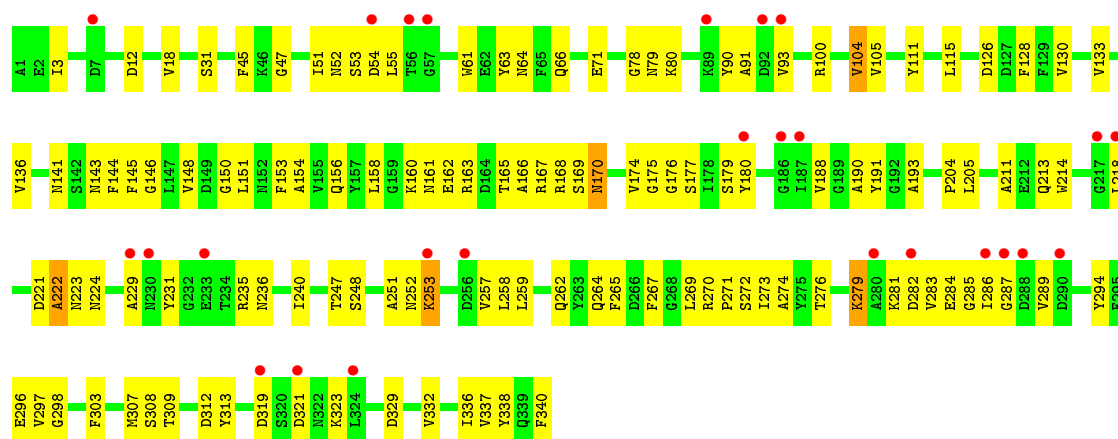


• Molecule 1: Outer membrane protein F



• Molecule 1: Outer membrane protein F





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 136.71Å 210.52Å 137.04Å 90.00° 100.49° 90.00° | Depositor |
| Resolution (Å) | 49.57 – 3.79 49.57 – 3.79 | Depositor EDS |
| % Data completeness (in resolution range) | 49.6 (49.57-3.79) 98.9 (49.57-3.79) | Depositor EDS |
| R_{merge} | 0.14 | Depositor |
| R_{sym} | 0.14 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.14 (at 3.77Å) | Xtriage |
| Refinement program | REFMAC 5.5.0066 | Depositor |
| R, R_{free} | 0.280 , 0.288 0.280 , 0.290 | Depositor DCC |
| R_{free} test set | 3786 reflections (5.32%) | DCC |
| Wilson B-factor (Å ²) | 70.6 | Xtriage |
| Anisotropy | 0.046 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 9.8 | EDS |
| Estimated twinning fraction | 0.003 for l,-k,h | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Outliers | 0 of 74966 reflections | Xtriage |
| F_o, F_c correlation | 0.78 | EDS |
| Total number of atoms | 31524 | wwPDB-VP |
| Average B, all atoms (Å ²) | 78.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 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 | 0.29 | 0/2683 | 0.41 | 0/3628 |
| 1 | B | 0.27 | 0/2683 | 0.41 | 0/3628 |
| 1 | C | 0.28 | 0/2683 | 0.41 | 0/3628 |
| 1 | D | 0.29 | 0/2683 | 0.41 | 0/3628 |
| 1 | E | 0.28 | 0/2683 | 0.41 | 0/3628 |
| 1 | F | 0.28 | 0/2683 | 0.41 | 0/3628 |
| 1 | G | 0.27 | 0/2683 | 0.41 | 0/3628 |
| 1 | H | 0.27 | 0/2683 | 0.41 | 0/3628 |
| 1 | I | 0.27 | 0/2683 | 0.41 | 0/3628 |
| 1 | J | 0.27 | 0/2683 | 0.41 | 0/3628 |
| 1 | K | 0.27 | 0/2683 | 0.41 | 0/3628 |
| 1 | L | 0.27 | 0/2683 | 0.41 | 0/3628 |
| All | All | 0.28 | 0/32196 | 0.41 | 0/43536 |

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 | 2627 | 0 | 2444 | 142 | 0 |
| 1 | B | 2627 | 0 | 2444 | 149 | 0 |
| 1 | C | 2627 | 0 | 2444 | 143 | 0 |
| 1 | D | 2627 | 0 | 2444 | 144 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | E | 2627 | 0 | 2444 | 144 | 0 |
| 1 | F | 2627 | 0 | 2444 | 148 | 0 |
| 1 | G | 2627 | 0 | 2444 | 151 | 0 |
| 1 | H | 2627 | 0 | 2444 | 146 | 0 |
| 1 | I | 2627 | 0 | 2444 | 151 | 0 |
| 1 | J | 2627 | 0 | 2444 | 143 | 0 |
| 1 | K | 2627 | 0 | 2444 | 146 | 0 |
| 1 | L | 2627 | 0 | 2444 | 150 | 0 |
| All | All | 31524 | 0 | 29328 | 1531 | 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 25.

All (1531) 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:E:321:ASP:OD1 | 1:K:287:GLY:HA2 | 1.18 | 1.35 |
| 1:E:287:GLY:CA | 1:I:321:ASP:OD1 | 1.76 | 1.33 |
| 1:I:287:GLY:CA | 1:K:321:ASP:OD1 | 1.75 | 1.32 |
| 1:B:287:GLY:CA | 1:L:321:ASP:OD1 | 1.76 | 1.32 |
| 1:C:287:GLY:HA2 | 1:G:321:ASP:OD1 | 1.17 | 1.31 |
| 1:H:321:ASP:OD1 | 1:L:287:GLY:CA | 1.78 | 1.29 |
| 1:B:321:ASP:OD1 | 1:H:287:GLY:HA2 | 1.22 | 1.28 |
| 1:C:287:GLY:CA | 1:G:321:ASP:OD1 | 1.83 | 1.27 |
| 1:C:321:ASP:OD1 | 1:D:287:GLY:HA2 | 1.11 | 1.27 |
| 1:A:321:ASP:OD1 | 1:J:287:GLY:CA | 1.82 | 1.25 |
| 1:D:321:ASP:OD1 | 1:G:287:GLY:CA | 1.83 | 1.25 |
| 1:F:287:GLY:CA | 1:J:321:ASP:OD1 | 1.82 | 1.25 |
| 1:A:287:GLY:HA2 | 1:F:321:ASP:OD1 | 1.10 | 1.25 |
| 1:E:321:ASP:OD1 | 1:K:287:GLY:CA | 1.84 | 1.24 |
| 1:F:287:GLY:HA2 | 1:J:321:ASP:OD1 | 1.11 | 1.23 |
| 1:C:321:ASP:OD1 | 1:D:287:GLY:CA | 1.85 | 1.21 |
| 1:D:321:ASP:OD1 | 1:G:287:GLY:HA2 | 1.06 | 1.19 |
| 1:A:287:GLY:CA | 1:F:321:ASP:OD1 | 1.90 | 1.18 |
| 1:E:287:GLY:HA2 | 1:I:321:ASP:OD1 | 1.02 | 1.17 |
| 1:B:287:GLY:HA2 | 1:L:321:ASP:OD1 | 1.02 | 1.17 |
| 1:I:287:GLY:HA2 | 1:K:321:ASP:OD1 | 1.00 | 1.15 |
| 1:A:321:ASP:OD1 | 1:J:287:GLY:HA2 | 0.98 | 1.15 |
| 1:B:321:ASP:OD1 | 1:H:287:GLY:CA | 1.94 | 1.15 |
| 1:H:321:ASP:OD1 | 1:L:287:GLY:HA2 | 0.98 | 1.13 |
| 1:G:71:GLU:HB3 | 1:H:80:LYS:HD2 | 1.34 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:71:GLU:HB3 | 1:E:80:LYS:HD2 | 1.36 | 1.07 |
| 1:L:313:TYR:CD1 | 1:L:332:VAL:HG22 | 1.92 | 1.04 |
| 1:A:80:LYS:HD2 | 1:C:71:GLU:HB3 | 1.37 | 1.04 |
| 1:I:313:TYR:CD1 | 1:I:332:VAL:HG22 | 1.92 | 1.04 |
| 1:K:313:TYR:CD1 | 1:K:332:VAL:HG22 | 1.93 | 1.03 |
| 1:C:313:TYR:CD1 | 1:C:332:VAL:HG22 | 1.94 | 1.03 |
| 1:J:313:TYR:CD1 | 1:J:332:VAL:HG22 | 1.93 | 1.03 |
| 1:H:313:TYR:CD1 | 1:H:332:VAL:HG22 | 1.92 | 1.03 |
| 1:G:80:LYS:HD2 | 1:I:71:GLU:HB3 | 1.40 | 1.02 |
| 1:A:313:TYR:CD1 | 1:A:332:VAL:HG22 | 1.94 | 1.02 |
| 1:G:313:TYR:CD1 | 1:G:332:VAL:HG22 | 1.93 | 1.02 |
| 1:J:71:GLU:HB3 | 1:K:80:LYS:HD2 | 1.41 | 1.02 |
| 1:F:313:TYR:CD1 | 1:F:332:VAL:HG22 | 1.94 | 1.02 |
| 1:B:313:TYR:CD1 | 1:B:332:VAL:HG22 | 1.93 | 1.02 |
| 1:H:71:GLU:HB3 | 1:I:80:LYS:HD2 | 1.40 | 1.01 |
| 1:D:313:TYR:CD1 | 1:D:332:VAL:HG22 | 1.96 | 1.00 |
| 1:K:71:GLU:HB3 | 1:L:80:LYS:HD2 | 1.43 | 1.00 |
| 1:E:313:TYR:CD1 | 1:E:332:VAL:HG22 | 1.94 | 1.00 |
| 1:D:80:LYS:HD2 | 1:F:71:GLU:HB3 | 1.44 | 1.00 |
| 1:A:71:GLU:HB3 | 1:B:80:LYS:HD2 | 1.39 | 1.00 |
| 1:B:71:GLU:HB3 | 1:C:80:LYS:HD2 | 1.40 | 0.99 |
| 1:J:80:LYS:HD2 | 1:L:71:GLU:HB3 | 1.41 | 0.99 |
| 1:E:71:GLU:HB3 | 1:F:80:LYS:HD2 | 1.41 | 0.98 |
| 1:E:165:THR:HG22 | 1:E:167:ARG:H | 1.30 | 0.97 |
| 1:D:165:THR:HG22 | 1:D:167:ARG:H | 1.29 | 0.96 |
| 1:C:165:THR:HG22 | 1:C:167:ARG:H | 1.30 | 0.96 |
| 1:B:165:THR:HG22 | 1:B:167:ARG:H | 1.29 | 0.95 |
| 1:J:165:THR:HG22 | 1:J:167:ARG:H | 1.30 | 0.95 |
| 1:F:165:THR:HG22 | 1:F:167:ARG:H | 1.30 | 0.95 |
| 1:K:165:THR:HG22 | 1:K:167:ARG:H | 1.28 | 0.94 |
| 1:A:165:THR:HG22 | 1:A:167:ARG:H | 1.30 | 0.94 |
| 1:L:165:THR:HG22 | 1:L:167:ARG:H | 1.27 | 0.94 |
| 1:I:165:THR:HG22 | 1:I:167:ARG:H | 1.29 | 0.94 |
| 1:G:165:THR:HG22 | 1:G:167:ARG:H | 1.31 | 0.92 |
| 1:H:165:THR:HG22 | 1:H:167:ARG:H | 1.31 | 0.92 |
| 1:A:321:ASP:CG | 1:J:287:GLY:HA2 | 1.91 | 0.91 |
| 1:B:287:GLY:CA | 1:L:321:ASP:CG | 2.39 | 0.91 |
| 1:I:27:ASN:HD22 | 1:I:29:GLU:HB2 | 1.36 | 0.90 |
| 1:A:321:ASP:CG | 1:J:287:GLY:CA | 2.41 | 0.89 |
| 1:L:165:THR:HG22 | 1:L:167:ARG:N | 1.87 | 0.89 |
| 1:A:165:THR:HG22 | 1:A:167:ARG:N | 1.89 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:287:GLY:CA | 1:K:321:ASP:CG | 2.42 | 0.88 |
| 1:F:165:THR:HG22 | 1:F:167:ARG:N | 1.89 | 0.88 |
| 1:K:165:THR:HG22 | 1:K:167:ARG:N | 1.88 | 0.88 |
| 1:E:165:THR:HG22 | 1:E:167:ARG:N | 1.89 | 0.87 |
| 1:B:279:LYS:HE3 | 1:B:281:LYS:HZ2 | 1.39 | 0.87 |
| 1:C:165:THR:HG22 | 1:C:167:ARG:N | 1.89 | 0.87 |
| 1:A:309:THR:HG22 | 1:A:336:ILE:HA | 1.57 | 0.87 |
| 1:E:287:GLY:CA | 1:I:321:ASP:CG | 2.42 | 0.87 |
| 1:D:165:THR:HG22 | 1:D:167:ARG:N | 1.89 | 0.87 |
| 1:C:313:TYR:HD1 | 1:C:332:VAL:HG22 | 1.40 | 0.86 |
| 1:J:165:THR:HG22 | 1:J:167:ARG:N | 1.89 | 0.86 |
| 1:B:165:THR:HG22 | 1:B:167:ARG:N | 1.89 | 0.86 |
| 1:G:165:THR:HG22 | 1:G:167:ARG:N | 1.90 | 0.86 |
| 1:H:321:ASP:CG | 1:L:287:GLY:CA | 2.44 | 0.85 |
| 1:H:165:THR:HG22 | 1:H:167:ARG:N | 1.90 | 0.85 |
| 1:H:279:LYS:HE3 | 1:H:281:LYS:HZ2 | 1.38 | 0.85 |
| 1:I:165:THR:HG22 | 1:I:167:ARG:N | 1.88 | 0.85 |
| 1:J:309:THR:HG22 | 1:J:336:ILE:HA | 1.58 | 0.85 |
| 1:I:279:LYS:HE3 | 1:I:281:LYS:HZ2 | 1.40 | 0.85 |
| 1:G:313:TYR:HD1 | 1:G:332:VAL:HG22 | 1.40 | 0.85 |
| 1:K:313:TYR:HD1 | 1:K:332:VAL:HG22 | 1.40 | 0.85 |
| 1:F:309:THR:HG22 | 1:F:336:ILE:HA | 1.59 | 0.85 |
| 1:K:279:LYS:HE3 | 1:K:281:LYS:HZ2 | 1.42 | 0.85 |
| 1:C:309:THR:HG22 | 1:C:336:ILE:HA | 1.59 | 0.84 |
| 1:K:71:GLU:HG3 | 1:L:100:ARG:NH2 | 1.91 | 0.84 |
| 1:G:309:THR:HG22 | 1:G:336:ILE:HA | 1.58 | 0.84 |
| 1:D:309:THR:HG22 | 1:D:336:ILE:HA | 1.57 | 0.84 |
| 1:J:313:TYR:HD1 | 1:J:332:VAL:HG22 | 1.39 | 0.84 |
| 1:L:286:ILE:HG21 | 1:L:289:VAL:HG21 | 1.58 | 0.84 |
| 1:A:313:TYR:HD1 | 1:A:332:VAL:HG22 | 1.40 | 0.84 |
| 1:B:309:THR:HG22 | 1:B:336:ILE:HA | 1.58 | 0.84 |
| 1:E:279:LYS:HE3 | 1:E:281:LYS:HZ2 | 1.42 | 0.84 |
| 1:E:286:ILE:HG21 | 1:E:289:VAL:HG21 | 1.60 | 0.84 |
| 1:F:286:ILE:HG21 | 1:F:289:VAL:HG21 | 1.60 | 0.83 |
| 1:L:279:LYS:HE3 | 1:L:281:LYS:HZ2 | 1.41 | 0.83 |
| 1:F:313:TYR:HD1 | 1:F:332:VAL:HG22 | 1.41 | 0.83 |
| 1:E:313:TYR:HD1 | 1:E:332:VAL:HG22 | 1.41 | 0.83 |
| 1:F:279:LYS:HE3 | 1:F:281:LYS:HZ2 | 1.41 | 0.83 |
| 1:B:287:GLY:HA2 | 1:L:321:ASP:CG | 1.96 | 0.83 |
| 1:K:309:THR:HG22 | 1:K:336:ILE:HA | 1.60 | 0.83 |
| 1:K:286:ILE:HG21 | 1:K:289:VAL:HG21 | 1.59 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:100:ARG:NH2 | 1:F:71:GLU:HG3 | 1.94 | 0.83 |
| 1:H:309:THR:HG22 | 1:H:336:ILE:HA | 1.60 | 0.83 |
| 1:K:31:SER:HA | 1:K:329:ASP:HB2 | 1.61 | 0.82 |
| 1:I:313:TYR:HD1 | 1:I:332:VAL:HG22 | 1.40 | 0.82 |
| 1:E:309:THR:HG22 | 1:E:336:ILE:HA | 1.59 | 0.82 |
| 1:H:111:TYR:CZ | 1:H:188:VAL:CG2 | 2.63 | 0.82 |
| 1:I:309:THR:HG22 | 1:I:336:ILE:HA | 1.61 | 0.82 |
| 1:C:31:SER:HA | 1:C:329:ASP:HB2 | 1.62 | 0.82 |
| 1:G:279:LYS:HE3 | 1:G:281:LYS:HZ2 | 1.45 | 0.82 |
| 1:H:313:TYR:HD1 | 1:H:332:VAL:HG22 | 1.39 | 0.82 |
| 1:L:309:THR:HG22 | 1:L:336:ILE:HA | 1.61 | 0.82 |
| 1:G:31:SER:HA | 1:G:329:ASP:HB2 | 1.62 | 0.81 |
| 1:I:286:ILE:HG21 | 1:I:289:VAL:HG21 | 1.59 | 0.81 |
| 1:J:286:ILE:HG21 | 1:J:289:VAL:HG21 | 1.61 | 0.81 |
| 1:H:321:ASP:CG | 1:L:287:GLY:HA2 | 1.99 | 0.81 |
| 1:D:321:ASP:CG | 1:G:287:GLY:CA | 2.48 | 0.81 |
| 1:H:31:SER:HA | 1:H:329:ASP:HB2 | 1.61 | 0.81 |
| 1:E:31:SER:HA | 1:E:329:ASP:HB2 | 1.61 | 0.81 |
| 1:B:286:ILE:HG21 | 1:B:289:VAL:HG21 | 1.61 | 0.81 |
| 1:C:286:ILE:HG21 | 1:C:289:VAL:HG21 | 1.61 | 0.81 |
| 1:J:31:SER:HA | 1:J:329:ASP:HB2 | 1.63 | 0.81 |
| 1:C:287:GLY:HA3 | 1:G:321:ASP:OD1 | 1.79 | 0.81 |
| 1:B:313:TYR:HD1 | 1:B:332:VAL:HG22 | 1.40 | 0.81 |
| 1:I:27:ASN:ND2 | 1:I:29:GLU:HB2 | 1.96 | 0.81 |
| 1:I:287:GLY:HA3 | 1:K:321:ASP:CG | 2.01 | 0.81 |
| 1:G:286:ILE:HG21 | 1:G:289:VAL:HG21 | 1.63 | 0.81 |
| 1:D:31:SER:HA | 1:D:329:ASP:HB2 | 1.63 | 0.81 |
| 1:A:286:ILE:HG21 | 1:A:289:VAL:HG21 | 1.63 | 0.80 |
| 1:B:71:GLU:HG3 | 1:C:100:ARG:NH2 | 1.96 | 0.80 |
| 1:H:286:ILE:HG21 | 1:H:289:VAL:HG21 | 1.61 | 0.80 |
| 1:J:279:LYS:HE3 | 1:J:281:LYS:HZ2 | 1.43 | 0.80 |
| 1:G:111:TYR:CZ | 1:G:188:VAL:CG2 | 2.64 | 0.80 |
| 1:B:31:SER:HA | 1:B:329:ASP:HB2 | 1.63 | 0.80 |
| 1:L:111:TYR:CZ | 1:L:188:VAL:CG2 | 2.64 | 0.80 |
| 1:J:71:GLU:HG3 | 1:K:100:ARG:NH2 | 1.96 | 0.80 |
| 1:I:111:TYR:CZ | 1:I:188:VAL:CG2 | 2.65 | 0.80 |
| 1:K:111:TYR:CZ | 1:K:188:VAL:CG2 | 2.65 | 0.80 |
| 1:F:31:SER:HA | 1:F:329:ASP:HB2 | 1.63 | 0.80 |
| 1:C:279:LYS:HE3 | 1:C:281:LYS:HZ2 | 1.46 | 0.80 |
| 1:L:31:SER:HA | 1:L:329:ASP:HB2 | 1.62 | 0.80 |
| 1:C:111:TYR:CZ | 1:C:188:VAL:CG2 | 2.64 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:313:TYR:HD1 | 1:L:332:VAL:HG22 | 1.39 | 0.79 |
| 1:A:31:SER:HA | 1:A:329:ASP:HB2 | 1.63 | 0.79 |
| 1:E:111:TYR:CZ | 1:E:188:VAL:CG2 | 2.66 | 0.79 |
| 1:D:286:ILE:HG21 | 1:D:289:VAL:HG21 | 1.62 | 0.79 |
| 1:B:111:TYR:CZ | 1:B:188:VAL:CG2 | 2.67 | 0.78 |
| 1:A:111:TYR:CZ | 1:A:188:VAL:CG2 | 2.65 | 0.78 |
| 1:I:31:SER:HA | 1:I:329:ASP:HB2 | 1.63 | 0.78 |
| 1:J:111:TYR:CZ | 1:J:188:VAL:CG2 | 2.66 | 0.78 |
| 1:B:287:GLY:HA3 | 1:L:321:ASP:CG | 2.01 | 0.78 |
| 1:E:321:ASP:OD1 | 1:K:287:GLY:HA3 | 1.81 | 0.78 |
| 1:E:287:GLY:HA3 | 1:I:321:ASP:CG | 2.03 | 0.78 |
| 1:F:111:TYR:CZ | 1:F:188:VAL:CG2 | 2.66 | 0.78 |
| 1:D:321:ASP:CG | 1:G:287:GLY:HA2 | 2.03 | 0.78 |
| 1:D:313:TYR:HD1 | 1:D:332:VAL:HG22 | 1.44 | 0.78 |
| 1:A:279:LYS:HE3 | 1:A:281:LYS:HZ2 | 1.48 | 0.77 |
| 1:D:279:LYS:HE3 | 1:D:281:LYS:HZ2 | 1.47 | 0.77 |
| 1:H:321:ASP:CG | 1:L:287:GLY:HA3 | 2.05 | 0.77 |
| 1:D:111:TYR:CZ | 1:D:188:VAL:CG2 | 2.68 | 0.77 |
| 1:E:287:GLY:HA2 | 1:I:321:ASP:CG | 2.00 | 0.76 |
| 1:C:321:ASP:CG | 1:D:287:GLY:CA | 2.53 | 0.76 |
| 1:G:160:LYS:HD3 | 1:G:162:GLU:OE2 | 1.86 | 0.76 |
| 1:H:160:LYS:HD3 | 1:H:162:GLU:OE2 | 1.86 | 0.76 |
| 1:H:279:LYS:HE3 | 1:H:281:LYS:NZ | 2.01 | 0.76 |
| 1:H:313:TYR:CD1 | 1:H:332:VAL:CG2 | 2.69 | 0.75 |
| 1:I:313:TYR:CD1 | 1:I:332:VAL:CG2 | 2.70 | 0.75 |
| 1:K:313:TYR:CD1 | 1:K:332:VAL:CG2 | 2.70 | 0.75 |
| 1:C:160:LYS:HD3 | 1:C:162:GLU:OE2 | 1.86 | 0.75 |
| 1:D:160:LYS:HD3 | 1:D:162:GLU:OE2 | 1.86 | 0.75 |
| 1:A:321:ASP:CG | 1:J:287:GLY:HA3 | 2.07 | 0.75 |
| 1:J:313:TYR:CD1 | 1:J:332:VAL:CG2 | 2.70 | 0.75 |
| 1:G:279:LYS:HE3 | 1:G:281:LYS:NZ | 2.02 | 0.75 |
| 1:L:160:LYS:HD3 | 1:L:162:GLU:OE2 | 1.86 | 0.74 |
| 1:K:160:LYS:HD3 | 1:K:162:GLU:OE2 | 1.87 | 0.74 |
| 1:J:160:LYS:HD3 | 1:J:162:GLU:OE2 | 1.87 | 0.74 |
| 1:L:313:TYR:CD1 | 1:L:332:VAL:CG2 | 2.69 | 0.74 |
| 1:E:71:GLU:HG3 | 1:F:100:ARG:NH2 | 2.03 | 0.74 |
| 1:E:313:TYR:CD1 | 1:E:332:VAL:CG2 | 2.71 | 0.74 |
| 1:E:160:LYS:HD3 | 1:E:162:GLU:OE2 | 1.88 | 0.74 |
| 1:A:160:LYS:HD3 | 1:A:162:GLU:OE2 | 1.87 | 0.74 |
| 1:A:279:LYS:HE3 | 1:A:281:LYS:NZ | 2.02 | 0.74 |
| 1:A:287:GLY:HA2 | 1:F:321:ASP:CG | 2.08 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:313:TYR:CD1 | 1:C:332:VAL:CG2 | 2.70 | 0.73 |
| 1:L:286:ILE:HG21 | 1:L:289:VAL:CG2 | 2.18 | 0.73 |
| 1:A:287:GLY:CA | 1:F:321:ASP:CG | 2.56 | 0.73 |
| 1:F:160:LYS:HD3 | 1:F:162:GLU:OE2 | 1.88 | 0.73 |
| 1:B:160:LYS:HD3 | 1:B:162:GLU:OE2 | 1.87 | 0.73 |
| 1:I:286:ILE:CG2 | 1:I:289:VAL:CG2 | 2.67 | 0.73 |
| 1:C:279:LYS:HE3 | 1:C:281:LYS:NZ | 2.03 | 0.73 |
| 1:D:279:LYS:HE3 | 1:D:281:LYS:NZ | 2.04 | 0.73 |
| 1:K:279:LYS:HE3 | 1:K:281:LYS:NZ | 2.03 | 0.73 |
| 1:I:279:LYS:HE3 | 1:I:281:LYS:NZ | 2.04 | 0.73 |
| 1:F:286:ILE:N | 1:F:286:ILE:HD12 | 2.02 | 0.73 |
| 1:L:279:LYS:HE3 | 1:L:281:LYS:NZ | 2.02 | 0.73 |
| 1:A:313:TYR:CD1 | 1:A:332:VAL:CG2 | 2.71 | 0.73 |
| 1:J:100:ARG:NH2 | 1:L:71:GLU:HG3 | 2.04 | 0.73 |
| 1:E:286:ILE:HD12 | 1:E:286:ILE:N | 2.03 | 0.73 |
| 1:E:279:LYS:HE3 | 1:E:281:LYS:NZ | 2.03 | 0.73 |
| 1:B:313:TYR:CD1 | 1:B:332:VAL:CG2 | 2.71 | 0.72 |
| 1:H:286:ILE:N | 1:H:286:ILE:HD12 | 2.04 | 0.72 |
| 1:H:71:GLU:HG3 | 1:I:100:ARG:NH2 | 2.04 | 0.72 |
| 1:L:286:ILE:CG2 | 1:L:289:VAL:CG2 | 2.66 | 0.72 |
| 1:J:279:LYS:HE3 | 1:J:281:LYS:NZ | 2.02 | 0.72 |
| 1:K:286:ILE:HG21 | 1:K:289:VAL:CG2 | 2.19 | 0.72 |
| 1:B:279:LYS:HE3 | 1:B:281:LYS:NZ | 2.04 | 0.72 |
| 1:K:286:ILE:CG2 | 1:K:289:VAL:CG2 | 2.68 | 0.72 |
| 1:I:286:ILE:N | 1:I:286:ILE:HD12 | 2.05 | 0.72 |
| 1:D:321:ASP:CG | 1:G:287:GLY:HA3 | 2.10 | 0.72 |
| 1:A:100:ARG:NH2 | 1:C:71:GLU:HG3 | 2.05 | 0.72 |
| 1:J:286:ILE:HD12 | 1:J:286:ILE:N | 2.05 | 0.72 |
| 1:D:313:TYR:CD1 | 1:D:332:VAL:CG2 | 2.73 | 0.72 |
| 1:I:286:ILE:HG21 | 1:I:289:VAL:CG2 | 2.19 | 0.72 |
| 1:I:160:LYS:HD3 | 1:I:162:GLU:OE2 | 1.88 | 0.72 |
| 1:G:313:TYR:CD1 | 1:G:332:VAL:CG2 | 2.70 | 0.71 |
| 1:F:279:LYS:HE3 | 1:F:281:LYS:NZ | 2.04 | 0.71 |
| 1:F:313:TYR:CD1 | 1:F:332:VAL:CG2 | 2.71 | 0.71 |
| 1:A:286:ILE:HD12 | 1:A:286:ILE:N | 2.04 | 0.71 |
| 1:C:111:TYR:OH | 1:C:188:VAL:CG2 | 2.38 | 0.71 |
| 1:L:111:TYR:OH | 1:L:188:VAL:CG2 | 2.39 | 0.71 |
| 1:K:111:TYR:OH | 1:K:188:VAL:CG2 | 2.39 | 0.71 |
| 1:D:286:ILE:N | 1:D:286:ILE:HD12 | 2.05 | 0.71 |
| 1:F:286:ILE:HG21 | 1:F:289:VAL:CG2 | 2.21 | 0.71 |
| 1:B:286:ILE:HD12 | 1:B:286:ILE:N | 2.04 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:286:ILE:HD12 | 1:L:286:ILE:N | 2.05 | 0.71 |
| 1:F:286:ILE:CG2 | 1:F:289:VAL:CG2 | 2.69 | 0.71 |
| 1:G:100:ARG:NH2 | 1:I:71:GLU:HG3 | 2.06 | 0.71 |
| 1:K:286:ILE:N | 1:K:286:ILE:HD12 | 2.04 | 0.71 |
| 1:G:286:ILE:HD12 | 1:G:286:ILE:N | 2.06 | 0.71 |
| 1:H:111:TYR:OH | 1:H:188:VAL:CG2 | 2.38 | 0.70 |
| 1:G:51:ILE:HD13 | 1:I:303:PHE:HB3 | 1.73 | 0.70 |
| 1:H:286:ILE:CG2 | 1:H:289:VAL:CG2 | 2.69 | 0.70 |
| 1:G:111:TYR:OH | 1:G:188:VAL:CG2 | 2.40 | 0.70 |
| 1:C:111:TYR:CZ | 1:C:188:VAL:HG21 | 2.27 | 0.70 |
| 1:A:71:GLU:HG3 | 1:B:100:ARG:NH2 | 2.07 | 0.70 |
| 1:A:111:TYR:OH | 1:A:188:VAL:CG2 | 2.39 | 0.70 |
| 1:E:286:ILE:CG2 | 1:E:289:VAL:CG2 | 2.69 | 0.70 |
| 1:C:286:ILE:N | 1:C:286:ILE:HD12 | 2.06 | 0.70 |
| 1:H:286:ILE:HG21 | 1:H:289:VAL:CG2 | 2.21 | 0.70 |
| 1:F:287:GLY:HA3 | 1:J:321:ASP:OD1 | 1.87 | 0.70 |
| 1:J:286:ILE:HG21 | 1:J:289:VAL:CG2 | 2.21 | 0.70 |
| 1:C:286:ILE:HG21 | 1:C:289:VAL:CG2 | 2.21 | 0.70 |
| 1:E:244:PHE:CZ | 1:K:285:GLY:HA3 | 2.27 | 0.70 |
| 1:D:286:ILE:HG21 | 1:D:289:VAL:CG2 | 2.22 | 0.70 |
| 1:B:286:ILE:HG21 | 1:B:289:VAL:CG2 | 2.21 | 0.69 |
| 1:C:286:ILE:CG2 | 1:C:289:VAL:CG2 | 2.70 | 0.69 |
| 1:C:321:ASP:CG | 1:D:287:GLY:HA3 | 2.13 | 0.69 |
| 1:E:286:ILE:HG21 | 1:E:289:VAL:CG2 | 2.21 | 0.69 |
| 1:D:286:ILE:CG2 | 1:D:289:VAL:CG2 | 2.70 | 0.69 |
| 1:F:287:GLY:CA | 1:J:321:ASP:CG | 2.61 | 0.69 |
| 1:H:111:TYR:CZ | 1:H:188:VAL:HG21 | 2.26 | 0.69 |
| 1:B:286:ILE:CG2 | 1:B:289:VAL:CG2 | 2.70 | 0.69 |
| 1:B:111:TYR:OH | 1:B:188:VAL:CG2 | 2.41 | 0.69 |
| 1:J:286:ILE:CG2 | 1:J:289:VAL:CG2 | 2.70 | 0.69 |
| 1:G:111:TYR:CZ | 1:G:188:VAL:HG21 | 2.27 | 0.69 |
| 1:A:111:TYR:CZ | 1:A:188:VAL:HG21 | 2.28 | 0.69 |
| 1:J:111:TYR:OH | 1:J:188:VAL:CG2 | 2.40 | 0.69 |
| 1:A:286:ILE:CG2 | 1:A:289:VAL:CG2 | 2.71 | 0.69 |
| 1:E:111:TYR:CZ | 1:E:188:VAL:HG21 | 2.28 | 0.68 |
| 1:I:111:TYR:CZ | 1:I:188:VAL:HG21 | 2.28 | 0.68 |
| 1:A:286:ILE:HG21 | 1:A:289:VAL:CG2 | 2.23 | 0.68 |
| 1:I:111:TYR:OH | 1:I:188:VAL:CG2 | 2.41 | 0.68 |
| 1:H:111:TYR:CZ | 1:H:188:VAL:HG23 | 2.28 | 0.68 |
| 1:B:111:TYR:CZ | 1:B:188:VAL:HG21 | 2.29 | 0.68 |
| 1:E:111:TYR:OH | 1:E:188:VAL:CG2 | 2.41 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:286:ILE:CG2 | 1:G:289:VAL:CG2 | 2.71 | 0.68 |
| 1:G:286:ILE:HG21 | 1:G:289:VAL:CG2 | 2.22 | 0.68 |
| 1:I:128:PHE:O | 1:I:133:VAL:HG11 | 1.94 | 0.68 |
| 1:F:111:TYR:OH | 1:F:188:VAL:CG2 | 2.42 | 0.68 |
| 1:I:111:TYR:CZ | 1:I:188:VAL:HG23 | 2.29 | 0.68 |
| 1:F:111:TYR:CZ | 1:F:188:VAL:HG21 | 2.28 | 0.68 |
| 1:K:111:TYR:CZ | 1:K:188:VAL:HG21 | 2.28 | 0.68 |
| 1:F:287:GLY:HA3 | 1:J:321:ASP:CG | 2.15 | 0.67 |
| 1:L:111:TYR:CZ | 1:L:188:VAL:HG21 | 2.28 | 0.67 |
| 1:G:47:GLY:HA3 | 1:I:338:TYR:CZ | 2.28 | 0.67 |
| 1:C:174:VAL:HG12 | 1:C:175:GLY:N | 2.10 | 0.67 |
| 1:L:111:TYR:CZ | 1:L:188:VAL:HG23 | 2.29 | 0.67 |
| 1:I:286:ILE:HG22 | 1:I:289:VAL:HG22 | 1.75 | 0.67 |
| 1:L:286:ILE:HG22 | 1:L:289:VAL:HG22 | 1.76 | 0.67 |
| 1:B:128:PHE:O | 1:B:133:VAL:HG11 | 1.94 | 0.67 |
| 1:G:128:PHE:O | 1:G:133:VAL:HG11 | 1.94 | 0.67 |
| 1:K:128:PHE:O | 1:K:133:VAL:HG11 | 1.94 | 0.67 |
| 1:E:244:PHE:CZ | 1:K:285:GLY:CA | 2.77 | 0.67 |
| 1:K:111:TYR:CZ | 1:K:188:VAL:HG23 | 2.29 | 0.67 |
| 1:J:128:PHE:O | 1:J:133:VAL:HG11 | 1.95 | 0.67 |
| 1:D:71:GLU:HG3 | 1:E:100:ARG:NH2 | 2.10 | 0.67 |
| 1:K:286:ILE:HG22 | 1:K:289:VAL:HG22 | 1.77 | 0.67 |
| 1:B:287:GLY:HA3 | 1:L:321:ASP:OD2 | 1.94 | 0.66 |
| 1:C:287:GLY:HA3 | 1:G:321:ASP:CG | 2.15 | 0.66 |
| 1:D:174:VAL:HG12 | 1:D:175:GLY:N | 2.10 | 0.66 |
| 1:C:128:PHE:O | 1:C:133:VAL:HG11 | 1.96 | 0.66 |
| 1:G:71:GLU:HG3 | 1:H:100:ARG:NH2 | 2.10 | 0.66 |
| 1:J:111:TYR:CZ | 1:J:188:VAL:HG21 | 2.28 | 0.66 |
| 1:D:128:PHE:O | 1:D:133:VAL:HG11 | 1.94 | 0.66 |
| 1:H:262:GLN:OE1 | 1:H:270:ARG:NH1 | 2.29 | 0.66 |
| 1:K:174:VAL:HG12 | 1:K:175:GLY:N | 2.11 | 0.66 |
| 1:D:111:TYR:CZ | 1:D:188:VAL:HG21 | 2.31 | 0.66 |
| 1:E:111:TYR:CZ | 1:E:188:VAL:HG23 | 2.31 | 0.66 |
| 1:E:174:VAL:HG12 | 1:E:175:GLY:N | 2.10 | 0.66 |
| 1:E:321:ASP:CG | 1:K:287:GLY:HA3 | 2.16 | 0.66 |
| 1:G:111:TYR:CZ | 1:G:188:VAL:HG23 | 2.29 | 0.66 |
| 1:G:338:TYR:CZ | 1:H:47:GLY:HA3 | 2.31 | 0.66 |
| 1:J:174:VAL:HG12 | 1:J:175:GLY:N | 2.11 | 0.66 |
| 1:F:286:ILE:HG22 | 1:F:289:VAL:HG22 | 1.77 | 0.66 |
| 1:C:111:TYR:CZ | 1:C:188:VAL:HG23 | 2.30 | 0.66 |
| 1:D:111:TYR:OH | 1:D:188:VAL:CG2 | 2.43 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:128:PHE:O | 1:E:133:VAL:HG11 | 1.95 | 0.66 |
| 1:F:128:PHE:O | 1:F:133:VAL:HG11 | 1.95 | 0.66 |
| 1:D:262:GLN:OE1 | 1:D:270:ARG:NH1 | 2.29 | 0.66 |
| 1:G:174:VAL:HG12 | 1:G:175:GLY:N | 2.11 | 0.66 |
| 1:E:205:LEU:HG | 1:E:247:THR:HG22 | 1.78 | 0.66 |
| 1:B:174:VAL:HG12 | 1:B:175:GLY:N | 2.11 | 0.66 |
| 1:A:128:PHE:O | 1:A:133:VAL:HG11 | 1.96 | 0.66 |
| 1:L:128:PHE:O | 1:L:133:VAL:HG11 | 1.96 | 0.65 |
| 1:F:286:ILE:HD12 | 1:F:286:ILE:H | 1.62 | 0.65 |
| 1:H:286:ILE:HG22 | 1:H:289:VAL:HG22 | 1.78 | 0.65 |
| 1:D:338:TYR:CZ | 1:E:47:GLY:HA3 | 2.31 | 0.65 |
| 1:C:262:GLN:OE1 | 1:C:270:ARG:NH1 | 2.30 | 0.65 |
| 1:J:262:GLN:OE1 | 1:J:270:ARG:NH1 | 2.28 | 0.65 |
| 1:C:285:GLY:HA3 | 1:G:244:PHE:CZ | 2.32 | 0.65 |
| 1:H:128:PHE:O | 1:H:133:VAL:HG11 | 1.95 | 0.65 |
| 1:D:191:TYR:HD1 | 1:D:214:TRP:HB3 | 1.62 | 0.65 |
| 1:E:262:GLN:OE1 | 1:E:270:ARG:NH1 | 2.30 | 0.65 |
| 1:J:286:ILE:HG22 | 1:J:289:VAL:HG22 | 1.79 | 0.65 |
| 1:C:286:ILE:HG22 | 1:C:289:VAL:HG22 | 1.79 | 0.65 |
| 1:B:111:TYR:CZ | 1:B:188:VAL:HG23 | 2.31 | 0.65 |
| 1:B:262:GLN:OE1 | 1:B:270:ARG:NH1 | 2.30 | 0.65 |
| 1:B:286:ILE:HG22 | 1:B:289:VAL:HG22 | 1.78 | 0.65 |
| 1:A:111:TYR:CZ | 1:A:188:VAL:HG23 | 2.30 | 0.65 |
| 1:L:265:PHE:HB3 | 1:L:267:PHE:CE1 | 2.32 | 0.65 |
| 1:B:205:LEU:HG | 1:B:247:THR:HG22 | 1.79 | 0.65 |
| 1:D:286:ILE:HG22 | 1:D:289:VAL:HG22 | 1.79 | 0.64 |
| 1:G:191:TYR:HD1 | 1:G:214:TRP:HB3 | 1.61 | 0.64 |
| 1:H:205:LEU:HG | 1:H:247:THR:HG22 | 1.79 | 0.64 |
| 1:J:191:TYR:HD1 | 1:J:214:TRP:HB3 | 1.62 | 0.64 |
| 1:F:262:GLN:OE1 | 1:F:270:ARG:NH1 | 2.30 | 0.64 |
| 1:F:223:ASN:O | 1:F:224:ASN:HB2 | 1.98 | 0.64 |
| 1:K:286:ILE:H | 1:K:286:ILE:HD12 | 1.63 | 0.64 |
| 1:J:111:TYR:CZ | 1:J:188:VAL:HG23 | 2.30 | 0.64 |
| 1:I:287:GLY:HA2 | 1:K:321:ASP:CG | 2.00 | 0.64 |
| 1:E:286:ILE:HG22 | 1:E:289:VAL:HG22 | 1.78 | 0.64 |
| 1:I:191:TYR:HD1 | 1:I:214:TRP:HB3 | 1.63 | 0.64 |
| 1:F:174:VAL:HG12 | 1:F:175:GLY:N | 2.12 | 0.64 |
| 1:L:262:GLN:OE1 | 1:L:270:ARG:NH1 | 2.31 | 0.64 |
| 1:H:265:PHE:HB3 | 1:H:267:PHE:CE1 | 2.32 | 0.64 |
| 1:A:47:GLY:HA3 | 1:C:338:TYR:CZ | 2.33 | 0.64 |
| 1:C:191:TYR:HD1 | 1:C:214:TRP:HB3 | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:262:GLN:OE1 | 1:A:270:ARG:NH1 | 2.30 | 0.64 |
| 1:G:262:GLN:OE1 | 1:G:270:ARG:NH1 | 2.30 | 0.64 |
| 1:L:286:ILE:CG2 | 1:L:289:VAL:HG22 | 2.28 | 0.64 |
| 1:L:174:VAL:HG12 | 1:L:175:GLY:N | 2.11 | 0.64 |
| 1:F:144:PHE:HB2 | 1:F:151:LEU:HD23 | 1.79 | 0.64 |
| 1:L:191:TYR:HD1 | 1:L:214:TRP:HB3 | 1.62 | 0.64 |
| 1:D:111:TYR:CZ | 1:D:188:VAL:HG23 | 2.33 | 0.64 |
| 1:A:174:VAL:HG12 | 1:A:175:GLY:N | 2.11 | 0.64 |
| 1:H:174:VAL:HG12 | 1:H:175:GLY:N | 2.12 | 0.64 |
| 1:A:191:TYR:HD1 | 1:A:214:TRP:HB3 | 1.62 | 0.64 |
| 1:K:262:GLN:OE1 | 1:K:270:ARG:NH1 | 2.31 | 0.64 |
| 1:A:286:ILE:HG22 | 1:A:289:VAL:HG22 | 1.79 | 0.64 |
| 1:H:144:PHE:HB2 | 1:H:151:LEU:HD23 | 1.80 | 0.64 |
| 1:B:144:PHE:HB2 | 1:B:151:LEU:HD23 | 1.79 | 0.64 |
| 1:I:174:VAL:HG12 | 1:I:175:GLY:N | 2.12 | 0.64 |
| 1:I:286:ILE:CG2 | 1:I:289:VAL:HG21 | 2.28 | 0.64 |
| 1:H:191:TYR:HD1 | 1:H:214:TRP:HB3 | 1.62 | 0.64 |
| 1:B:191:TYR:HD1 | 1:B:214:TRP:HB3 | 1.63 | 0.64 |
| 1:C:144:PHE:HB2 | 1:C:151:LEU:HD23 | 1.81 | 0.63 |
| 1:E:191:TYR:HD1 | 1:E:214:TRP:HB3 | 1.62 | 0.63 |
| 1:I:262:GLN:OE1 | 1:I:270:ARG:NH1 | 2.31 | 0.63 |
| 1:D:205:LEU:HG | 1:D:247:THR:HG22 | 1.80 | 0.63 |
| 1:F:191:TYR:HD1 | 1:F:214:TRP:HB3 | 1.63 | 0.63 |
| 1:G:286:ILE:HG22 | 1:G:289:VAL:HG22 | 1.79 | 0.63 |
| 1:F:111:TYR:CZ | 1:F:188:VAL:HG23 | 2.31 | 0.63 |
| 1:E:265:PHE:HB3 | 1:E:267:PHE:CE1 | 2.33 | 0.63 |
| 1:K:191:TYR:HD1 | 1:K:214:TRP:HB3 | 1.63 | 0.63 |
| 1:K:265:PHE:HB3 | 1:K:267:PHE:CE1 | 2.33 | 0.63 |
| 1:B:303:PHE:HB3 | 1:C:51:ILE:HD13 | 1.79 | 0.63 |
| 1:I:165:THR:HG21 | 1:I:167:ARG:HB3 | 1.81 | 0.63 |
| 1:I:286:ILE:CG2 | 1:I:289:VAL:HG22 | 2.28 | 0.63 |
| 1:G:205:LEU:HG | 1:G:247:THR:HG22 | 1.80 | 0.63 |
| 1:A:287:GLY:HA3 | 1:F:321:ASP:CG | 2.19 | 0.63 |
| 1:F:265:PHE:HB3 | 1:F:267:PHE:CE1 | 2.33 | 0.63 |
| 1:L:205:LEU:HG | 1:L:247:THR:HG22 | 1.80 | 0.63 |
| 1:K:286:ILE:CG2 | 1:K:289:VAL:HG22 | 2.29 | 0.63 |
| 1:G:144:PHE:HB2 | 1:G:151:LEU:HD23 | 1.81 | 0.63 |
| 1:A:144:PHE:HB2 | 1:A:151:LEU:HD23 | 1.80 | 0.63 |
| 1:G:18:VAL:HG13 | 1:G:337:VAL:HG22 | 1.80 | 0.63 |
| 1:K:18:VAL:HG13 | 1:K:337:VAL:HG22 | 1.81 | 0.63 |
| 1:J:18:VAL:HG13 | 1:J:337:VAL:HG22 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:165:THR:HG21 | 1:K:167:ARG:HB3 | 1.81 | 0.63 |
| 1:I:144:PHE:HB2 | 1:I:151:LEU:HD23 | 1.80 | 0.63 |
| 1:J:265:PHE:HB3 | 1:J:267:PHE:CE1 | 2.33 | 0.63 |
| 1:J:47:GLY:HA3 | 1:L:338:TYR:CZ | 2.34 | 0.62 |
| 1:C:205:LEU:HG | 1:C:247:THR:HG22 | 1.81 | 0.62 |
| 1:D:144:PHE:HB2 | 1:D:151:LEU:HD23 | 1.80 | 0.62 |
| 1:C:265:PHE:HB3 | 1:C:267:PHE:CE1 | 2.34 | 0.62 |
| 1:D:303:PHE:HB3 | 1:E:51:ILE:HD13 | 1.81 | 0.62 |
| 1:A:265:PHE:HB3 | 1:A:267:PHE:CE1 | 2.34 | 0.62 |
| 1:A:18:VAL:HG13 | 1:A:337:VAL:HG22 | 1.80 | 0.62 |
| 1:I:265:PHE:HB3 | 1:I:267:PHE:CE1 | 2.34 | 0.62 |
| 1:L:223:ASN:O | 1:L:224:ASN:HB2 | 1.99 | 0.62 |
| 1:J:144:PHE:HB2 | 1:J:151:LEU:HD23 | 1.81 | 0.62 |
| 1:I:223:ASN:O | 1:I:224:ASN:HB2 | 2.00 | 0.62 |
| 1:G:265:PHE:HB3 | 1:G:267:PHE:CE1 | 2.34 | 0.62 |
| 1:B:18:VAL:HG13 | 1:B:337:VAL:HG22 | 1.82 | 0.62 |
| 1:D:51:ILE:HD13 | 1:F:303:PHE:HB3 | 1.81 | 0.62 |
| 1:B:286:ILE:HD12 | 1:B:286:ILE:H | 1.63 | 0.62 |
| 1:A:286:ILE:H | 1:A:286:ILE:HD12 | 1.65 | 0.62 |
| 1:B:265:PHE:HB3 | 1:B:267:PHE:CE1 | 2.34 | 0.62 |
| 1:H:296:GLU:OE2 | 1:H:312:ASP:OD1 | 2.18 | 0.62 |
| 1:L:286:ILE:HD12 | 1:L:286:ILE:H | 1.64 | 0.62 |
| 1:E:303:PHE:HB3 | 1:F:51:ILE:HD13 | 1.80 | 0.62 |
| 1:A:205:LEU:HG | 1:A:247:THR:HG22 | 1.81 | 0.62 |
| 1:E:205:LEU:HG | 1:E:247:THR:CG2 | 2.30 | 0.62 |
| 1:L:18:VAL:HG13 | 1:L:337:VAL:HG22 | 1.82 | 0.62 |
| 1:B:338:TYR:CZ | 1:C:47:GLY:HA3 | 2.35 | 0.62 |
| 1:K:144:PHE:HB2 | 1:K:151:LEU:HD23 | 1.81 | 0.62 |
| 1:B:205:LEU:HG | 1:B:247:THR:CG2 | 2.30 | 0.62 |
| 1:L:144:PHE:HB2 | 1:L:151:LEU:HD23 | 1.80 | 0.62 |
| 1:G:296:GLU:OE2 | 1:G:312:ASP:OD1 | 2.18 | 0.62 |
| 1:F:285:GLY:HA3 | 1:J:244:PHE:CZ | 2.35 | 0.62 |
| 1:L:165:THR:HG21 | 1:L:167:ARG:HB3 | 1.82 | 0.61 |
| 1:I:205:LEU:HG | 1:I:247:THR:HG22 | 1.80 | 0.61 |
| 1:K:205:LEU:HG | 1:K:247:THR:HG22 | 1.82 | 0.61 |
| 1:D:18:VAL:HG13 | 1:D:337:VAL:HG22 | 1.81 | 0.61 |
| 1:D:100:ARG:HH21 | 1:F:71:GLU:HG3 | 1.65 | 0.61 |
| 1:G:286:ILE:HD12 | 1:G:286:ILE:H | 1.64 | 0.61 |
| 1:H:286:ILE:H | 1:H:286:ILE:HD12 | 1.63 | 0.61 |
| 1:E:223:ASN:O | 1:E:224:ASN:HB2 | 2.00 | 0.61 |
| 1:G:303:PHE:HB3 | 1:H:51:ILE:HD13 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:286:ILE:H | 1:E:286:ILE:HD12 | 1.63 | 0.61 |
| 1:G:205:LEU:HG | 1:G:247:THR:CG2 | 2.30 | 0.61 |
| 1:D:265:PHE:HB3 | 1:D:267:PHE:CE1 | 2.35 | 0.61 |
| 1:D:47:GLY:HA3 | 1:F:338:TYR:CZ | 2.36 | 0.61 |
| 1:F:18:VAL:HG13 | 1:F:337:VAL:HG22 | 1.81 | 0.61 |
| 1:B:165:THR:HG21 | 1:B:167:ARG:HB3 | 1.83 | 0.61 |
| 1:J:165:THR:HG21 | 1:J:167:ARG:HB3 | 1.83 | 0.61 |
| 1:B:223:ASN:O | 1:B:224:ASN:HB2 | 2.01 | 0.61 |
| 1:F:205:LEU:HG | 1:F:247:THR:HG22 | 1.82 | 0.61 |
| 1:E:287:GLY:HA3 | 1:I:321:ASP:OD2 | 2.00 | 0.61 |
| 1:B:71:GLU:HG3 | 1:C:100:ARG:HH21 | 1.65 | 0.61 |
| 1:J:296:GLU:OE2 | 1:J:312:ASP:OD1 | 2.19 | 0.61 |
| 1:F:286:ILE:CG2 | 1:F:289:VAL:HG22 | 2.30 | 0.61 |
| 1:D:205:LEU:HG | 1:D:247:THR:CG2 | 2.31 | 0.61 |
| 1:C:18:VAL:HG13 | 1:C:337:VAL:HG22 | 1.82 | 0.61 |
| 1:I:296:GLU:OE2 | 1:I:312:ASP:OD1 | 2.19 | 0.61 |
| 1:H:286:ILE:CG2 | 1:H:289:VAL:HG22 | 2.31 | 0.61 |
| 1:D:286:ILE:H | 1:D:286:ILE:HD12 | 1.64 | 0.61 |
| 1:L:205:LEU:HG | 1:L:247:THR:CG2 | 2.31 | 0.61 |
| 1:K:71:GLU:HG3 | 1:L:100:ARG:HH21 | 1.64 | 0.61 |
| 1:I:286:ILE:H | 1:I:286:ILE:HD12 | 1.64 | 0.61 |
| 1:J:286:ILE:CG2 | 1:J:289:VAL:HG22 | 2.31 | 0.61 |
| 1:B:286:ILE:CG2 | 1:B:289:VAL:HG21 | 2.30 | 0.61 |
| 1:J:51:ILE:HD13 | 1:L:303:PHE:HB3 | 1.82 | 0.61 |
| 1:G:165:THR:HG21 | 1:G:167:ARG:HB3 | 1.83 | 0.61 |
| 1:H:165:THR:HG21 | 1:H:167:ARG:HB3 | 1.83 | 0.61 |
| 1:H:18:VAL:HG13 | 1:H:337:VAL:HG22 | 1.83 | 0.61 |
| 1:E:338:TYR:CZ | 1:F:47:GLY:HA3 | 2.35 | 0.60 |
| 1:H:205:LEU:HG | 1:H:247:THR:CG2 | 2.30 | 0.60 |
| 1:K:223:ASN:O | 1:K:224:ASN:HB2 | 2.01 | 0.60 |
| 1:B:286:ILE:CG2 | 1:B:289:VAL:HG22 | 2.31 | 0.60 |
| 1:D:165:THR:HG21 | 1:D:167:ARG:HB3 | 1.83 | 0.60 |
| 1:C:286:ILE:CG2 | 1:C:289:VAL:HG22 | 2.31 | 0.60 |
| 1:G:286:ILE:CG2 | 1:G:289:VAL:HG22 | 2.32 | 0.60 |
| 1:D:286:ILE:CG2 | 1:D:289:VAL:HG22 | 2.31 | 0.60 |
| 1:E:144:PHE:HB2 | 1:E:151:LEU:HD23 | 1.83 | 0.60 |
| 1:E:286:ILE:CG2 | 1:E:289:VAL:HG22 | 2.31 | 0.60 |
| 1:J:205:LEU:HG | 1:J:247:THR:HG22 | 1.82 | 0.60 |
| 1:F:296:GLU:OE2 | 1:F:312:ASP:OD1 | 2.20 | 0.60 |
| 1:C:205:LEU:HG | 1:C:247:THR:CG2 | 2.32 | 0.60 |
| 1:I:205:LEU:HG | 1:I:247:THR:CG2 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:18:VAL:HG13 | 1:E:337:VAL:HG22 | 1.81 | 0.60 |
| 1:F:319:ASP:OD2 | 1:F:321:ASP:HB2 | 2.02 | 0.60 |
| 1:A:165:THR:HG21 | 1:A:167:ARG:HB3 | 1.84 | 0.60 |
| 1:F:165:THR:HG21 | 1:F:167:ARG:HB3 | 1.83 | 0.60 |
| 1:L:286:ILE:CG2 | 1:L:289:VAL:HG21 | 2.28 | 0.60 |
| 1:D:286:ILE:CG2 | 1:D:289:VAL:HG21 | 2.31 | 0.60 |
| 1:K:27:ASN:HD22 | 1:K:29:GLU:HB2 | 1.67 | 0.60 |
| 1:L:296:GLU:OE2 | 1:L:312:ASP:OD1 | 2.20 | 0.60 |
| 1:E:258:LEU:CD1 | 1:E:276:THR:HG23 | 2.32 | 0.60 |
| 1:C:258:LEU:CD1 | 1:C:276:THR:HG23 | 2.32 | 0.60 |
| 1:C:296:GLU:OE2 | 1:C:312:ASP:OD1 | 2.19 | 0.60 |
| 1:A:338:TYR:CZ | 1:B:47:GLY:HA3 | 2.37 | 0.60 |
| 1:J:286:ILE:HD12 | 1:J:286:ILE:H | 1.64 | 0.59 |
| 1:F:205:LEU:HG | 1:F:247:THR:CG2 | 2.32 | 0.59 |
| 1:F:286:ILE:CG2 | 1:F:289:VAL:HG21 | 2.29 | 0.59 |
| 1:G:286:ILE:CG2 | 1:G:289:VAL:HG21 | 2.32 | 0.59 |
| 1:A:205:LEU:HG | 1:A:247:THR:CG2 | 2.32 | 0.59 |
| 1:I:18:VAL:HG13 | 1:I:337:VAL:HG22 | 1.82 | 0.59 |
| 1:A:286:ILE:CG2 | 1:A:289:VAL:HG22 | 2.31 | 0.59 |
| 1:J:307:MET:O | 1:J:308:SER:HB3 | 2.02 | 0.59 |
| 1:A:223:ASN:O | 1:A:224:ASN:HB2 | 2.02 | 0.59 |
| 1:K:205:LEU:HG | 1:K:247:THR:CG2 | 2.32 | 0.59 |
| 1:D:223:ASN:O | 1:D:224:ASN:HB2 | 2.01 | 0.59 |
| 1:H:286:ILE:CG2 | 1:H:289:VAL:HG21 | 2.30 | 0.59 |
| 1:B:258:LEU:CD1 | 1:B:276:THR:HG23 | 2.32 | 0.59 |
| 1:E:165:THR:HG21 | 1:E:167:ARG:HB3 | 1.84 | 0.59 |
| 1:J:205:LEU:HG | 1:J:247:THR:CG2 | 2.32 | 0.59 |
| 1:C:286:ILE:H | 1:C:286:ILE:HD12 | 1.65 | 0.59 |
| 1:F:258:LEU:CD1 | 1:F:276:THR:HG23 | 2.33 | 0.59 |
| 1:B:296:GLU:OE2 | 1:B:312:ASP:OD1 | 2.21 | 0.59 |
| 1:G:319:ASP:OD2 | 1:G:321:ASP:HB2 | 2.03 | 0.59 |
| 1:C:165:THR:HG21 | 1:C:167:ARG:HB3 | 1.84 | 0.59 |
| 1:K:258:LEU:CD1 | 1:K:276:THR:HG23 | 2.32 | 0.59 |
| 1:G:307:MET:O | 1:G:308:SER:HB3 | 2.03 | 0.59 |
| 1:K:296:GLU:OE2 | 1:K:312:ASP:OD1 | 2.21 | 0.59 |
| 1:H:258:LEU:CD1 | 1:H:276:THR:HG23 | 2.33 | 0.59 |
| 1:H:223:ASN:O | 1:H:224:ASN:HB2 | 2.02 | 0.59 |
| 1:H:338:TYR:CZ | 1:I:47:GLY:HA3 | 2.38 | 0.59 |
| 1:D:258:LEU:CD1 | 1:D:276:THR:HG23 | 2.33 | 0.59 |
| 1:D:296:GLU:OE2 | 1:D:312:ASP:OD1 | 2.20 | 0.58 |
| 1:J:223:ASN:O | 1:J:224:ASN:HB2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:286:ILE:CG2 | 1:J:289:VAL:HG21 | 2.31 | 0.58 |
| 1:C:285:GLY:CA | 1:G:244:PHE:CZ | 2.85 | 0.58 |
| 1:F:307:MET:O | 1:F:308:SER:HB3 | 2.02 | 0.58 |
| 1:I:287:GLY:HA3 | 1:K:321:ASP:OD2 | 2.03 | 0.58 |
| 1:A:303:PHE:HB3 | 1:B:51:ILE:HD13 | 1.85 | 0.58 |
| 1:B:319:ASP:OD2 | 1:B:321:ASP:HB2 | 2.02 | 0.58 |
| 1:C:319:ASP:OD2 | 1:C:321:ASP:HB2 | 2.04 | 0.58 |
| 1:J:319:ASP:OD2 | 1:J:321:ASP:HB2 | 2.04 | 0.58 |
| 1:I:258:LEU:CD1 | 1:I:276:THR:HG23 | 2.34 | 0.58 |
| 1:A:307:MET:O | 1:A:308:SER:HB3 | 2.04 | 0.58 |
| 1:A:258:LEU:CD1 | 1:A:276:THR:HG23 | 2.32 | 0.58 |
| 1:L:307:MET:O | 1:L:308:SER:HB3 | 2.03 | 0.58 |
| 1:A:296:GLU:OE2 | 1:A:312:ASP:OD1 | 2.21 | 0.58 |
| 1:H:45:PHE:CD1 | 1:H:45:PHE:O | 2.57 | 0.58 |
| 1:I:319:ASP:OD2 | 1:I:321:ASP:HB2 | 2.02 | 0.58 |
| 1:J:71:GLU:HG3 | 1:K:100:ARG:HH21 | 1.69 | 0.58 |
| 1:C:104:VAL:HG22 | 1:C:156:GLN:OE1 | 2.04 | 0.58 |
| 1:J:258:LEU:CD1 | 1:J:276:THR:HG23 | 2.34 | 0.58 |
| 1:B:244:PHE:CZ | 1:H:285:GLY:HA3 | 2.39 | 0.58 |
| 1:K:319:ASP:OD2 | 1:K:321:ASP:HB2 | 2.04 | 0.57 |
| 1:E:296:GLU:OE2 | 1:E:312:ASP:OD1 | 2.21 | 0.57 |
| 1:D:104:VAL:HG22 | 1:D:156:GLN:OE1 | 2.04 | 0.57 |
| 1:G:223:ASN:O | 1:G:224:ASN:HB2 | 2.03 | 0.57 |
| 1:B:307:MET:O | 1:B:308:SER:HB3 | 2.05 | 0.57 |
| 1:I:45:PHE:O | 1:I:45:PHE:CD1 | 2.57 | 0.57 |
| 1:A:319:ASP:OD2 | 1:A:321:ASP:HB2 | 2.05 | 0.57 |
| 1:I:307:MET:O | 1:I:308:SER:HB3 | 2.04 | 0.57 |
| 1:A:105:VAL:O | 1:A:105:VAL:HG12 | 2.03 | 0.57 |
| 1:C:223:ASN:O | 1:C:224:ASN:HB2 | 2.03 | 0.57 |
| 1:B:143:ASN:O | 1:B:146:GLY:N | 2.38 | 0.57 |
| 1:H:303:PHE:HB3 | 1:I:51:ILE:HD13 | 1.86 | 0.57 |
| 1:L:258:LEU:CD1 | 1:L:276:THR:HG23 | 2.34 | 0.57 |
| 1:G:105:VAL:O | 1:G:105:VAL:HG12 | 2.04 | 0.57 |
| 1:G:47:GLY:HA3 | 1:I:338:TYR:CE2 | 2.40 | 0.57 |
| 1:K:307:MET:O | 1:K:308:SER:HB3 | 2.05 | 0.57 |
| 1:H:319:ASP:OD2 | 1:H:321:ASP:HB2 | 2.05 | 0.56 |
| 1:G:104:VAL:HG22 | 1:G:156:GLN:OE1 | 2.04 | 0.56 |
| 1:A:45:PHE:CD1 | 1:A:45:PHE:O | 2.58 | 0.56 |
| 1:L:319:ASP:OD2 | 1:L:321:ASP:HB2 | 2.04 | 0.56 |
| 1:D:240:ILE:HD13 | 1:D:251:ALA:HB2 | 1.87 | 0.56 |
| 1:B:321:ASP:OD1 | 1:H:287:GLY:HA3 | 1.96 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:286:ILE:HG22 | 1:I:289:VAL:CG2 | 2.34 | 0.56 |
| 1:A:286:ILE:CG2 | 1:A:289:VAL:HG21 | 2.33 | 0.56 |
| 1:H:307:MET:O | 1:H:308:SER:HB3 | 2.05 | 0.56 |
| 1:C:270:ARG:HG2 | 1:C:270:ARG:O | 2.05 | 0.56 |
| 1:E:143:ASN:O | 1:E:146:GLY:N | 2.38 | 0.56 |
| 1:D:307:MET:O | 1:D:308:SER:HB3 | 2.04 | 0.56 |
| 1:B:45:PHE:O | 1:B:45:PHE:CD1 | 2.58 | 0.56 |
| 1:I:104:VAL:HG22 | 1:I:156:GLN:OE1 | 2.05 | 0.56 |
| 1:E:319:ASP:OD2 | 1:E:321:ASP:HB2 | 2.05 | 0.56 |
| 1:D:319:ASP:OD2 | 1:D:321:ASP:HB2 | 2.04 | 0.56 |
| 1:D:105:VAL:O | 1:D:105:VAL:HG12 | 2.05 | 0.56 |
| 1:H:111:TYR:CE2 | 1:H:188:VAL:HG23 | 2.40 | 0.56 |
| 1:B:303:PHE:CB | 1:C:51:ILE:HD13 | 2.36 | 0.56 |
| 1:E:307:MET:O | 1:E:308:SER:HB3 | 2.04 | 0.56 |
| 1:C:143:ASN:O | 1:C:146:GLY:N | 2.39 | 0.56 |
| 1:A:143:ASN:O | 1:A:146:GLY:N | 2.38 | 0.56 |
| 1:D:143:ASN:O | 1:D:146:GLY:N | 2.38 | 0.56 |
| 1:B:244:PHE:CZ | 1:H:285:GLY:CA | 2.89 | 0.56 |
| 1:G:45:PHE:O | 1:G:45:PHE:CD1 | 2.59 | 0.56 |
| 1:E:45:PHE:O | 1:E:45:PHE:CD1 | 2.58 | 0.56 |
| 1:B:270:ARG:O | 1:B:270:ARG:HG2 | 2.05 | 0.56 |
| 1:F:285:GLY:CA | 1:J:244:PHE:CZ | 2.89 | 0.56 |
| 1:B:104:VAL:HG22 | 1:B:156:GLN:OE1 | 2.06 | 0.56 |
| 1:G:11:VAL:HG21 | 1:I:340:PHE:HB2 | 1.88 | 0.56 |
| 1:A:104:VAL:HG22 | 1:A:156:GLN:OE1 | 2.06 | 0.56 |
| 1:E:286:ILE:CG2 | 1:E:289:VAL:HG21 | 2.30 | 0.56 |
| 1:K:105:VAL:O | 1:K:105:VAL:HG12 | 2.05 | 0.56 |
| 1:C:307:MET:O | 1:C:308:SER:HB3 | 2.06 | 0.56 |
| 1:K:286:ILE:CG2 | 1:K:289:VAL:HG21 | 2.29 | 0.55 |
| 1:I:270:ARG:O | 1:I:270:ARG:HG2 | 2.06 | 0.55 |
| 1:C:105:VAL:HG12 | 1:C:105:VAL:O | 2.05 | 0.55 |
| 1:G:258:LEU:CD1 | 1:G:276:THR:HG23 | 2.36 | 0.55 |
| 1:E:104:VAL:HG22 | 1:E:156:GLN:OE1 | 2.06 | 0.55 |
| 1:J:45:PHE:O | 1:J:45:PHE:CD1 | 2.59 | 0.55 |
| 1:K:165:THR:CG2 | 1:K:167:ARG:HB3 | 2.37 | 0.55 |
| 1:I:27:ASN:HD22 | 1:I:29:GLU:CB | 2.12 | 0.55 |
| 1:A:281:LYS:O | 1:A:282:ASP:HB2 | 2.06 | 0.55 |
| 1:E:270:ARG:O | 1:E:270:ARG:HG2 | 2.06 | 0.55 |
| 1:L:45:PHE:O | 1:L:45:PHE:CD1 | 2.59 | 0.55 |
| 1:B:281:LYS:O | 1:B:282:ASP:HB2 | 2.07 | 0.55 |
| 1:F:111:TYR:CE2 | 1:F:188:VAL:HG23 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:143:ASN:HA | 1:L:148:VAL:O | 2.07 | 0.55 |
| 1:H:221:ASP:O | 1:H:222:ALA:HB2 | 2.05 | 0.55 |
| 1:I:165:THR:CG2 | 1:I:167:ARG:HB3 | 2.37 | 0.55 |
| 1:G:51:ILE:HD13 | 1:I:303:PHE:CB | 2.34 | 0.55 |
| 1:K:281:LYS:O | 1:K:282:ASP:HB2 | 2.07 | 0.55 |
| 1:L:286:ILE:HG22 | 1:L:289:VAL:CG2 | 2.34 | 0.55 |
| 1:B:309:THR:HG22 | 1:B:336:ILE:CA | 2.35 | 0.55 |
| 1:I:221:ASP:O | 1:I:222:ALA:HB2 | 2.07 | 0.55 |
| 1:K:143:ASN:O | 1:K:146:GLY:N | 2.39 | 0.55 |
| 1:I:105:VAL:O | 1:I:105:VAL:HG12 | 2.07 | 0.55 |
| 1:J:303:PHE:HB3 | 1:K:51:ILE:HD13 | 1.89 | 0.55 |
| 1:J:338:TYR:CZ | 1:K:47:GLY:HA3 | 2.42 | 0.55 |
| 1:B:321:ASP:CG | 1:H:287:GLY:HA3 | 2.26 | 0.55 |
| 1:K:71:GLU:CG | 1:L:100:ARG:HH21 | 2.19 | 0.55 |
| 1:J:105:VAL:HG12 | 1:J:105:VAL:O | 2.06 | 0.55 |
| 1:F:281:LYS:O | 1:F:282:ASP:HB2 | 2.07 | 0.55 |
| 1:J:111:TYR:CE2 | 1:J:188:VAL:HG23 | 2.42 | 0.55 |
| 1:F:143:ASN:O | 1:F:146:GLY:N | 2.39 | 0.55 |
| 1:H:286:ILE:HG22 | 1:H:289:VAL:CG2 | 2.36 | 0.55 |
| 1:L:111:TYR:CE2 | 1:L:188:VAL:HG23 | 2.41 | 0.55 |
| 1:A:221:ASP:O | 1:A:222:ALA:HB2 | 2.06 | 0.55 |
| 1:K:104:VAL:HG22 | 1:K:156:GLN:OE1 | 2.06 | 0.55 |
| 1:J:104:VAL:HG22 | 1:J:156:GLN:OE1 | 2.07 | 0.55 |
| 1:H:281:LYS:O | 1:H:282:ASP:HB2 | 2.07 | 0.54 |
| 1:I:111:TYR:CE2 | 1:I:188:VAL:HG23 | 2.41 | 0.54 |
| 1:E:111:TYR:CE2 | 1:E:188:VAL:HG23 | 2.42 | 0.54 |
| 1:I:143:ASN:HA | 1:I:148:VAL:O | 2.07 | 0.54 |
| 1:K:45:PHE:CD1 | 1:K:45:PHE:O | 2.59 | 0.54 |
| 1:B:321:ASP:CG | 1:H:287:GLY:CA | 2.72 | 0.54 |
| 1:A:321:ASP:OD2 | 1:J:287:GLY:HA3 | 2.06 | 0.54 |
| 1:A:111:TYR:CE2 | 1:A:188:VAL:HG23 | 2.43 | 0.54 |
| 1:B:338:TYR:CE2 | 1:C:47:GLY:HA3 | 2.43 | 0.54 |
| 1:L:143:ASN:O | 1:L:146:GLY:N | 2.41 | 0.54 |
| 1:G:111:TYR:CE2 | 1:G:188:VAL:HG23 | 2.41 | 0.54 |
| 1:G:143:ASN:HA | 1:G:148:VAL:O | 2.07 | 0.54 |
| 1:L:221:ASP:O | 1:L:222:ALA:HB2 | 2.07 | 0.54 |
| 1:H:143:ASN:O | 1:H:146:GLY:N | 2.40 | 0.54 |
| 1:D:221:ASP:O | 1:D:222:ALA:HB2 | 2.07 | 0.54 |
| 1:I:141:ASN:HB3 | 1:I:153:PHE:CE1 | 2.43 | 0.54 |
| 1:F:105:VAL:HG12 | 1:F:105:VAL:O | 2.08 | 0.54 |
| 1:D:100:ARG:HH21 | 1:F:71:GLU:CG | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:281:LYS:O | 1:J:282:ASP:HB2 | 2.08 | 0.54 |
| 1:C:111:TYR:CE2 | 1:C:188:VAL:HG23 | 2.42 | 0.54 |
| 1:F:165:THR:CG2 | 1:F:167:ARG:HB3 | 2.38 | 0.54 |
| 1:G:143:ASN:O | 1:G:146:GLY:N | 2.41 | 0.54 |
| 1:H:104:VAL:HG22 | 1:H:156:GLN:OE1 | 2.08 | 0.54 |
| 1:F:45:PHE:CD1 | 1:F:45:PHE:O | 2.60 | 0.54 |
| 1:F:104:VAL:HG22 | 1:F:156:GLN:OE1 | 2.07 | 0.54 |
| 1:L:165:THR:CG2 | 1:L:167:ARG:HB3 | 2.37 | 0.54 |
| 1:F:221:ASP:O | 1:F:222:ALA:HB2 | 2.07 | 0.54 |
| 1:H:143:ASN:HA | 1:H:148:VAL:O | 2.08 | 0.54 |
| 1:B:143:ASN:HA | 1:B:148:VAL:O | 2.08 | 0.54 |
| 1:A:240:ILE:HD13 | 1:A:251:ALA:HB2 | 1.90 | 0.54 |
| 1:E:281:LYS:O | 1:E:282:ASP:HB2 | 2.07 | 0.53 |
| 1:K:111:TYR:CE2 | 1:K:188:VAL:HG23 | 2.43 | 0.53 |
| 1:F:270:ARG:O | 1:F:270:ARG:HG2 | 2.07 | 0.53 |
| 1:K:144:PHE:O | 1:K:145:PHE:HB2 | 2.08 | 0.53 |
| 1:A:51:ILE:HD13 | 1:C:303:PHE:HB3 | 1.89 | 0.53 |
| 1:H:165:THR:CG2 | 1:H:167:ARG:HB3 | 2.38 | 0.53 |
| 1:K:270:ARG:HG2 | 1:K:270:ARG:O | 2.08 | 0.53 |
| 1:I:143:ASN:O | 1:I:146:GLY:N | 2.41 | 0.53 |
| 1:B:105:VAL:O | 1:B:105:VAL:HG12 | 2.08 | 0.53 |
| 1:B:111:TYR:CE2 | 1:B:188:VAL:HG23 | 2.43 | 0.53 |
| 1:B:221:ASP:O | 1:B:222:ALA:HB2 | 2.07 | 0.53 |
| 1:H:105:VAL:O | 1:H:105:VAL:HG12 | 2.08 | 0.53 |
| 1:C:174:VAL:CG1 | 1:C:175:GLY:N | 2.72 | 0.53 |
| 1:G:144:PHE:O | 1:G:145:PHE:HB2 | 2.09 | 0.53 |
| 1:K:221:ASP:O | 1:K:222:ALA:HB2 | 2.07 | 0.53 |
| 1:D:45:PHE:O | 1:D:45:PHE:CD1 | 2.61 | 0.53 |
| 1:B:240:ILE:HD13 | 1:B:251:ALA:HB2 | 1.91 | 0.53 |
| 1:D:165:THR:CG2 | 1:D:167:ARG:HB3 | 2.39 | 0.53 |
| 1:G:165:THR:CG2 | 1:G:167:ARG:HB3 | 2.38 | 0.53 |
| 1:F:286:ILE:CD1 | 1:F:286:ILE:H | 2.22 | 0.53 |
| 1:C:281:LYS:O | 1:C:282:ASP:HB2 | 2.08 | 0.53 |
| 1:J:221:ASP:O | 1:J:222:ALA:HB2 | 2.08 | 0.53 |
| 1:G:141:ASN:HB3 | 1:G:153:PHE:CE1 | 2.44 | 0.53 |
| 1:G:3:ILE:HD12 | 1:I:3:ILE:HG21 | 1.91 | 0.53 |
| 1:A:270:ARG:O | 1:A:270:ARG:HG2 | 2.08 | 0.53 |
| 1:D:281:LYS:O | 1:D:282:ASP:HB2 | 2.08 | 0.53 |
| 1:K:174:VAL:CG1 | 1:K:175:GLY:N | 2.72 | 0.53 |
| 1:E:221:ASP:O | 1:E:222:ALA:HB2 | 2.08 | 0.53 |
| 1:G:221:ASP:O | 1:G:222:ALA:HB2 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:221:ASP:O | 1:C:222:ALA:HB2 | 2.08 | 0.53 |
| 1:E:321:ASP:CG | 1:K:287:GLY:CA | 2.68 | 0.53 |
| 1:C:286:ILE:HG22 | 1:C:289:VAL:CG2 | 2.37 | 0.53 |
| 1:F:143:ASN:HA | 1:F:148:VAL:O | 2.08 | 0.53 |
| 1:A:144:PHE:O | 1:A:145:PHE:HB2 | 2.09 | 0.53 |
| 1:L:144:PHE:O | 1:L:145:PHE:HB2 | 2.09 | 0.53 |
| 1:K:240:ILE:HD13 | 1:K:251:ALA:HB2 | 1.91 | 0.53 |
| 1:D:321:ASP:OD2 | 1:G:287:GLY:HA3 | 2.09 | 0.53 |
| 1:I:281:LYS:O | 1:I:282:ASP:HB2 | 2.09 | 0.53 |
| 1:J:144:PHE:O | 1:J:145:PHE:HB2 | 2.08 | 0.53 |
| 1:E:143:ASN:HA | 1:E:148:VAL:O | 2.09 | 0.53 |
| 1:J:222:ALA:O | 1:J:223:ASN:HB2 | 2.09 | 0.53 |
| 1:C:45:PHE:O | 1:C:45:PHE:CD1 | 2.62 | 0.53 |
| 1:F:286:ILE:HG22 | 1:F:289:VAL:CG2 | 2.36 | 0.52 |
| 1:D:111:TYR:CE2 | 1:D:188:VAL:HG23 | 2.44 | 0.52 |
| 1:D:174:VAL:CG1 | 1:D:175:GLY:N | 2.71 | 0.52 |
| 1:G:222:ALA:O | 1:G:223:ASN:HB2 | 2.09 | 0.52 |
| 1:E:105:VAL:HG12 | 1:E:105:VAL:O | 2.08 | 0.52 |
| 1:B:340:PHE:HB2 | 1:C:11:VAL:HG21 | 1.91 | 0.52 |
| 1:B:71:GLU:CG | 1:C:100:ARG:HH21 | 2.23 | 0.52 |
| 1:C:165:THR:CG2 | 1:C:167:ARG:HB3 | 2.39 | 0.52 |
| 1:B:165:THR:CG2 | 1:B:167:ARG:HB3 | 2.39 | 0.52 |
| 1:E:286:ILE:CD1 | 1:E:286:ILE:N | 2.72 | 0.52 |
| 1:G:281:LYS:O | 1:G:282:ASP:HB2 | 2.09 | 0.52 |
| 1:H:270:ARG:O | 1:H:270:ARG:HG2 | 2.08 | 0.52 |
| 1:G:338:TYR:CE2 | 1:H:47:GLY:HA3 | 2.45 | 0.52 |
| 1:L:270:ARG:HG2 | 1:L:270:ARG:O | 2.09 | 0.52 |
| 1:L:174:VAL:CG1 | 1:L:175:GLY:N | 2.72 | 0.52 |
| 1:J:143:ASN:HA | 1:J:148:VAL:O | 2.09 | 0.52 |
| 1:L:105:VAL:HG12 | 1:L:105:VAL:O | 2.10 | 0.52 |
| 1:A:309:THR:HG22 | 1:A:336:ILE:CA | 2.34 | 0.52 |
| 1:H:144:PHE:O | 1:H:145:PHE:HB2 | 2.08 | 0.52 |
| 1:E:222:ALA:O | 1:E:223:ASN:HB2 | 2.09 | 0.52 |
| 1:J:165:THR:CG2 | 1:J:167:ARG:HB3 | 2.38 | 0.52 |
| 1:L:281:LYS:O | 1:L:282:ASP:HB2 | 2.09 | 0.52 |
| 1:E:174:VAL:CG1 | 1:E:175:GLY:N | 2.72 | 0.52 |
| 1:J:174:VAL:CG1 | 1:J:175:GLY:N | 2.72 | 0.52 |
| 1:C:143:ASN:HA | 1:C:148:VAL:O | 2.08 | 0.52 |
| 1:I:264:GLN:OE1 | 1:I:270:ARG:HB2 | 2.09 | 0.52 |
| 1:I:144:PHE:O | 1:I:145:PHE:HB2 | 2.10 | 0.52 |
| 1:D:143:ASN:HA | 1:D:148:VAL:O | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:141:ASN:HB3 | 1:H:153:PHE:CE1 | 2.45 | 0.52 |
| 1:D:309:THR:HG22 | 1:D:336:ILE:CA | 2.34 | 0.52 |
| 1:C:286:ILE:CG2 | 1:C:289:VAL:HG21 | 2.31 | 0.52 |
| 1:C:222:ALA:O | 1:C:223:ASN:HB2 | 2.09 | 0.52 |
| 1:J:309:THR:HG22 | 1:J:336:ILE:CA | 2.35 | 0.52 |
| 1:G:309:THR:HG22 | 1:G:336:ILE:CA | 2.35 | 0.52 |
| 1:B:174:VAL:CG1 | 1:B:175:GLY:N | 2.73 | 0.52 |
| 1:B:303:PHE:CG | 1:C:51:ILE:HD13 | 2.45 | 0.52 |
| 1:A:143:ASN:HA | 1:A:148:VAL:O | 2.09 | 0.52 |
| 1:K:143:ASN:HA | 1:K:148:VAL:O | 2.08 | 0.52 |
| 1:H:240:ILE:HD13 | 1:H:251:ALA:HB2 | 1.92 | 0.52 |
| 1:L:104:VAL:HG22 | 1:L:156:GLN:OE1 | 2.08 | 0.52 |
| 1:E:165:THR:CG2 | 1:E:167:ARG:HB3 | 2.39 | 0.52 |
| 1:D:51:ILE:HD13 | 1:F:303:PHE:CB | 2.39 | 0.52 |
| 1:F:258:LEU:HD13 | 1:F:276:THR:HG23 | 1.92 | 0.52 |
| 1:E:286:ILE:H | 1:E:286:ILE:CD1 | 2.23 | 0.52 |
| 1:C:144:PHE:O | 1:C:145:PHE:HB2 | 2.10 | 0.52 |
| 1:A:165:THR:CG2 | 1:A:167:ARG:HB3 | 2.39 | 0.52 |
| 1:F:286:ILE:N | 1:F:286:ILE:CD1 | 2.71 | 0.52 |
| 1:E:303:PHE:CB | 1:F:51:ILE:HD13 | 2.40 | 0.52 |
| 1:F:161:ASN:HB2 | 1:F:170:ASN:OD1 | 2.11 | 0.52 |
| 1:K:154:ALA:O | 1:K:176:GLY:HA2 | 2.10 | 0.52 |
| 1:G:174:VAL:CG1 | 1:G:175:GLY:N | 2.73 | 0.51 |
| 1:K:286:ILE:H | 1:K:286:ILE:CD1 | 2.23 | 0.51 |
| 1:I:309:THR:HG22 | 1:I:336:ILE:CA | 2.38 | 0.51 |
| 1:G:270:ARG:O | 1:G:270:ARG:HG2 | 2.10 | 0.51 |
| 1:A:174:VAL:CG1 | 1:A:175:GLY:N | 2.73 | 0.51 |
| 1:B:141:ASN:HB3 | 1:B:153:PHE:CE1 | 2.46 | 0.51 |
| 1:B:154:ALA:O | 1:B:176:GLY:HA2 | 2.11 | 0.51 |
| 1:I:240:ILE:HD13 | 1:I:251:ALA:HB2 | 1.92 | 0.51 |
| 1:I:161:ASN:HB2 | 1:I:170:ASN:OD1 | 2.09 | 0.51 |
| 1:J:270:ARG:HG2 | 1:J:270:ARG:O | 2.09 | 0.51 |
| 1:F:144:PHE:O | 1:F:145:PHE:HB2 | 2.10 | 0.51 |
| 1:H:244:PHE:CZ | 1:L:285:GLY:HA3 | 2.45 | 0.51 |
| 1:D:141:ASN:HB3 | 1:D:153:PHE:CE1 | 2.45 | 0.51 |
| 1:D:270:ARG:HG2 | 1:D:270:ARG:O | 2.08 | 0.51 |
| 1:K:264:GLN:OE1 | 1:K:270:ARG:HB2 | 2.10 | 0.51 |
| 1:F:240:ILE:HD13 | 1:F:251:ALA:HB2 | 1.92 | 0.51 |
| 1:A:141:ASN:HB3 | 1:A:153:PHE:CE1 | 2.45 | 0.51 |
| 1:J:141:ASN:HB3 | 1:J:153:PHE:CE1 | 2.45 | 0.51 |
| 1:F:174:VAL:CG1 | 1:F:175:GLY:N | 2.73 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:204:PRO:HD2 | 1:G:248:SER:O | 2.10 | 0.51 |
| 1:D:47:GLY:HA3 | 1:F:338:TYR:CE2 | 2.45 | 0.51 |
| 1:C:258:LEU:HD13 | 1:C:276:THR:HG23 | 1.93 | 0.51 |
| 1:B:340:PHE:CB | 1:C:11:VAL:HG21 | 2.40 | 0.51 |
| 1:E:154:ALA:O | 1:E:176:GLY:HA2 | 2.10 | 0.51 |
| 1:B:130:VAL:HG13 | 1:B:213:GLN:CD | 2.31 | 0.51 |
| 1:L:141:ASN:HB3 | 1:L:153:PHE:CE1 | 2.46 | 0.51 |
| 1:H:174:VAL:CG1 | 1:H:175:GLY:N | 2.73 | 0.51 |
| 1:D:144:PHE:O | 1:D:145:PHE:HB2 | 2.10 | 0.51 |
| 1:K:204:PRO:HB2 | 1:K:247:THR:CG2 | 2.41 | 0.51 |
| 1:E:144:PHE:O | 1:E:145:PHE:HB2 | 2.09 | 0.51 |
| 1:K:141:ASN:HB3 | 1:K:153:PHE:CE1 | 2.46 | 0.51 |
| 1:L:165:THR:CG2 | 1:L:167:ARG:H | 2.13 | 0.51 |
| 1:E:286:ILE:HG22 | 1:E:289:VAL:CG2 | 2.37 | 0.51 |
| 1:J:143:ASN:O | 1:J:146:GLY:N | 2.43 | 0.51 |
| 1:A:154:ALA:O | 1:A:176:GLY:HA2 | 2.10 | 0.51 |
| 1:G:240:ILE:HD13 | 1:G:251:ALA:HB2 | 1.92 | 0.51 |
| 1:F:154:ALA:O | 1:F:176:GLY:HA2 | 2.11 | 0.51 |
| 1:D:338:TYR:CE2 | 1:E:47:GLY:HA3 | 2.46 | 0.51 |
| 1:B:264:GLN:OE1 | 1:B:270:ARG:HB2 | 2.11 | 0.51 |
| 1:I:174:VAL:CG1 | 1:I:175:GLY:N | 2.73 | 0.51 |
| 1:E:258:LEU:HD13 | 1:E:276:THR:HG23 | 1.92 | 0.51 |
| 1:D:258:LEU:HD13 | 1:D:276:THR:HG23 | 1.92 | 0.51 |
| 1:A:258:LEU:HD13 | 1:A:276:THR:HG23 | 1.93 | 0.51 |
| 1:E:141:ASN:HB3 | 1:E:153:PHE:CE1 | 2.46 | 0.51 |
| 1:J:286:ILE:N | 1:J:286:ILE:CD1 | 2.74 | 0.51 |
| 1:B:144:PHE:O | 1:B:145:PHE:HB2 | 2.11 | 0.51 |
| 1:L:222:ALA:O | 1:L:223:ASN:HB2 | 2.11 | 0.51 |
| 1:H:222:ALA:O | 1:H:223:ASN:HB2 | 2.11 | 0.51 |
| 1:J:258:LEU:HD13 | 1:J:276:THR:HG23 | 1.93 | 0.51 |
| 1:G:11:VAL:HG21 | 1:I:340:PHE:CB | 2.41 | 0.51 |
| 1:J:240:ILE:HD13 | 1:J:251:ALA:HB2 | 1.92 | 0.50 |
| 1:L:136:VAL:CG1 | 1:L:158:LEU:HD13 | 2.41 | 0.50 |
| 1:H:321:ASP:OD2 | 1:L:287:GLY:HA3 | 2.11 | 0.50 |
| 1:D:222:ALA:O | 1:D:223:ASN:HB2 | 2.11 | 0.50 |
| 1:I:154:ALA:O | 1:I:176:GLY:HA2 | 2.11 | 0.50 |
| 1:K:130:VAL:HG13 | 1:K:213:GLN:CD | 2.32 | 0.50 |
| 1:E:240:ILE:HD13 | 1:E:251:ALA:HB2 | 1.91 | 0.50 |
| 1:J:154:ALA:O | 1:J:176:GLY:HA2 | 2.11 | 0.50 |
| 1:G:136:VAL:CG1 | 1:G:158:LEU:HD13 | 2.42 | 0.50 |
| 1:C:309:THR:HG22 | 1:C:336:ILE:CA | 2.36 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:136:VAL:CG1 | 1:H:158:LEU:HD13 | 2.41 | 0.50 |
| 1:L:154:ALA:O | 1:L:176:GLY:HA2 | 2.11 | 0.50 |
| 1:F:309:THR:HG22 | 1:F:336:ILE:CA | 2.36 | 0.50 |
| 1:J:286:ILE:H | 1:J:286:ILE:CD1 | 2.25 | 0.50 |
| 1:J:286:ILE:HG22 | 1:J:289:VAL:CG2 | 2.38 | 0.50 |
| 1:I:204:PRO:HB2 | 1:I:247:THR:CG2 | 2.42 | 0.50 |
| 1:A:222:ALA:O | 1:A:223:ASN:HB2 | 2.11 | 0.50 |
| 1:G:340:PHE:HB2 | 1:H:11:VAL:HG21 | 1.93 | 0.50 |
| 1:H:161:ASN:HB2 | 1:H:170:ASN:OD1 | 2.11 | 0.50 |
| 1:D:154:ALA:O | 1:D:176:GLY:HA2 | 2.11 | 0.50 |
| 1:G:286:ILE:CD1 | 1:G:286:ILE:N | 2.74 | 0.50 |
| 1:H:130:VAL:HG13 | 1:H:213:GLN:CD | 2.32 | 0.50 |
| 1:K:161:ASN:HB2 | 1:K:170:ASN:OD1 | 2.12 | 0.50 |
| 1:B:286:ILE:CD1 | 1:B:286:ILE:H | 2.24 | 0.50 |
| 1:A:286:ILE:CD1 | 1:A:286:ILE:H | 2.25 | 0.50 |
| 1:I:258:LEU:HD13 | 1:I:276:THR:HG23 | 1.93 | 0.50 |
| 1:G:154:ALA:O | 1:G:176:GLY:HA2 | 2.11 | 0.50 |
| 1:F:130:VAL:HG13 | 1:F:213:GLN:CD | 2.32 | 0.50 |
| 1:J:161:ASN:HB2 | 1:J:170:ASN:OD1 | 2.11 | 0.50 |
| 1:C:321:ASP:OD2 | 1:D:287:GLY:HA3 | 2.12 | 0.50 |
| 1:I:286:ILE:H | 1:I:286:ILE:CD1 | 2.24 | 0.50 |
| 1:B:286:ILE:CD1 | 1:B:286:ILE:N | 2.73 | 0.50 |
| 1:L:204:PRO:HD2 | 1:L:248:SER:O | 2.11 | 0.50 |
| 1:E:130:VAL:HG13 | 1:E:213:GLN:CD | 2.32 | 0.50 |
| 1:J:294:TYR:C | 1:J:294:TYR:CD1 | 2.85 | 0.50 |
| 1:J:71:GLU:CG | 1:K:100:ARG:HH21 | 2.25 | 0.50 |
| 1:L:286:ILE:H | 1:L:286:ILE:CD1 | 2.25 | 0.50 |
| 1:G:286:ILE:CD1 | 1:G:286:ILE:H | 2.25 | 0.50 |
| 1:E:204:PRO:HB2 | 1:E:247:THR:CG2 | 2.42 | 0.50 |
| 1:E:153:PHE:HA | 1:E:177:SER:O | 2.12 | 0.50 |
| 1:I:136:VAL:CG1 | 1:I:158:LEU:HD13 | 2.41 | 0.50 |
| 1:G:313:TYR:HD1 | 1:G:332:VAL:CG2 | 2.18 | 0.50 |
| 1:I:286:ILE:N | 1:I:286:ILE:CD1 | 2.74 | 0.50 |
| 1:H:204:PRO:HD2 | 1:H:248:SER:O | 2.12 | 0.50 |
| 1:G:105:VAL:HA | 1:G:190:ALA:HB1 | 1.94 | 0.50 |
| 1:G:153:PHE:HA | 1:G:177:SER:O | 2.12 | 0.50 |
| 1:E:161:ASN:HB2 | 1:E:170:ASN:OD1 | 2.12 | 0.50 |
| 1:G:161:ASN:HB2 | 1:G:170:ASN:OD1 | 2.11 | 0.50 |
| 1:H:286:ILE:H | 1:H:286:ILE:CD1 | 2.24 | 0.49 |
| 1:L:264:GLN:OE1 | 1:L:270:ARG:HB2 | 2.12 | 0.49 |
| 1:D:204:PRO:HB2 | 1:D:247:THR:CG2 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:204:PRO:HD2 | 1:C:248:SER:O | 2.12 | 0.49 |
| 1:C:154:ALA:O | 1:C:176:GLY:HA2 | 2.12 | 0.49 |
| 1:D:11:VAL:HG21 | 1:F:340:PHE:HB2 | 1.93 | 0.49 |
| 1:K:294:TYR:CD1 | 1:K:294:TYR:C | 2.85 | 0.49 |
| 1:L:240:ILE:HD13 | 1:L:251:ALA:HB2 | 1.92 | 0.49 |
| 1:I:204:PRO:HD2 | 1:I:248:SER:O | 2.12 | 0.49 |
| 1:H:154:ALA:O | 1:H:176:GLY:HA2 | 2.11 | 0.49 |
| 1:F:153:PHE:HA | 1:F:177:SER:O | 2.13 | 0.49 |
| 1:C:240:ILE:HD13 | 1:C:251:ALA:HB2 | 1.94 | 0.49 |
| 1:B:161:ASN:HB2 | 1:B:170:ASN:OD1 | 2.11 | 0.49 |
| 1:L:130:VAL:HG13 | 1:L:213:GLN:CD | 2.32 | 0.49 |
| 1:K:309:THR:HG22 | 1:K:336:ILE:CA | 2.37 | 0.49 |
| 1:L:309:THR:HG22 | 1:L:336:ILE:CA | 2.37 | 0.49 |
| 1:D:286:ILE:HG22 | 1:D:289:VAL:CG2 | 2.38 | 0.49 |
| 1:B:303:PHE:HB3 | 1:C:51:ILE:HG21 | 1.94 | 0.49 |
| 1:J:153:PHE:HA | 1:J:177:SER:O | 2.12 | 0.49 |
| 1:F:141:ASN:HB3 | 1:F:153:PHE:CE1 | 2.47 | 0.49 |
| 1:K:286:ILE:N | 1:K:286:ILE:CD1 | 2.73 | 0.49 |
| 1:J:51:ILE:HD13 | 1:L:303:PHE:CB | 2.43 | 0.49 |
| 1:K:222:ALA:O | 1:K:223:ASN:HB2 | 2.12 | 0.49 |
| 1:L:258:LEU:HD13 | 1:L:276:THR:HG23 | 1.94 | 0.49 |
| 1:I:66:GLN:HG3 | 1:I:78:GLY:HA3 | 1.94 | 0.49 |
| 1:K:338:TYR:CZ | 1:L:47:GLY:HA3 | 2.48 | 0.49 |
| 1:C:136:VAL:CG1 | 1:C:158:LEU:HD13 | 2.42 | 0.49 |
| 1:J:136:VAL:CG1 | 1:J:158:LEU:HD13 | 2.42 | 0.49 |
| 1:K:236:ASN:OD1 | 1:K:252:ASN:HA | 2.12 | 0.49 |
| 1:K:204:PRO:HD2 | 1:K:248:SER:O | 2.12 | 0.49 |
| 1:E:136:VAL:CG1 | 1:E:158:LEU:HD13 | 2.42 | 0.49 |
| 1:C:236:ASN:OD1 | 1:C:252:ASN:HA | 2.13 | 0.49 |
| 1:L:286:ILE:N | 1:L:286:ILE:CD1 | 2.73 | 0.49 |
| 1:I:267:PHE:HD1 | 1:I:267:PHE:H | 1.61 | 0.49 |
| 1:C:141:ASN:HB3 | 1:C:153:PHE:CE1 | 2.47 | 0.49 |
| 1:H:66:GLN:HG3 | 1:H:78:GLY:HA3 | 1.94 | 0.49 |
| 1:D:340:PHE:HB2 | 1:E:11:VAL:HG21 | 1.94 | 0.49 |
| 1:A:294:TYR:CD1 | 1:A:294:TYR:C | 2.85 | 0.49 |
| 1:B:204:PRO:HB2 | 1:B:247:THR:CG2 | 2.43 | 0.49 |
| 1:A:47:GLY:HA3 | 1:C:338:TYR:CE2 | 2.48 | 0.49 |
| 1:I:222:ALA:O | 1:I:223:ASN:HB2 | 2.11 | 0.49 |
| 1:L:161:ASN:HB2 | 1:L:170:ASN:OD1 | 2.13 | 0.49 |
| 1:K:136:VAL:CG1 | 1:K:158:LEU:HD13 | 2.43 | 0.49 |
| 1:E:244:PHE:HZ | 1:K:285:GLY:CA | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:258:LEU:HD13 | 1:B:276:THR:HG23 | 1.94 | 0.49 |
| 1:K:258:LEU:HD13 | 1:K:276:THR:HG23 | 1.93 | 0.49 |
| 1:H:258:LEU:HD13 | 1:H:276:THR:HG23 | 1.94 | 0.49 |
| 1:B:153:PHE:HA | 1:B:177:SER:O | 2.13 | 0.49 |
| 1:D:161:ASN:HB2 | 1:D:170:ASN:OD1 | 2.12 | 0.49 |
| 1:E:71:GLU:HG3 | 1:F:100:ARG:HH21 | 1.77 | 0.49 |
| 1:F:31:SER:CA | 1:F:329:ASP:HB2 | 2.40 | 0.49 |
| 1:H:264:GLN:OE1 | 1:H:270:ARG:HB2 | 2.12 | 0.49 |
| 1:E:264:GLN:OE1 | 1:E:270:ARG:HB2 | 2.13 | 0.49 |
| 1:L:269:LEU:HG | 1:L:271:PRO:HD3 | 1.95 | 0.49 |
| 1:H:309:THR:HG22 | 1:H:336:ILE:CA | 2.37 | 0.49 |
| 1:A:286:ILE:HG22 | 1:A:289:VAL:CG2 | 2.39 | 0.49 |
| 1:G:204:PRO:HB2 | 1:G:247:THR:CG2 | 2.43 | 0.49 |
| 1:J:204:PRO:HB2 | 1:J:247:THR:CG2 | 2.43 | 0.49 |
| 1:E:236:ASN:OD1 | 1:E:252:ASN:HA | 2.13 | 0.49 |
| 1:A:100:ARG:HH21 | 1:C:71:GLU:HG3 | 1.76 | 0.48 |
| 1:I:165:THR:CG2 | 1:I:167:ARG:H | 2.15 | 0.48 |
| 1:G:267:PHE:HD1 | 1:G:267:PHE:H | 1.61 | 0.48 |
| 1:C:286:ILE:CD1 | 1:C:286:ILE:H | 2.26 | 0.48 |
| 1:D:286:ILE:H | 1:D:286:ILE:CD1 | 2.25 | 0.48 |
| 1:C:204:PRO:HB2 | 1:C:247:THR:CG2 | 2.43 | 0.48 |
| 1:F:204:PRO:HD2 | 1:F:248:SER:O | 2.13 | 0.48 |
| 1:I:153:PHE:HA | 1:I:177:SER:O | 2.13 | 0.48 |
| 1:B:105:VAL:HA | 1:B:190:ALA:HB1 | 1.94 | 0.48 |
| 1:A:153:PHE:HA | 1:A:177:SER:O | 2.12 | 0.48 |
| 1:I:236:ASN:OD1 | 1:I:252:ASN:HA | 2.13 | 0.48 |
| 1:K:66:GLN:HG3 | 1:K:78:GLY:HA3 | 1.95 | 0.48 |
| 1:I:130:VAL:HG13 | 1:I:213:GLN:CD | 2.34 | 0.48 |
| 1:H:236:ASN:OD1 | 1:H:252:ASN:HA | 2.13 | 0.48 |
| 1:A:11:VAL:HG21 | 1:C:340:PHE:HB2 | 1.95 | 0.48 |
| 1:H:61:TRP:CZ2 | 1:H:63:TYR:HB2 | 2.48 | 0.48 |
| 1:A:3:ILE:HD12 | 1:C:3:ILE:HG21 | 1.95 | 0.48 |
| 1:J:269:LEU:HG | 1:J:271:PRO:HD3 | 1.95 | 0.48 |
| 1:L:294:TYR:CD1 | 1:L:294:TYR:C | 2.86 | 0.48 |
| 1:K:165:THR:CG2 | 1:K:167:ARG:H | 2.14 | 0.48 |
| 1:A:31:SER:CA | 1:A:329:ASP:HB2 | 2.40 | 0.48 |
| 1:A:264:GLN:OE1 | 1:A:270:ARG:HB2 | 2.12 | 0.48 |
| 1:L:204:PRO:HB2 | 1:L:247:THR:CG2 | 2.42 | 0.48 |
| 1:D:61:TRP:CZ2 | 1:D:63:TYR:HB2 | 2.48 | 0.48 |
| 1:A:161:ASN:HB2 | 1:A:170:ASN:OD1 | 2.13 | 0.48 |
| 1:C:294:TYR:C | 1:C:294:TYR:CD1 | 2.87 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:267:PHE:HD1 | 1:E:267:PHE:H | 1.62 | 0.48 |
| 1:A:204:PRO:HB2 | 1:A:247:THR:CG2 | 2.43 | 0.48 |
| 1:A:66:GLN:HG3 | 1:A:78:GLY:HA3 | 1.96 | 0.48 |
| 1:F:136:VAL:CG1 | 1:F:158:LEU:HD13 | 2.43 | 0.48 |
| 1:H:31:SER:CA | 1:H:329:ASP:HB2 | 2.39 | 0.48 |
| 1:E:204:PRO:HB2 | 1:E:247:THR:HG23 | 1.95 | 0.48 |
| 1:H:204:PRO:HB2 | 1:H:247:THR:CG2 | 2.43 | 0.48 |
| 1:J:105:VAL:HA | 1:J:190:ALA:HB1 | 1.96 | 0.48 |
| 1:L:153:PHE:HA | 1:L:177:SER:O | 2.13 | 0.48 |
| 1:I:61:TRP:CZ2 | 1:I:63:TYR:HB2 | 2.48 | 0.48 |
| 1:L:236:ASN:OD1 | 1:L:252:ASN:HA | 2.14 | 0.48 |
| 1:G:130:VAL:HG13 | 1:G:213:GLN:CD | 2.33 | 0.48 |
| 1:E:313:TYR:HD1 | 1:E:332:VAL:CG2 | 2.19 | 0.48 |
| 1:K:204:PRO:HB2 | 1:K:247:THR:HG23 | 1.95 | 0.48 |
| 1:E:31:SER:CA | 1:E:329:ASP:HB2 | 2.39 | 0.48 |
| 1:F:267:PHE:H | 1:F:267:PHE:HD1 | 1.60 | 0.48 |
| 1:B:222:ALA:O | 1:B:223:ASN:HB2 | 2.12 | 0.48 |
| 1:C:130:VAL:HG13 | 1:C:213:GLN:CD | 2.33 | 0.48 |
| 1:B:136:VAL:CG1 | 1:B:158:LEU:HD13 | 2.44 | 0.48 |
| 1:J:130:VAL:HG13 | 1:J:213:GLN:CD | 2.34 | 0.48 |
| 1:H:269:LEU:HG | 1:H:271:PRO:HD3 | 1.96 | 0.48 |
| 1:G:66:GLN:HG3 | 1:G:78:GLY:HA3 | 1.96 | 0.48 |
| 1:I:294:TYR:CD1 | 1:I:294:TYR:C | 2.87 | 0.48 |
| 1:B:294:TYR:C | 1:B:294:TYR:CD1 | 2.86 | 0.48 |
| 1:J:47:GLY:HA3 | 1:L:338:TYR:CE2 | 2.48 | 0.48 |
| 1:D:66:GLN:HG3 | 1:D:78:GLY:HA3 | 1.96 | 0.48 |
| 1:L:272:SER:N | 1:L:298:GLY:O | 2.44 | 0.48 |
| 1:D:130:VAL:HG13 | 1:D:213:GLN:CD | 2.34 | 0.48 |
| 1:D:236:ASN:OD1 | 1:D:252:ASN:HA | 2.14 | 0.48 |
| 1:E:294:TYR:C | 1:E:294:TYR:CD1 | 2.86 | 0.48 |
| 1:F:294:TYR:CD1 | 1:F:294:TYR:C | 2.86 | 0.48 |
| 1:J:165:THR:CG2 | 1:J:167:ARG:H | 2.16 | 0.48 |
| 1:C:264:GLN:OE1 | 1:C:270:ARG:HB2 | 2.14 | 0.48 |
| 1:L:267:PHE:HD1 | 1:L:267:PHE:H | 1.60 | 0.48 |
| 1:D:204:PRO:HD2 | 1:D:248:SER:O | 2.13 | 0.48 |
| 1:J:204:PRO:HD2 | 1:J:248:SER:O | 2.13 | 0.48 |
| 1:C:153:PHE:HA | 1:C:177:SER:O | 2.14 | 0.48 |
| 1:G:236:ASN:OD1 | 1:G:252:ASN:HA | 2.13 | 0.48 |
| 1:C:66:GLN:HG3 | 1:C:78:GLY:HA3 | 1.96 | 0.48 |
| 1:A:236:ASN:OD1 | 1:A:252:ASN:HA | 2.14 | 0.48 |
| 1:F:313:TYR:HD1 | 1:F:332:VAL:CG2 | 2.19 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:165:THR:HG22 | 1:G:166:ALA:N | 2.28 | 0.47 |
| 1:F:264:GLN:OE1 | 1:F:270:ARG:HB2 | 2.14 | 0.47 |
| 1:D:105:VAL:HA | 1:D:190:ALA:HB1 | 1.96 | 0.47 |
| 1:F:269:LEU:HG | 1:F:271:PRO:HD3 | 1.96 | 0.47 |
| 1:B:66:GLN:HG3 | 1:B:78:GLY:HA3 | 1.96 | 0.47 |
| 1:K:286:ILE:HG22 | 1:K:289:VAL:CG2 | 2.36 | 0.47 |
| 1:D:264:GLN:OE1 | 1:D:270:ARG:HB2 | 2.13 | 0.47 |
| 1:F:222:ALA:O | 1:F:223:ASN:HB2 | 2.13 | 0.47 |
| 1:D:204:PRO:HB2 | 1:D:247:THR:HG23 | 1.96 | 0.47 |
| 1:F:204:PRO:HB2 | 1:F:247:THR:CG2 | 2.43 | 0.47 |
| 1:I:105:VAL:HA | 1:I:190:ALA:HB1 | 1.96 | 0.47 |
| 1:G:340:PHE:CB | 1:H:11:VAL:HG21 | 2.43 | 0.47 |
| 1:J:273:ILE:CD1 | 1:J:297:VAL:HG22 | 2.45 | 0.47 |
| 1:B:165:THR:HG22 | 1:B:166:ALA:N | 2.29 | 0.47 |
| 1:J:165:THR:HG22 | 1:J:166:ALA:N | 2.29 | 0.47 |
| 1:K:31:SER:CA | 1:K:329:ASP:HB2 | 2.39 | 0.47 |
| 1:B:204:PRO:HB2 | 1:B:247:THR:HG23 | 1.96 | 0.47 |
| 1:L:169:SER:O | 1:L:170:ASN:HB3 | 2.15 | 0.47 |
| 1:F:61:TRP:CZ2 | 1:F:63:TYR:HB2 | 2.49 | 0.47 |
| 1:D:294:TYR:C | 1:D:294:TYR:CD1 | 2.88 | 0.47 |
| 1:A:136:VAL:CG1 | 1:A:158:LEU:HD13 | 2.44 | 0.47 |
| 1:C:31:SER:CA | 1:C:329:ASP:HB2 | 2.39 | 0.47 |
| 1:D:31:SER:CA | 1:D:329:ASP:HB2 | 2.41 | 0.47 |
| 1:H:267:PHE:HD1 | 1:H:267:PHE:H | 1.60 | 0.47 |
| 1:A:267:PHE:H | 1:A:267:PHE:HD1 | 1.60 | 0.47 |
| 1:E:338:TYR:CE2 | 1:F:47:GLY:HA3 | 2.49 | 0.47 |
| 1:D:153:PHE:HA | 1:D:177:SER:O | 2.13 | 0.47 |
| 1:D:165:THR:HG22 | 1:D:166:ALA:N | 2.29 | 0.47 |
| 1:B:286:ILE:HG22 | 1:B:289:VAL:CG2 | 2.37 | 0.47 |
| 1:G:286:ILE:HG22 | 1:G:289:VAL:CG2 | 2.38 | 0.47 |
| 1:C:267:PHE:H | 1:C:267:PHE:HD1 | 1.61 | 0.47 |
| 1:J:144:PHE:CD2 | 1:J:144:PHE:O | 2.68 | 0.47 |
| 1:G:303:PHE:CB | 1:H:51:ILE:HD13 | 2.42 | 0.47 |
| 1:E:61:TRP:CZ2 | 1:E:63:TYR:HB2 | 2.50 | 0.47 |
| 1:E:66:GLN:HG3 | 1:E:78:GLY:HA3 | 1.96 | 0.47 |
| 1:H:313:TYR:HD1 | 1:H:332:VAL:CG2 | 2.17 | 0.47 |
| 1:B:179:SER:HB3 | 1:B:188:VAL:HG13 | 1.96 | 0.47 |
| 1:E:169:SER:O | 1:E:170:ASN:HB3 | 2.15 | 0.47 |
| 1:C:61:TRP:CZ2 | 1:C:63:TYR:HB2 | 2.49 | 0.47 |
| 1:B:236:ASN:OD1 | 1:B:252:ASN:HA | 2.14 | 0.47 |
| 1:L:61:TRP:CZ2 | 1:L:63:TYR:HB2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:66:GLN:HG3 | 1:L:78:GLY:HA3 | 1.96 | 0.47 |
| 1:A:80:LYS:HD2 | 1:C:71:GLU:CB | 2.28 | 0.47 |
| 1:L:165:THR:HG22 | 1:L:166:ALA:N | 2.30 | 0.47 |
| 1:B:31:SER:CA | 1:B:329:ASP:HB2 | 2.41 | 0.47 |
| 1:B:303:PHE:HB3 | 1:C:51:ILE:CG2 | 2.44 | 0.47 |
| 1:G:144:PHE:CD2 | 1:G:144:PHE:O | 2.68 | 0.47 |
| 1:J:267:PHE:HD1 | 1:J:267:PHE:H | 1.62 | 0.47 |
| 1:D:267:PHE:H | 1:D:267:PHE:HD1 | 1.61 | 0.47 |
| 1:E:143:ASN:O | 1:E:144:PHE:C | 2.53 | 0.47 |
| 1:H:258:LEU:N | 1:H:258:LEU:HD22 | 2.30 | 0.47 |
| 1:H:153:PHE:HA | 1:H:177:SER:O | 2.13 | 0.47 |
| 1:D:169:SER:O | 1:D:170:ASN:HB3 | 2.14 | 0.47 |
| 1:C:161:ASN:HB2 | 1:C:170:ASN:OD1 | 2.13 | 0.47 |
| 1:A:130:VAL:HG13 | 1:A:213:GLN:CD | 2.35 | 0.47 |
| 1:F:236:ASN:OD1 | 1:F:252:ASN:HA | 2.14 | 0.47 |
| 1:H:294:TYR:C | 1:H:294:TYR:CD1 | 2.87 | 0.47 |
| 1:E:244:PHE:CZ | 1:K:285:GLY:HA2 | 2.50 | 0.47 |
| 1:G:264:GLN:OE1 | 1:G:270:ARG:HB2 | 2.14 | 0.47 |
| 1:K:105:VAL:HA | 1:K:190:ALA:HB1 | 1.96 | 0.47 |
| 1:H:105:VAL:HA | 1:H:190:ALA:HB1 | 1.96 | 0.47 |
| 1:F:169:SER:O | 1:F:170:ASN:HB3 | 2.14 | 0.47 |
| 1:K:61:TRP:CZ2 | 1:K:63:TYR:HB2 | 2.50 | 0.47 |
| 1:G:71:GLU:HG3 | 1:H:100:ARG:HH21 | 1.80 | 0.47 |
| 1:L:31:SER:CA | 1:L:329:ASP:HB2 | 2.39 | 0.47 |
| 1:I:269:LEU:HG | 1:I:271:PRO:HD3 | 1.96 | 0.47 |
| 1:C:269:LEU:HG | 1:C:271:PRO:HD3 | 1.97 | 0.47 |
| 1:B:165:THR:CG2 | 1:B:167:ARG:H | 2.15 | 0.47 |
| 1:C:286:ILE:N | 1:C:286:ILE:CD1 | 2.75 | 0.47 |
| 1:H:286:ILE:N | 1:H:286:ILE:CD1 | 2.73 | 0.47 |
| 1:B:204:PRO:HD2 | 1:B:248:SER:O | 2.14 | 0.47 |
| 1:L:204:PRO:HB2 | 1:L:247:THR:HG23 | 1.96 | 0.47 |
| 1:E:105:VAL:HA | 1:E:190:ALA:HB1 | 1.96 | 0.47 |
| 1:K:153:PHE:HA | 1:K:177:SER:O | 2.14 | 0.47 |
| 1:A:61:TRP:CZ2 | 1:A:63:TYR:HB2 | 2.50 | 0.47 |
| 1:L:313:TYR:HD1 | 1:L:332:VAL:CG2 | 2.17 | 0.46 |
| 1:G:204:PRO:HB2 | 1:G:247:THR:HG23 | 1.96 | 0.46 |
| 1:C:204:PRO:HB2 | 1:C:247:THR:HG23 | 1.98 | 0.46 |
| 1:B:51:ILE:HB | 1:B:55:LEU:HB3 | 1.98 | 0.46 |
| 1:G:258:LEU:HD13 | 1:G:276:THR:HG23 | 1.96 | 0.46 |
| 1:D:11:VAL:HG21 | 1:F:340:PHE:CB | 2.45 | 0.46 |
| 1:A:169:SER:O | 1:A:170:ASN:HB3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:269:LEU:HG | 1:E:271:PRO:HD3 | 1.96 | 0.46 |
| 1:E:340:PHE:HB2 | 1:F:11:VAL:HG21 | 1.97 | 0.46 |
| 1:J:3:ILE:HD12 | 1:L:3:ILE:HG21 | 1.97 | 0.46 |
| 1:K:303:PHE:HB3 | 1:L:51:ILE:HD13 | 1.98 | 0.46 |
| 1:F:272:SER:N | 1:F:298:GLY:O | 2.46 | 0.46 |
| 1:J:236:ASN:OD1 | 1:J:252:ASN:HA | 2.15 | 0.46 |
| 1:E:165:THR:HG22 | 1:E:166:ALA:N | 2.29 | 0.46 |
| 1:J:264:GLN:OE1 | 1:J:270:ARG:HB2 | 2.15 | 0.46 |
| 1:A:273:ILE:CD1 | 1:A:297:VAL:HG22 | 2.44 | 0.46 |
| 1:J:11:VAL:HG21 | 1:L:340:PHE:HB2 | 1.96 | 0.46 |
| 1:G:100:ARG:HH21 | 1:I:71:GLU:HG3 | 1.76 | 0.46 |
| 1:A:165:THR:HG22 | 1:A:166:ALA:N | 2.29 | 0.46 |
| 1:G:51:ILE:HD13 | 1:I:303:PHE:CG | 2.50 | 0.46 |
| 1:H:204:PRO:HB2 | 1:H:247:THR:HG23 | 1.96 | 0.46 |
| 1:H:143:ASN:O | 1:H:144:PHE:C | 2.54 | 0.46 |
| 1:K:191:TYR:CD1 | 1:K:214:TRP:HB3 | 2.49 | 0.46 |
| 1:D:303:PHE:CB | 1:E:51:ILE:HD13 | 2.44 | 0.46 |
| 1:K:273:ILE:CD1 | 1:K:297:VAL:HG22 | 2.46 | 0.46 |
| 1:K:165:THR:HG22 | 1:K:166:ALA:N | 2.30 | 0.46 |
| 1:E:204:PRO:HD2 | 1:E:248:SER:O | 2.15 | 0.46 |
| 1:G:191:TYR:CD1 | 1:G:214:TRP:HB3 | 2.48 | 0.46 |
| 1:A:204:PRO:HD2 | 1:A:248:SER:O | 2.15 | 0.46 |
| 1:K:144:PHE:CD2 | 1:K:144:PHE:O | 2.69 | 0.46 |
| 1:G:3:ILE:HG21 | 1:H:3:ILE:HD12 | 1.98 | 0.46 |
| 1:H:169:SER:O | 1:H:170:ASN:HB3 | 2.15 | 0.46 |
| 1:D:340:PHE:CB | 1:E:11:VAL:HG21 | 2.46 | 0.46 |
| 1:D:3:ILE:HG21 | 1:E:3:ILE:HD12 | 1.97 | 0.46 |
| 1:D:136:VAL:CG1 | 1:D:158:LEU:HD13 | 2.45 | 0.46 |
| 1:H:273:ILE:CD1 | 1:H:297:VAL:HG22 | 2.45 | 0.46 |
| 1:B:336:ILE:O | 1:B:336:ILE:HG23 | 2.16 | 0.46 |
| 1:E:309:THR:HG22 | 1:E:336:ILE:CA | 2.37 | 0.46 |
| 1:D:51:ILE:HD13 | 1:F:303:PHE:CG | 2.50 | 0.46 |
| 1:K:169:SER:O | 1:K:170:ASN:HB3 | 2.15 | 0.46 |
| 1:D:52:ASN:OD1 | 1:D:53:SER:N | 2.48 | 0.46 |
| 1:H:340:PHE:HB2 | 1:I:11:VAL:HG21 | 1.98 | 0.46 |
| 1:I:204:PRO:HB2 | 1:I:247:THR:HG23 | 1.96 | 0.46 |
| 1:E:144:PHE:CD2 | 1:E:144:PHE:O | 2.69 | 0.46 |
| 1:J:204:PRO:HB2 | 1:J:247:THR:HG23 | 1.97 | 0.46 |
| 1:L:105:VAL:HA | 1:L:190:ALA:HB1 | 1.96 | 0.46 |
| 1:A:11:VAL:HG21 | 1:C:340:PHE:CB | 2.46 | 0.46 |
| 1:J:191:TYR:CD1 | 1:J:214:TRP:HB3 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:143:ASN:O | 1:B:144:PHE:C | 2.53 | 0.46 |
| 1:A:143:ASN:O | 1:A:144:PHE:C | 2.54 | 0.46 |
| 1:A:204:PRO:HB2 | 1:A:247:THR:HG23 | 1.96 | 0.46 |
| 1:A:105:VAL:HA | 1:A:190:ALA:HB1 | 1.96 | 0.46 |
| 1:J:193:ALA:HA | 1:J:211:ALA:O | 2.16 | 0.46 |
| 1:B:61:TRP:CZ2 | 1:B:63:TYR:HB2 | 2.50 | 0.46 |
| 1:D:286:ILE:N | 1:D:286:ILE:CD1 | 2.74 | 0.46 |
| 1:F:143:ASN:O | 1:F:144:PHE:C | 2.54 | 0.46 |
| 1:A:191:TYR:CD1 | 1:A:214:TRP:HB3 | 2.48 | 0.46 |
| 1:F:204:PRO:HB2 | 1:F:247:THR:HG23 | 1.97 | 0.46 |
| 1:C:105:VAL:HA | 1:C:190:ALA:HB1 | 1.97 | 0.46 |
| 1:D:3:ILE:HD12 | 1:F:3:ILE:HG21 | 1.97 | 0.46 |
| 1:E:193:ALA:HA | 1:E:211:ALA:O | 2.16 | 0.46 |
| 1:K:193:ALA:HA | 1:K:211:ALA:O | 2.16 | 0.46 |
| 1:G:61:TRP:CZ2 | 1:G:63:TYR:HB2 | 2.50 | 0.46 |
| 1:J:100:ARG:HH21 | 1:L:71:GLU:HG3 | 1.77 | 0.46 |
| 1:I:165:THR:HG22 | 1:I:166:ALA:N | 2.30 | 0.46 |
| 1:F:309:THR:HG22 | 1:F:336:ILE:HG13 | 1.98 | 0.46 |
| 1:G:309:THR:HG22 | 1:G:336:ILE:HG13 | 1.98 | 0.46 |
| 1:L:286:ILE:HG23 | 1:L:323:LYS:CB | 2.46 | 0.46 |
| 1:D:143:ASN:O | 1:D:144:PHE:C | 2.55 | 0.46 |
| 1:I:51:ILE:HB | 1:I:55:LEU:HB3 | 1.97 | 0.46 |
| 1:J:169:SER:O | 1:J:170:ASN:HB3 | 2.16 | 0.46 |
| 1:J:61:TRP:CZ2 | 1:J:63:TYR:HB2 | 2.50 | 0.46 |
| 1:I:179:SER:HB3 | 1:I:188:VAL:HG13 | 1.98 | 0.46 |
| 1:I:191:TYR:CD1 | 1:I:214:TRP:HB3 | 2.49 | 0.46 |
| 1:I:144:PHE:CD2 | 1:I:144:PHE:O | 2.69 | 0.46 |
| 1:L:193:ALA:HA | 1:L:211:ALA:O | 2.16 | 0.46 |
| 1:B:287:GLY:CA | 1:L:321:ASP:OD2 | 2.61 | 0.45 |
| 1:H:71:GLU:HG3 | 1:I:100:ARG:HH21 | 1.78 | 0.45 |
| 1:C:165:THR:HG22 | 1:C:166:ALA:N | 2.30 | 0.45 |
| 1:B:267:PHE:H | 1:B:267:PHE:HD1 | 1.62 | 0.45 |
| 1:H:163:ARG:HD2 | 1:H:168:ARG:O | 2.16 | 0.45 |
| 1:B:193:ALA:HA | 1:B:211:ALA:O | 2.16 | 0.45 |
| 1:G:294:TYR:C | 1:G:294:TYR:CD1 | 2.88 | 0.45 |
| 1:F:165:THR:HG22 | 1:F:166:ALA:N | 2.31 | 0.45 |
| 1:H:165:THR:HG22 | 1:H:166:ALA:N | 2.30 | 0.45 |
| 1:I:169:SER:O | 1:I:170:ASN:HB3 | 2.16 | 0.45 |
| 1:G:193:ALA:HA | 1:G:211:ALA:O | 2.17 | 0.45 |
| 1:A:52:ASN:OD1 | 1:A:53:SER:N | 2.50 | 0.45 |
| 1:A:336:ILE:HG23 | 1:A:336:ILE:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:191:TYR:CD1 | 1:H:214:TRP:HB3 | 2.48 | 0.45 |
| 1:E:273:ILE:CD1 | 1:E:297:VAL:HG22 | 2.46 | 0.45 |
| 1:F:66:GLN:HG3 | 1:F:78:GLY:HA3 | 1.96 | 0.45 |
| 1:B:150:GLY:O | 1:B:180:TYR:HA | 2.17 | 0.45 |
| 1:K:71:GLU:CG | 1:L:100:ARG:NH2 | 2.70 | 0.45 |
| 1:C:309:THR:HG22 | 1:C:336:ILE:HG13 | 1.98 | 0.45 |
| 1:G:286:ILE:HG23 | 1:G:323:LYS:CB | 2.47 | 0.45 |
| 1:C:143:ASN:O | 1:C:144:PHE:C | 2.54 | 0.45 |
| 1:A:144:PHE:O | 1:A:144:PHE:CD2 | 2.70 | 0.45 |
| 1:K:51:ILE:HB | 1:K:55:LEU:HB3 | 1.99 | 0.45 |
| 1:I:193:ALA:HA | 1:I:211:ALA:O | 2.16 | 0.45 |
| 1:D:272:SER:N | 1:D:298:GLY:O | 2.43 | 0.45 |
| 1:G:309:THR:CG2 | 1:G:336:ILE:HG13 | 2.46 | 0.45 |
| 1:K:179:SER:HB3 | 1:K:188:VAL:HG13 | 1.97 | 0.45 |
| 1:F:51:ILE:HB | 1:F:55:LEU:HB3 | 1.99 | 0.45 |
| 1:E:258:LEU:N | 1:E:258:LEU:HD22 | 2.32 | 0.45 |
| 1:A:105:VAL:O | 1:A:105:VAL:CG1 | 2.65 | 0.45 |
| 1:D:269:LEU:HG | 1:D:271:PRO:HD3 | 1.98 | 0.45 |
| 1:J:52:ASN:OD1 | 1:J:53:SER:N | 2.50 | 0.45 |
| 1:A:269:LEU:HG | 1:A:271:PRO:HD3 | 1.99 | 0.45 |
| 1:G:273:ILE:CD1 | 1:G:297:VAL:HG22 | 2.47 | 0.45 |
| 1:B:269:LEU:HG | 1:B:271:PRO:HD3 | 1.98 | 0.45 |
| 1:H:193:ALA:HA | 1:H:211:ALA:O | 2.16 | 0.45 |
| 1:H:272:SER:N | 1:H:298:GLY:O | 2.46 | 0.45 |
| 1:K:336:ILE:HG23 | 1:K:336:ILE:O | 2.17 | 0.45 |
| 1:D:144:PHE:CD2 | 1:D:144:PHE:O | 2.70 | 0.45 |
| 1:J:338:TYR:CE2 | 1:K:47:GLY:HA3 | 2.52 | 0.45 |
| 1:F:105:VAL:HA | 1:F:190:ALA:HB1 | 1.97 | 0.45 |
| 1:J:11:VAL:HG21 | 1:L:340:PHE:CB | 2.47 | 0.45 |
| 1:J:66:GLN:HG3 | 1:J:78:GLY:HA3 | 1.98 | 0.45 |
| 1:L:309:THR:HG22 | 1:L:336:ILE:HG13 | 1.99 | 0.45 |
| 1:L:144:PHE:CD2 | 1:L:144:PHE:O | 2.70 | 0.45 |
| 1:G:169:SER:O | 1:G:170:ASN:HB3 | 2.16 | 0.45 |
| 1:B:3:ILE:HG21 | 1:C:3:ILE:HD12 | 1.99 | 0.45 |
| 1:F:193:ALA:HA | 1:F:211:ALA:O | 2.17 | 0.45 |
| 1:B:273:ILE:CD1 | 1:B:297:VAL:HG22 | 2.47 | 0.45 |
| 1:I:286:ILE:HG23 | 1:I:323:LYS:CB | 2.47 | 0.45 |
| 1:D:286:ILE:HG23 | 1:D:323:LYS:CB | 2.47 | 0.45 |
| 1:E:272:SER:N | 1:E:298:GLY:O | 2.45 | 0.45 |
| 1:I:150:GLY:O | 1:I:180:TYR:HA | 2.17 | 0.45 |
| 1:K:163:ARG:HD2 | 1:K:168:ARG:O | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:273:ILE:CD1 | 1:D:297:VAL:HG22 | 2.46 | 0.45 |
| 1:J:336:ILE:O | 1:J:336:ILE:HG23 | 2.17 | 0.45 |
| 1:H:179:SER:HB3 | 1:H:188:VAL:HG13 | 1.99 | 0.45 |
| 1:B:286:ILE:HG23 | 1:B:323:LYS:CB | 2.47 | 0.45 |
| 1:L:179:SER:HB3 | 1:L:188:VAL:HG13 | 1.97 | 0.45 |
| 1:I:143:ASN:O | 1:I:144:PHE:C | 2.55 | 0.45 |
| 1:L:273:ILE:CD1 | 1:L:297:VAL:HG22 | 2.46 | 0.45 |
| 1:C:193:ALA:HA | 1:C:211:ALA:O | 2.17 | 0.45 |
| 1:K:269:LEU:HG | 1:K:271:PRO:HD3 | 1.97 | 0.45 |
| 1:J:179:SER:HB3 | 1:J:188:VAL:HG13 | 1.98 | 0.45 |
| 1:B:191:TYR:CD1 | 1:B:214:TRP:HB3 | 2.49 | 0.45 |
| 1:K:143:ASN:O | 1:K:144:PHE:C | 2.56 | 0.45 |
| 1:L:258:LEU:N | 1:L:258:LEU:HD22 | 2.32 | 0.45 |
| 1:G:258:LEU:HD22 | 1:G:258:LEU:N | 2.32 | 0.45 |
| 1:B:169:SER:O | 1:B:170:ASN:HB3 | 2.16 | 0.45 |
| 1:C:163:ARG:HD2 | 1:C:168:ARG:O | 2.17 | 0.45 |
| 1:E:229:ALA:CB | 1:E:259:LEU:HD23 | 2.47 | 0.45 |
| 1:I:273:ILE:CD1 | 1:I:297:VAL:HG22 | 2.47 | 0.45 |
| 1:C:165:THR:CG2 | 1:C:167:ARG:H | 2.16 | 0.44 |
| 1:F:336:ILE:O | 1:F:336:ILE:HG23 | 2.17 | 0.44 |
| 1:C:51:ILE:HB | 1:C:55:LEU:HB3 | 1.99 | 0.44 |
| 1:D:51:ILE:HB | 1:D:55:LEU:HB3 | 1.99 | 0.44 |
| 1:A:258:LEU:N | 1:A:258:LEU:HD22 | 2.32 | 0.44 |
| 1:G:272:SER:N | 1:G:298:GLY:O | 2.44 | 0.44 |
| 1:C:287:GLY:CA | 1:G:321:ASP:CG | 2.67 | 0.44 |
| 1:E:309:THR:HG22 | 1:E:336:ILE:HG13 | 1.98 | 0.44 |
| 1:E:336:ILE:O | 1:E:336:ILE:HG23 | 2.16 | 0.44 |
| 1:A:286:ILE:HG23 | 1:A:323:LYS:CB | 2.47 | 0.44 |
| 1:G:51:ILE:HB | 1:G:55:LEU:HB3 | 1.99 | 0.44 |
| 1:C:258:LEU:HD22 | 1:C:258:LEU:N | 2.33 | 0.44 |
| 1:E:3:ILE:HG21 | 1:F:3:ILE:HD12 | 1.99 | 0.44 |
| 1:K:272:SER:N | 1:K:298:GLY:O | 2.45 | 0.44 |
| 1:A:309:THR:CG2 | 1:A:336:ILE:HG13 | 2.48 | 0.44 |
| 1:H:51:ILE:HB | 1:H:55:LEU:HB3 | 1.99 | 0.44 |
| 1:H:338:TYR:CE2 | 1:I:47:GLY:HA3 | 2.52 | 0.44 |
| 1:J:90:TYR:CD2 | 1:J:93:VAL:HG21 | 2.52 | 0.44 |
| 1:I:229:ALA:CB | 1:I:259:LEU:HD23 | 2.47 | 0.44 |
| 1:A:165:THR:CG2 | 1:A:167:ARG:H | 2.15 | 0.44 |
| 1:F:286:ILE:HG23 | 1:F:323:LYS:CB | 2.48 | 0.44 |
| 1:E:309:THR:CG2 | 1:E:336:ILE:HG13 | 2.48 | 0.44 |
| 1:H:286:ILE:HG23 | 1:H:323:LYS:CB | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:143:ASN:O | 1:L:144:PHE:C | 2.56 | 0.44 |
| 1:K:258:LEU:N | 1:K:258:LEU:HD22 | 2.32 | 0.44 |
| 1:H:303:PHE:CB | 1:I:51:ILE:HD13 | 2.48 | 0.44 |
| 1:J:303:PHE:CB | 1:K:51:ILE:HD13 | 2.47 | 0.44 |
| 1:A:51:ILE:HB | 1:A:55:LEU:HB3 | 1.98 | 0.44 |
| 1:H:3:ILE:HG21 | 1:I:3:ILE:HD12 | 1.99 | 0.44 |
| 1:A:229:ALA:CB | 1:A:259:LEU:HD23 | 2.47 | 0.44 |
| 1:I:309:THR:HG22 | 1:I:336:ILE:HG13 | 1.98 | 0.44 |
| 1:L:51:ILE:HB | 1:L:55:LEU:HB3 | 1.99 | 0.44 |
| 1:A:193:ALA:HA | 1:A:211:ALA:O | 2.17 | 0.44 |
| 1:I:163:ARG:HD2 | 1:I:168:ARG:O | 2.18 | 0.44 |
| 1:D:71:GLU:HG3 | 1:E:100:ARG:HH21 | 1.81 | 0.44 |
| 1:J:309:THR:CG2 | 1:J:336:ILE:HG13 | 2.48 | 0.44 |
| 1:F:309:THR:CG2 | 1:F:336:ILE:HG13 | 2.47 | 0.44 |
| 1:C:309:THR:CG2 | 1:C:336:ILE:HG13 | 2.47 | 0.44 |
| 1:L:336:ILE:O | 1:L:336:ILE:HG23 | 2.17 | 0.44 |
| 1:B:144:PHE:CD2 | 1:B:144:PHE:O | 2.70 | 0.44 |
| 1:D:51:ILE:HG21 | 1:F:303:PHE:HB3 | 2.00 | 0.44 |
| 1:J:51:ILE:HB | 1:J:55:LEU:HB3 | 2.00 | 0.44 |
| 1:G:235:ARG:HA | 1:G:235:ARG:HD3 | 1.79 | 0.44 |
| 1:J:54:ASP:HB3 | 1:J:91:ALA:HB2 | 2.00 | 0.44 |
| 1:B:283:VAL:O | 1:B:284:GLU:C | 2.56 | 0.44 |
| 1:E:71:GLU:CG | 1:F:100:ARG:HH21 | 2.31 | 0.44 |
| 1:K:286:ILE:HG23 | 1:K:323:LYS:CB | 2.48 | 0.44 |
| 1:F:144:PHE:CD2 | 1:F:144:PHE:O | 2.71 | 0.44 |
| 1:I:235:ARG:HD3 | 1:I:235:ARG:HA | 1.80 | 0.44 |
| 1:E:90:TYR:CD2 | 1:E:93:VAL:HG21 | 2.53 | 0.44 |
| 1:D:336:ILE:HG23 | 1:D:336:ILE:O | 2.17 | 0.44 |
| 1:E:286:ILE:HG23 | 1:E:323:LYS:CB | 2.47 | 0.44 |
| 1:K:309:THR:HG22 | 1:K:336:ILE:HG13 | 2.00 | 0.44 |
| 1:I:336:ILE:HG23 | 1:I:336:ILE:O | 2.17 | 0.44 |
| 1:I:31:SER:CA | 1:I:329:ASP:HB2 | 2.40 | 0.44 |
| 1:C:191:TYR:CD1 | 1:C:214:TRP:HB3 | 2.48 | 0.44 |
| 1:G:105:VAL:O | 1:G:105:VAL:CG1 | 2.66 | 0.44 |
| 1:C:105:VAL:O | 1:C:105:VAL:CG1 | 2.66 | 0.44 |
| 1:G:269:LEU:HG | 1:G:271:PRO:HD3 | 1.99 | 0.44 |
| 1:I:313:TYR:HD1 | 1:I:332:VAL:CG2 | 2.17 | 0.44 |
| 1:C:179:SER:HB3 | 1:C:188:VAL:HG13 | 1.99 | 0.44 |
| 1:J:143:ASN:O | 1:J:144:PHE:C | 2.56 | 0.44 |
| 1:L:273:ILE:HA | 1:L:273:ILE:HD13 | 1.86 | 0.44 |
| 1:J:272:SER:N | 1:J:298:GLY:O | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:229:ALA:CB | 1:B:259:LEU:HD23 | 2.48 | 0.44 |
| 1:E:52:ASN:OD1 | 1:E:53:SER:N | 2.51 | 0.44 |
| 1:G:336:ILE:O | 1:G:336:ILE:HG23 | 2.17 | 0.43 |
| 1:J:286:ILE:HG23 | 1:J:323:LYS:CB | 2.48 | 0.43 |
| 1:E:51:ILE:HB | 1:E:55:LEU:HB3 | 1.99 | 0.43 |
| 1:K:283:VAL:O | 1:K:284:GLU:C | 2.56 | 0.43 |
| 1:C:229:ALA:CB | 1:C:259:LEU:HD23 | 2.47 | 0.43 |
| 1:H:235:ARG:HA | 1:H:235:ARG:HD3 | 1.80 | 0.43 |
| 1:C:336:ILE:HG23 | 1:C:336:ILE:O | 2.17 | 0.43 |
| 1:A:286:ILE:CD1 | 1:A:286:ILE:N | 2.73 | 0.43 |
| 1:G:303:PHE:CG | 1:H:51:ILE:HD13 | 2.53 | 0.43 |
| 1:H:150:GLY:O | 1:H:180:TYR:HA | 2.19 | 0.43 |
| 1:A:272:SER:N | 1:A:298:GLY:O | 2.46 | 0.43 |
| 1:B:272:SER:N | 1:B:298:GLY:O | 2.44 | 0.43 |
| 1:B:52:ASN:OD1 | 1:B:53:SER:N | 2.50 | 0.43 |
| 1:G:229:ALA:CB | 1:G:259:LEU:HD23 | 2.48 | 0.43 |
| 1:C:272:SER:N | 1:C:298:GLY:O | 2.44 | 0.43 |
| 1:D:71:GLU:CB | 1:E:80:LYS:HD2 | 2.26 | 0.43 |
| 1:A:309:THR:HG22 | 1:A:336:ILE:HG13 | 2.00 | 0.43 |
| 1:J:309:THR:HG22 | 1:J:336:ILE:HG13 | 1.99 | 0.43 |
| 1:E:286:ILE:HG23 | 1:E:323:LYS:HB3 | 2.00 | 0.43 |
| 1:B:258:LEU:HD22 | 1:B:258:LEU:N | 2.33 | 0.43 |
| 1:H:144:PHE:CD2 | 1:H:144:PHE:O | 2.71 | 0.43 |
| 1:A:303:PHE:CB | 1:B:51:ILE:HD13 | 2.48 | 0.43 |
| 1:E:303:PHE:CG | 1:F:51:ILE:HD13 | 2.54 | 0.43 |
| 1:D:163:ARG:HD2 | 1:D:168:ARG:O | 2.19 | 0.43 |
| 1:H:309:THR:HG22 | 1:H:336:ILE:HG13 | 2.00 | 0.43 |
| 1:G:179:SER:HB3 | 1:G:188:VAL:HG13 | 2.00 | 0.43 |
| 1:A:111:TYR:OH | 1:A:188:VAL:HG23 | 2.18 | 0.43 |
| 1:C:144:PHE:O | 1:C:144:PHE:CD2 | 2.72 | 0.43 |
| 1:D:105:VAL:CG1 | 1:D:105:VAL:O | 2.66 | 0.43 |
| 1:C:169:SER:O | 1:C:170:ASN:HB3 | 2.18 | 0.43 |
| 1:G:90:TYR:CD2 | 1:G:93:VAL:HG21 | 2.54 | 0.43 |
| 1:F:283:VAL:O | 1:F:284:GLU:C | 2.56 | 0.43 |
| 1:K:229:ALA:CB | 1:K:259:LEU:HD23 | 2.48 | 0.43 |
| 1:D:150:GLY:O | 1:D:180:TYR:HA | 2.19 | 0.43 |
| 1:F:165:THR:CG2 | 1:F:167:ARG:H | 2.16 | 0.43 |
| 1:D:309:THR:HG22 | 1:D:336:ILE:HG13 | 2.00 | 0.43 |
| 1:I:286:ILE:HG23 | 1:I:323:LYS:HB3 | 2.01 | 0.43 |
| 1:C:286:ILE:HG23 | 1:C:323:LYS:CB | 2.48 | 0.43 |
| 1:D:179:SER:HB3 | 1:D:188:VAL:HG13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:143:ASN:O | 1:G:144:PHE:C | 2.57 | 0.43 |
| 1:A:338:TYR:CE2 | 1:B:47:GLY:HA3 | 2.52 | 0.43 |
| 1:A:55:LEU:HD12 | 1:A:55:LEU:HA | 1.90 | 0.43 |
| 1:D:193:ALA:HA | 1:D:211:ALA:O | 2.18 | 0.43 |
| 1:H:229:ALA:CB | 1:H:259:LEU:HD23 | 2.49 | 0.43 |
| 1:A:340:PHE:HB2 | 1:B:11:VAL:HG21 | 2.00 | 0.43 |
| 1:F:273:ILE:CD1 | 1:F:297:VAL:HG22 | 2.49 | 0.43 |
| 1:F:52:ASN:OD1 | 1:F:53:SER:N | 2.51 | 0.43 |
| 1:D:229:ALA:CB | 1:D:259:LEU:HD23 | 2.48 | 0.43 |
| 1:E:163:ARG:HD2 | 1:E:168:ARG:O | 2.19 | 0.43 |
| 1:K:309:THR:CG2 | 1:K:336:ILE:HG13 | 2.49 | 0.43 |
| 1:H:336:ILE:O | 1:H:336:ILE:HG23 | 2.19 | 0.43 |
| 1:L:309:THR:CG2 | 1:L:336:ILE:HG13 | 2.49 | 0.43 |
| 1:C:285:GLY:CA | 1:G:244:PHE:HZ | 2.31 | 0.43 |
| 1:B:115:LEU:HD21 | 1:B:274:ALA:HB2 | 2.01 | 0.43 |
| 1:G:12:ASP:O | 1:G:45:PHE:HA | 2.18 | 0.43 |
| 1:E:340:PHE:CB | 1:F:11:VAL:HG21 | 2.49 | 0.43 |
| 1:L:54:ASP:HB3 | 1:L:91:ALA:HB2 | 2.01 | 0.43 |
| 1:D:309:THR:CG2 | 1:D:336:ILE:HG13 | 2.48 | 0.43 |
| 1:G:51:ILE:HG21 | 1:I:303:PHE:HB3 | 2.01 | 0.43 |
| 1:F:235:ARG:HD3 | 1:F:235:ARG:HA | 1.80 | 0.43 |
| 1:L:150:GLY:O | 1:L:180:TYR:HA | 2.19 | 0.43 |
| 1:B:235:ARG:NH2 | 1:B:253:LYS:HZ3 | 2.17 | 0.43 |
| 1:C:235:ARG:HA | 1:C:235:ARG:HD3 | 1.80 | 0.43 |
| 1:B:313:TYR:HD1 | 1:B:332:VAL:CG2 | 2.19 | 0.43 |
| 1:B:309:THR:CG2 | 1:B:336:ILE:HG13 | 2.49 | 0.43 |
| 1:G:31:SER:CA | 1:G:329:ASP:HB2 | 2.39 | 0.43 |
| 1:B:286:ILE:HG23 | 1:B:323:LYS:HB3 | 2.00 | 0.43 |
| 1:G:286:ILE:HG23 | 1:G:323:LYS:HB3 | 2.01 | 0.43 |
| 1:K:267:PHE:HD1 | 1:K:267:PHE:H | 1.62 | 0.43 |
| 1:I:12:ASP:O | 1:I:45:PHE:HA | 2.19 | 0.43 |
| 1:I:45:PHE:C | 1:I:45:PHE:CD1 | 2.92 | 0.43 |
| 1:H:244:PHE:CZ | 1:L:285:GLY:CA | 3.02 | 0.43 |
| 1:E:235:ARG:NH2 | 1:E:253:LYS:HZ3 | 2.17 | 0.43 |
| 1:L:229:ALA:CB | 1:L:259:LEU:HD23 | 2.49 | 0.43 |
| 1:F:229:ALA:CB | 1:F:259:LEU:HD23 | 2.48 | 0.43 |
| 1:C:273:ILE:CD1 | 1:C:297:VAL:HG22 | 2.49 | 0.43 |
| 1:G:165:THR:CG2 | 1:G:167:ARG:H | 2.16 | 0.42 |
| 1:K:286:ILE:HG23 | 1:K:323:LYS:HB3 | 2.01 | 0.42 |
| 1:F:179:SER:HB3 | 1:F:188:VAL:HG13 | 2.01 | 0.42 |
| 1:H:340:PHE:CB | 1:I:11:VAL:HG21 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:283:VAL:O | 1:J:284:GLU:C | 2.57 | 0.42 |
| 1:L:283:VAL:O | 1:L:284:GLU:C | 2.57 | 0.42 |
| 1:L:52:ASN:OD1 | 1:L:53:SER:N | 2.52 | 0.42 |
| 1:J:229:ALA:CB | 1:J:259:LEU:HD23 | 2.48 | 0.42 |
| 1:I:272:SER:N | 1:I:298:GLY:O | 2.45 | 0.42 |
| 1:J:313:TYR:HD1 | 1:J:332:VAL:CG2 | 2.17 | 0.42 |
| 1:D:100:ARG:NH2 | 1:F:71:GLU:CG | 2.73 | 0.42 |
| 1:A:71:GLU:HG3 | 1:B:100:ARG:HH21 | 1.80 | 0.42 |
| 1:J:286:ILE:HG23 | 1:J:323:LYS:HB3 | 2.01 | 0.42 |
| 1:C:235:ARG:NH2 | 1:C:253:LYS:HZ3 | 2.16 | 0.42 |
| 1:C:54:ASP:HB3 | 1:C:91:ALA:HB2 | 2.01 | 0.42 |
| 1:G:150:GLY:O | 1:G:180:TYR:HA | 2.19 | 0.42 |
| 1:L:90:TYR:CD2 | 1:L:93:VAL:HG21 | 2.54 | 0.42 |
| 1:B:287:GLY:N | 1:L:321:ASP:OD1 | 2.45 | 0.42 |
| 1:L:265:PHE:CB | 1:L:267:PHE:CE1 | 3.02 | 0.42 |
| 1:E:235:ARG:NE | 1:E:253:LYS:HG2 | 2.34 | 0.42 |
| 1:H:283:VAL:O | 1:H:284:GLU:C | 2.57 | 0.42 |
| 1:B:309:THR:HG22 | 1:B:336:ILE:HG13 | 2.00 | 0.42 |
| 1:K:179:SER:HB2 | 1:K:188:VAL:HG22 | 2.02 | 0.42 |
| 1:C:55:LEU:HD12 | 1:C:55:LEU:HA | 1.89 | 0.42 |
| 1:L:12:ASP:O | 1:L:45:PHE:HA | 2.19 | 0.42 |
| 1:H:235:ARG:NE | 1:H:253:LYS:HG2 | 2.33 | 0.42 |
| 1:D:283:VAL:O | 1:D:284:GLU:C | 2.57 | 0.42 |
| 1:A:150:GLY:O | 1:A:180:TYR:HA | 2.19 | 0.42 |
| 1:K:90:TYR:CD2 | 1:K:93:VAL:HG21 | 2.54 | 0.42 |
| 1:E:179:SER:HB3 | 1:E:188:VAL:HG13 | 2.01 | 0.42 |
| 1:I:258:LEU:HD22 | 1:I:258:LEU:N | 2.34 | 0.42 |
| 1:L:136:VAL:CG1 | 1:L:158:LEU:CD1 | 2.98 | 0.42 |
| 1:H:235:ARG:NH2 | 1:H:253:LYS:HZ3 | 2.17 | 0.42 |
| 1:A:283:VAL:O | 1:A:284:GLU:C | 2.58 | 0.42 |
| 1:E:150:GLY:O | 1:E:180:TYR:HA | 2.19 | 0.42 |
| 1:I:309:THR:CG2 | 1:I:336:ILE:HG13 | 2.49 | 0.42 |
| 1:A:179:SER:HB3 | 1:A:188:VAL:HG13 | 2.01 | 0.42 |
| 1:I:285:GLY:HA3 | 1:K:244:PHE:CZ | 2.54 | 0.42 |
| 1:H:90:TYR:CD2 | 1:H:93:VAL:HG21 | 2.54 | 0.42 |
| 1:L:286:ILE:HG23 | 1:L:323:LYS:HB3 | 2.00 | 0.42 |
| 1:H:309:THR:CG2 | 1:H:336:ILE:HG13 | 2.50 | 0.42 |
| 1:E:303:PHE:HB3 | 1:F:51:ILE:HG21 | 2.01 | 0.42 |
| 1:F:258:LEU:N | 1:F:258:LEU:HD22 | 2.34 | 0.42 |
| 1:D:258:LEU:HD22 | 1:D:258:LEU:N | 2.35 | 0.42 |
| 1:B:12:ASP:O | 1:B:45:PHE:HA | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:273:ILE:HD13 | 1:D:273:ILE:HA | 1.86 | 0.42 |
| 1:L:231:TYR:HD1 | 1:L:257:VAL:HG22 | 1.85 | 0.42 |
| 1:C:52:ASN:OD1 | 1:C:53:SER:N | 2.53 | 0.42 |
| 1:H:71:GLU:CG | 1:I:100:ARG:HH21 | 2.32 | 0.42 |
| 1:E:283:VAL:O | 1:E:284:GLU:C | 2.58 | 0.42 |
| 1:K:54:ASP:HB3 | 1:K:91:ALA:HB2 | 2.02 | 0.42 |
| 1:K:235:ARG:NE | 1:K:253:LYS:HG2 | 2.35 | 0.42 |
| 1:G:283:VAL:O | 1:G:284:GLU:C | 2.57 | 0.42 |
| 1:F:54:ASP:HB3 | 1:F:91:ALA:HB2 | 2.02 | 0.42 |
| 1:J:100:ARG:HH21 | 1:L:71:GLU:CG | 2.32 | 0.42 |
| 1:A:286:ILE:HG23 | 1:A:323:LYS:HB3 | 2.00 | 0.42 |
| 1:J:303:PHE:CG | 1:K:51:ILE:HD13 | 2.55 | 0.42 |
| 1:K:12:ASP:O | 1:K:45:PHE:HA | 2.20 | 0.42 |
| 1:F:235:ARG:NE | 1:F:253:LYS:HG2 | 2.35 | 0.42 |
| 1:G:54:ASP:HB3 | 1:G:91:ALA:HB2 | 2.02 | 0.42 |
| 1:D:54:ASP:HB3 | 1:D:91:ALA:HB2 | 2.02 | 0.42 |
| 1:B:55:LEU:HA | 1:B:55:LEU:HD12 | 1.91 | 0.42 |
| 1:C:283:VAL:O | 1:C:284:GLU:C | 2.58 | 0.42 |
| 1:F:150:GLY:O | 1:F:180:TYR:HA | 2.20 | 0.42 |
| 1:A:54:ASP:HB3 | 1:A:91:ALA:HB2 | 2.02 | 0.42 |
| 1:H:286:ILE:HG23 | 1:H:323:LYS:HB3 | 2.01 | 0.41 |
| 1:B:179:SER:HB2 | 1:B:188:VAL:HG22 | 2.02 | 0.41 |
| 1:H:265:PHE:CB | 1:H:267:PHE:CE1 | 3.02 | 0.41 |
| 1:L:191:TYR:CD1 | 1:L:214:TRP:HB3 | 2.49 | 0.41 |
| 1:H:45:PHE:CD1 | 1:H:45:PHE:C | 2.93 | 0.41 |
| 1:K:105:VAL:O | 1:K:105:VAL:CG1 | 2.67 | 0.41 |
| 1:A:90:TYR:CD2 | 1:A:93:VAL:HG21 | 2.55 | 0.41 |
| 1:K:52:ASN:OD1 | 1:K:53:SER:N | 2.53 | 0.41 |
| 1:F:90:TYR:CD2 | 1:F:93:VAL:HG21 | 2.55 | 0.41 |
| 1:H:52:ASN:OD1 | 1:H:53:SER:N | 2.53 | 0.41 |
| 1:D:286:ILE:HG23 | 1:D:323:LYS:HB3 | 2.01 | 0.41 |
| 1:L:45:PHE:CD1 | 1:L:45:PHE:C | 2.93 | 0.41 |
| 1:J:105:VAL:CG1 | 1:J:105:VAL:O | 2.67 | 0.41 |
| 1:C:1:ALA:N | 1:C:340:PHE:OXT | 2.42 | 0.41 |
| 1:K:150:GLY:O | 1:K:180:TYR:HA | 2.19 | 0.41 |
| 1:G:163:ARG:HD2 | 1:G:168:ARG:O | 2.20 | 0.41 |
| 1:A:163:ARG:HD2 | 1:A:168:ARG:O | 2.20 | 0.41 |
| 1:G:100:ARG:HH21 | 1:I:71:GLU:CG | 2.34 | 0.41 |
| 1:K:71:GLU:CD | 1:L:100:ARG:HH21 | 2.24 | 0.41 |
| 1:J:309:THR:HG22 | 1:J:336:ILE:CB | 2.51 | 0.41 |
| 1:L:223:ASN:O | 1:L:224:ASN:CB | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:12:ASP:O | 1:H:45:PHE:HA | 2.19 | 0.41 |
| 1:E:12:ASP:O | 1:E:45:PHE:HA | 2.20 | 0.41 |
| 1:I:180:TYR:CE2 | 1:I:182:TYR:HB2 | 2.55 | 0.41 |
| 1:B:54:ASP:HB3 | 1:B:91:ALA:HB2 | 2.01 | 0.41 |
| 1:G:115:LEU:HD21 | 1:G:274:ALA:HB2 | 2.02 | 0.41 |
| 1:C:150:GLY:O | 1:C:180:TYR:HA | 2.19 | 0.41 |
| 1:E:265:PHE:CB | 1:E:267:PHE:CE1 | 3.02 | 0.41 |
| 1:G:203:GLN:HA | 1:G:204:PRO:HD3 | 1.86 | 0.41 |
| 1:J:303:PHE:HB3 | 1:K:51:ILE:HG21 | 2.01 | 0.41 |
| 1:L:163:ARG:HD2 | 1:L:168:ARG:O | 2.20 | 0.41 |
| 1:B:163:ARG:HD2 | 1:B:168:ARG:O | 2.20 | 0.41 |
| 1:A:309:THR:HG22 | 1:A:336:ILE:CB | 2.50 | 0.41 |
| 1:C:286:ILE:HG23 | 1:C:323:LYS:HB3 | 2.03 | 0.41 |
| 1:C:174:VAL:CG1 | 1:C:175:GLY:H | 2.34 | 0.41 |
| 1:H:104:VAL:HG13 | 1:H:156:GLN:HB2 | 2.03 | 0.41 |
| 1:I:235:ARG:NE | 1:I:253:LYS:HG2 | 2.35 | 0.41 |
| 1:F:253:LYS:HD2 | 1:F:254:THR:N | 2.36 | 0.41 |
| 1:K:115:LEU:HD21 | 1:K:274:ALA:HB2 | 2.03 | 0.41 |
| 1:E:54:ASP:HB3 | 1:E:91:ALA:HB2 | 2.01 | 0.41 |
| 1:D:142:SER:HA | 1:D:152:ASN:OD1 | 2.21 | 0.41 |
| 1:F:45:PHE:CD1 | 1:F:45:PHE:C | 2.94 | 0.41 |
| 1:G:1:ALA:N | 1:G:340:PHE:OXT | 2.41 | 0.41 |
| 1:H:235:ARG:NH2 | 1:H:253:LYS:NZ | 2.69 | 0.41 |
| 1:I:90:TYR:CD2 | 1:I:93:VAL:HG21 | 2.55 | 0.41 |
| 1:G:52:ASN:OD1 | 1:G:53:SER:N | 2.53 | 0.41 |
| 1:I:52:ASN:OD1 | 1:I:53:SER:N | 2.53 | 0.41 |
| 1:G:104:VAL:HG13 | 1:G:156:GLN:HB2 | 2.03 | 0.41 |
| 1:A:45:PHE:CD1 | 1:A:45:PHE:C | 2.93 | 0.41 |
| 1:G:235:ARG:NE | 1:G:253:LYS:HG2 | 2.36 | 0.41 |
| 1:A:244:PHE:CZ | 1:J:285:GLY:HA3 | 2.55 | 0.41 |
| 1:A:235:ARG:HA | 1:A:235:ARG:HD3 | 1.80 | 0.41 |
| 1:A:100:ARG:HH21 | 1:C:71:GLU:CG | 2.32 | 0.41 |
| 1:J:31:SER:CA | 1:J:329:ASP:HB2 | 2.40 | 0.41 |
| 1:A:179:SER:HB2 | 1:A:188:VAL:HG22 | 2.03 | 0.41 |
| 1:D:51:ILE:CG2 | 1:F:303:PHE:HB3 | 2.50 | 0.41 |
| 1:I:115:LEU:HD13 | 1:I:296:GLU:HG3 | 2.03 | 0.41 |
| 1:J:51:ILE:HG21 | 1:L:303:PHE:HB3 | 2.03 | 0.41 |
| 1:J:258:LEU:HD22 | 1:J:258:LEU:N | 2.36 | 0.41 |
| 1:F:105:VAL:CG1 | 1:F:105:VAL:O | 2.69 | 0.41 |
| 1:B:235:ARG:NE | 1:B:253:LYS:HG2 | 2.35 | 0.41 |
| 1:L:235:ARG:NE | 1:L:253:LYS:HG2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:340:PHE:HB2 | 1:K:11:VAL:HG21 | 2.03 | 0.41 |
| 1:J:1:ALA:N | 1:J:340:PHE:OXT | 2.42 | 0.41 |
| 1:D:253:LYS:HD2 | 1:D:254:THR:N | 2.36 | 0.41 |
| 1:K:313:TYR:HD1 | 1:K:332:VAL:CG2 | 2.18 | 0.41 |
| 1:B:309:THR:HG22 | 1:B:336:ILE:CB | 2.51 | 0.41 |
| 1:F:286:ILE:HG23 | 1:F:323:LYS:HB3 | 2.02 | 0.41 |
| 1:L:309:THR:HG22 | 1:L:336:ILE:CB | 2.51 | 0.41 |
| 1:D:174:VAL:HG12 | 1:D:175:GLY:H | 1.84 | 0.41 |
| 1:D:174:VAL:CG1 | 1:D:175:GLY:H | 2.33 | 0.41 |
| 1:G:143:ASN:CA | 1:G:148:VAL:O | 2.69 | 0.41 |
| 1:D:55:LEU:HD12 | 1:D:55:LEU:HA | 1.90 | 0.41 |
| 1:I:115:LEU:HD21 | 1:I:274:ALA:HB2 | 2.02 | 0.41 |
| 1:B:115:LEU:HD13 | 1:B:296:GLU:HG3 | 2.02 | 0.41 |
| 1:B:45:PHE:C | 1:B:45:PHE:CD1 | 2.94 | 0.41 |
| 1:E:45:PHE:C | 1:E:45:PHE:CD1 | 2.93 | 0.41 |
| 1:J:45:PHE:C | 1:J:45:PHE:CD1 | 2.94 | 0.41 |
| 1:K:45:PHE:CD1 | 1:K:45:PHE:C | 2.94 | 0.41 |
| 1:I:136:VAL:CG1 | 1:I:158:LEU:CD1 | 2.99 | 0.41 |
| 1:D:1:ALA:N | 1:D:340:PHE:OXT | 2.44 | 0.41 |
| 1:A:235:ARG:NE | 1:A:253:LYS:HG2 | 2.36 | 0.41 |
| 1:B:90:TYR:CD2 | 1:B:93:VAL:HG21 | 2.55 | 0.41 |
| 1:H:24:SER:H | 1:H:35:ASN:ND2 | 2.19 | 0.41 |
| 1:J:150:GLY:O | 1:J:180:TYR:HA | 2.20 | 0.41 |
| 1:E:174:VAL:CG1 | 1:E:175:GLY:H | 2.35 | 0.41 |
| 1:L:115:LEU:HD21 | 1:L:274:ALA:HB2 | 2.03 | 0.41 |
| 1:F:163:ARG:HD2 | 1:F:168:ARG:O | 2.21 | 0.41 |
| 1:I:54:ASP:HB3 | 1:I:91:ALA:HB2 | 2.02 | 0.41 |
| 1:E:124:TYR:O | 1:E:131:GLY:HA3 | 2.21 | 0.41 |
| 1:L:64:ASN:O | 1:L:79:ASN:HA | 2.21 | 0.41 |
| 1:J:163:ARG:HD2 | 1:J:168:ARG:O | 2.21 | 0.41 |
| 1:H:54:ASP:HB3 | 1:H:91:ALA:HB2 | 2.02 | 0.41 |
| 1:G:71:GLU:CB | 1:H:80:LYS:HD2 | 2.25 | 0.40 |
| 1:I:105:VAL:CG1 | 1:I:105:VAL:O | 2.68 | 0.40 |
| 1:A:253:LYS:HD2 | 1:A:254:THR:N | 2.36 | 0.40 |
| 1:F:231:TYR:HD1 | 1:F:257:VAL:HG22 | 1.86 | 0.40 |
| 1:I:124:TYR:O | 1:I:131:GLY:HA3 | 2.21 | 0.40 |
| 1:D:111:TYR:OH | 1:D:188:VAL:HG23 | 2.21 | 0.40 |
| 1:E:203:GLN:HA | 1:E:204:PRO:HD3 | 1.86 | 0.40 |
| 1:I:265:PHE:CB | 1:I:267:PHE:CE1 | 3.04 | 0.40 |
| 1:B:105:VAL:O | 1:B:105:VAL:CG1 | 2.68 | 0.40 |
| 1:G:265:PHE:CB | 1:G:267:PHE:CE1 | 3.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:45:PHE:C | 1:G:45:PHE:CD1 | 2.94 | 0.40 |
| 1:H:136:VAL:CG1 | 1:H:158:LEU:CD1 | 2.99 | 0.40 |
| 1:J:180:TYR:CE2 | 1:J:182:TYR:HB2 | 2.56 | 0.40 |
| 1:I:231:TYR:HD1 | 1:I:257:VAL:HG22 | 1.86 | 0.40 |
| 1:I:283:VAL:O | 1:I:284:GLU:C | 2.60 | 0.40 |
| 1:K:309:THR:HG22 | 1:K:336:ILE:CB | 2.51 | 0.40 |
| 1:K:265:PHE:CB | 1:K:267:PHE:CE1 | 3.03 | 0.40 |
| 1:J:51:ILE:HD13 | 1:L:303:PHE:CG | 2.56 | 0.40 |
| 1:D:12:ASP:O | 1:D:45:PHE:HA | 2.22 | 0.40 |
| 1:G:136:VAL:CG1 | 1:G:158:LEU:CD1 | 3.00 | 0.40 |
| 1:K:206:GLY:H | 1:K:284:GLU:CD | 2.25 | 0.40 |
| 1:A:340:PHE:CB | 1:B:11:VAL:HG21 | 2.52 | 0.40 |
| 1:F:64:ASN:O | 1:F:79:ASN:HA | 2.22 | 0.40 |
| 1:A:115:LEU:HD23 | 1:A:115:LEU:N | 2.36 | 0.40 |
| 1:D:115:LEU:HD21 | 1:D:274:ALA:HB2 | 2.04 | 0.40 |
| 1:C:309:THR:HG22 | 1:C:336:ILE:CB | 2.52 | 0.40 |
| 1:G:309:THR:HG22 | 1:G:336:ILE:CB | 2.51 | 0.40 |
| 1:K:111:TYR:OH | 1:K:188:VAL:HG23 | 2.17 | 0.40 |
| 1:L:126:ASP:HA | 1:L:133:VAL:HG12 | 2.04 | 0.40 |
| 1:F:191:TYR:CD1 | 1:F:214:TRP:HB3 | 2.49 | 0.40 |
| 1:L:143:ASN:CA | 1:L:148:VAL:O | 2.69 | 0.40 |
| 1:L:115:LEU:HD13 | 1:L:296:GLU:HG3 | 2.03 | 0.40 |
| 1:A:12:ASP:O | 1:A:45:PHE:HA | 2.21 | 0.40 |
| 1:F:12:ASP:O | 1:F:45:PHE:HA | 2.20 | 0.40 |
| 1:C:12:ASP:O | 1:C:45:PHE:HA | 2.21 | 0.40 |
| 1:A:3:ILE:HG21 | 1:B:3:ILE:HD12 | 2.03 | 0.40 |
| 1:B:180:TYR:CE2 | 1:B:182:TYR:HB2 | 2.56 | 0.40 |
| 1:F:206:GLY:H | 1:F:284:GLU:CD | 2.24 | 0.40 |
| 1:J:340:PHE:CB | 1:K:11:VAL:HG21 | 2.52 | 0.40 |
| 1:D:235:ARG:HD3 | 1:D:235:ARG:HA | 1.79 | 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 | 338/340 (99%) | 311 (92%) | 26 (8%) | 1 (0%) | 46 | 83 |
| 1 | B | 338/340 (99%) | 312 (92%) | 25 (7%) | 1 (0%) | 46 | 83 |
| 1 | C | 338/340 (99%) | 311 (92%) | 25 (7%) | 2 (1%) | 30 | 74 |
| 1 | D | 338/340 (99%) | 312 (92%) | 25 (7%) | 1 (0%) | 46 | 83 |
| 1 | E | 338/340 (99%) | 312 (92%) | 25 (7%) | 1 (0%) | 46 | 83 |
| 1 | F | 338/340 (99%) | 311 (92%) | 25 (7%) | 2 (1%) | 30 | 74 |
| 1 | G | 338/340 (99%) | 311 (92%) | 26 (8%) | 1 (0%) | 46 | 83 |
| 1 | H | 338/340 (99%) | 311 (92%) | 26 (8%) | 1 (0%) | 46 | 83 |
| 1 | I | 338/340 (99%) | 311 (92%) | 25 (7%) | 2 (1%) | 30 | 74 |
| 1 | J | 338/340 (99%) | 310 (92%) | 27 (8%) | 1 (0%) | 46 | 83 |
| 1 | K | 338/340 (99%) | 313 (93%) | 24 (7%) | 1 (0%) | 46 | 83 |
| 1 | L | 338/340 (99%) | 311 (92%) | 26 (8%) | 1 (0%) | 46 | 83 |
| All | All | 4056/4080 (99%) | 3736 (92%) | 305 (8%) | 15 (0%) | 39 | 80 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 222 | ALA |
| 1 | I | 222 | ALA |
| 1 | L | 222 | ALA |
| 1 | A | 222 | ALA |
| 1 | B | 222 | ALA |
| 1 | C | 222 | ALA |
| 1 | E | 222 | ALA |
| 1 | F | 222 | ALA |
| 1 | G | 222 | ALA |
| 1 | H | 222 | ALA |
| 1 | J | 222 | ALA |
| 1 | K | 222 | ALA |
| 1 | C | 284 | GLU |
| 1 | F | 284 | GLU |
| 1 | I | 284 | GLU |

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 | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | B | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | C | 263/263 (100%) | 257 (98%) | 6 (2%) | 58 | 84 |
| 1 | D | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | E | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | F | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | G | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | H | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | I | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | J | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | K | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| 1 | L | 263/263 (100%) | 258 (98%) | 5 (2%) | 65 | 87 |
| All | All | 3156/3156 (100%) | 3095 (98%) | 61 (2%) | 65 | 87 |

All (61) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 104 | VAL |
| 1 | A | 170 | ASN |
| 1 | A | 218 | LEU |
| 1 | A | 253 | LYS |
| 1 | A | 279 | LYS |
| 1 | B | 104 | VAL |
| 1 | B | 170 | ASN |
| 1 | B | 218 | LEU |
| 1 | B | 253 | LYS |
| 1 | B | 279 | LYS |
| 1 | C | 27 | ASN |
| 1 | C | 104 | VAL |
| 1 | C | 170 | ASN |
| 1 | C | 218 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 253 | LYS |
| 1 | C | 279 | LYS |
| 1 | D | 104 | VAL |
| 1 | D | 170 | ASN |
| 1 | D | 218 | LEU |
| 1 | D | 253 | LYS |
| 1 | D | 279 | LYS |
| 1 | E | 104 | VAL |
| 1 | E | 170 | ASN |
| 1 | E | 218 | LEU |
| 1 | E | 253 | LYS |
| 1 | E | 279 | LYS |
| 1 | F | 104 | VAL |
| 1 | F | 170 | ASN |
| 1 | F | 218 | LEU |
| 1 | F | 253 | LYS |
| 1 | F | 279 | LYS |
| 1 | G | 104 | VAL |
| 1 | G | 170 | ASN |
| 1 | G | 218 | LEU |
| 1 | G | 253 | LYS |
| 1 | G | 279 | LYS |
| 1 | H | 104 | VAL |
| 1 | H | 170 | ASN |
| 1 | H | 218 | LEU |
| 1 | H | 253 | LYS |
| 1 | H | 279 | LYS |
| 1 | I | 104 | VAL |
| 1 | I | 170 | ASN |
| 1 | I | 218 | LEU |
| 1 | I | 253 | LYS |
| 1 | I | 279 | LYS |
| 1 | J | 104 | VAL |
| 1 | J | 170 | ASN |
| 1 | J | 218 | LEU |
| 1 | J | 253 | LYS |
| 1 | J | 279 | LYS |
| 1 | K | 104 | VAL |
| 1 | K | 170 | ASN |
| 1 | K | 218 | LEU |
| 1 | K | 253 | LYS |
| 1 | K | 279 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 104 | VAL |
| 1 | L | 170 | ASN |
| 1 | L | 218 | LEU |
| 1 | L | 253 | LYS |
| 1 | L | 279 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 35 | ASN |
| 1 | A | 60 | GLN |
| 1 | A | 223 | ASN |
| 1 | A | 255 | GLN |
| 1 | B | 35 | ASN |
| 1 | B | 60 | GLN |
| 1 | B | 223 | ASN |
| 1 | B | 255 | GLN |
| 1 | C | 35 | ASN |
| 1 | C | 60 | GLN |
| 1 | C | 223 | ASN |
| 1 | C | 255 | GLN |
| 1 | D | 35 | ASN |
| 1 | D | 60 | GLN |
| 1 | D | 223 | ASN |
| 1 | D | 255 | GLN |
| 1 | E | 35 | ASN |
| 1 | E | 60 | GLN |
| 1 | E | 223 | ASN |
| 1 | E | 255 | GLN |
| 1 | F | 35 | ASN |
| 1 | F | 60 | GLN |
| 1 | F | 223 | ASN |
| 1 | F | 255 | GLN |
| 1 | G | 35 | ASN |
| 1 | G | 60 | GLN |
| 1 | G | 223 | ASN |
| 1 | G | 255 | GLN |
| 1 | H | 35 | ASN |
| 1 | H | 60 | GLN |
| 1 | H | 223 | ASN |
| 1 | H | 255 | GLN |
| 1 | I | 27 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 35 | ASN |
| 1 | I | 60 | GLN |
| 1 | I | 223 | ASN |
| 1 | I | 255 | GLN |
| 1 | J | 35 | ASN |
| 1 | J | 60 | GLN |
| 1 | J | 223 | ASN |
| 1 | J | 255 | GLN |
| 1 | K | 27 | ASN |
| 1 | K | 35 | ASN |
| 1 | K | 60 | GLN |
| 1 | K | 223 | ASN |
| 1 | K | 255 | GLN |
| 1 | L | 35 | ASN |
| 1 | L | 60 | GLN |
| 1 | L | 223 | ASN |
| 1 | L | 255 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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 | 339/340 (99%) | 0.25 | 13 (3%) 44 30 | 76, 78, 80, 81 | 0 |
| 1 | B | 340/340 (100%) | 0.21 | 3 (0%) 85 74 | 76, 78, 80, 82 | 0 |
| 1 | C | 340/340 (100%) | 0.27 | 6 (1%) 71 56 | 76, 78, 80, 81 | 0 |
| 1 | D | 339/340 (99%) | 0.28 | 4 (1%) 81 67 | 76, 78, 80, 81 | 0 |
| 1 | E | 340/340 (100%) | 0.25 | 5 (1%) 76 62 | 76, 78, 80, 81 | 0 |
| 1 | F | 340/340 (100%) | 0.24 | 4 (1%) 81 67 | 76, 78, 80, 82 | 0 |
| 1 | G | 339/340 (99%) | 0.38 | 19 (5%) 28 18 | 76, 78, 80, 81 | 0 |
| 1 | H | 340/340 (100%) | 0.45 | 17 (5%) 32 21 | 76, 78, 80, 82 | 0 |
| 1 | I | 340/340 (100%) | 0.49 | 22 (6%) 22 13 | 76, 78, 80, 82 | 0 |
| 1 | J | 339/340 (99%) | 0.37 | 12 (3%) 48 32 | 76, 78, 80, 81 | 0 |
| 1 | K | 340/340 (100%) | 0.30 | 14 (4%) 41 27 | 76, 78, 80, 82 | 0 |
| 1 | L | 340/340 (100%) | 0.48 | 26 (7%) 17 10 | 76, 78, 80, 82 | 0 |
| All | All | 4076/4080 (99%) | 0.33 | 145 (3%) 46 32 | 76, 78, 80, 82 | 0 |

All (145) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | L | 229 | ALA | 4.5 |
| 1 | H | 1 | ALA | 3.7 |
| 1 | A | 230 | ASN | 3.5 |
| 1 | L | 218 | LEU | 3.5 |
| 1 | L | 230 | ASN | 3.4 |
| 1 | L | 288 | ASP | 3.4 |
| 1 | G | 7 | ASP | 3.4 |
| 1 | L | 319 | ASP | 3.3 |
| 1 | I | 216 | THR | 3.3 |
| 1 | L | 253 | LYS | 3.2 |
| 1 | H | 94 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | J | 256 | ASP | 3.1 |
| 1 | C | 92 | ASP | 3.1 |
| 1 | K | 243 | LYS | 3.0 |
| 1 | H | 8 | GLY | 3.0 |
| 1 | I | 59 | GLY | 3.0 |
| 1 | L | 93 | VAL | 3.0 |
| 1 | J | 340 | PHE | 2.9 |
| 1 | J | 248 | SER | 2.9 |
| 1 | E | 275 | TYR | 2.9 |
| 1 | K | 1 | ALA | 2.9 |
| 1 | I | 250 | PHE | 2.9 |
| 1 | K | 317 | GLN | 2.9 |
| 1 | H | 321 | ASP | 2.9 |
| 1 | H | 229 | ALA | 2.8 |
| 1 | H | 2 | GLU | 2.8 |
| 1 | H | 320 | SER | 2.8 |
| 1 | G | 242 | ASN | 2.7 |
| 1 | G | 321 | ASP | 2.7 |
| 1 | A | 277 | LYS | 2.7 |
| 1 | A | 94 | GLY | 2.7 |
| 1 | L | 54 | ASP | 2.7 |
| 1 | I | 249 | GLY | 2.6 |
| 1 | L | 290 | ASP | 2.6 |
| 1 | J | 243 | LYS | 2.6 |
| 1 | F | 220 | TYR | 2.6 |
| 1 | L | 186 | GLY | 2.6 |
| 1 | I | 220 | TYR | 2.6 |
| 1 | K | 93 | VAL | 2.6 |
| 1 | D | 180 | TYR | 2.6 |
| 1 | K | 244 | PHE | 2.6 |
| 1 | G | 149 | ASP | 2.6 |
| 1 | A | 229 | ALA | 2.5 |
| 1 | L | 56 | THR | 2.5 |
| 1 | L | 287 | GLY | 2.5 |
| 1 | H | 244 | PHE | 2.5 |
| 1 | B | 288 | ASP | 2.5 |
| 1 | I | 306 | ASN | 2.5 |
| 1 | C | 279 | LYS | 2.5 |
| 1 | A | 276 | THR | 2.5 |
| 1 | I | 89 | LYS | 2.5 |
| 1 | A | 92 | ASP | 2.5 |
| 1 | E | 290 | ASP | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | I | 230 | ASN | 2.5 |
| 1 | I | 248 | SER | 2.5 |
| 1 | A | 216 | THR | 2.4 |
| 1 | E | 243 | LYS | 2.4 |
| 1 | L | 180 | TYR | 2.4 |
| 1 | L | 282 | ASP | 2.4 |
| 1 | I | 286 | ILE | 2.4 |
| 1 | G | 1 | ALA | 2.4 |
| 1 | J | 217 | GLY | 2.4 |
| 1 | G | 10 | LYS | 2.4 |
| 1 | B | 290 | ASP | 2.4 |
| 1 | I | 47 | GLY | 2.4 |
| 1 | J | 288 | ASP | 2.4 |
| 1 | K | 323 | LYS | 2.3 |
| 1 | L | 89 | LYS | 2.3 |
| 1 | K | 303 | PHE | 2.3 |
| 1 | H | 183 | GLU | 2.3 |
| 1 | H | 10 | LYS | 2.3 |
| 1 | I | 10 | LYS | 2.3 |
| 1 | I | 8 | GLY | 2.3 |
| 1 | L | 286 | ILE | 2.3 |
| 1 | H | 216 | THR | 2.3 |
| 1 | H | 271 | PRO | 2.3 |
| 1 | I | 262 | GLN | 2.3 |
| 1 | L | 92 | ASP | 2.3 |
| 1 | F | 221 | ASP | 2.3 |
| 1 | K | 188 | VAL | 2.3 |
| 1 | I | 1 | ALA | 2.3 |
| 1 | I | 48 | GLU | 2.3 |
| 1 | L | 256 | ASP | 2.3 |
| 1 | A | 144 | PHE | 2.3 |
| 1 | A | 275 | TYR | 2.3 |
| 1 | I | 49 | THR | 2.3 |
| 1 | G | 223 | ASN | 2.3 |
| 1 | G | 109 | LEU | 2.3 |
| 1 | I | 290 | ASP | 2.3 |
| 1 | B | 280 | ALA | 2.3 |
| 1 | I | 218 | LEU | 2.3 |
| 1 | J | 290 | ASP | 2.3 |
| 1 | K | 301 | TYR | 2.3 |
| 1 | I | 187 | ILE | 2.2 |
| 1 | C | 320 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | H | 53 | SER | 2.2 |
| 1 | J | 250 | PHE | 2.2 |
| 1 | D | 215 | ALA | 2.2 |
| 1 | K | 187 | ILE | 2.2 |
| 1 | F | 222 | ALA | 2.2 |
| 1 | H | 218 | LEU | 2.2 |
| 1 | K | 268 | GLY | 2.2 |
| 1 | G | 107 | ASP | 2.2 |
| 1 | C | 276 | THR | 2.2 |
| 1 | H | 298 | GLY | 2.2 |
| 1 | L | 280 | ALA | 2.2 |
| 1 | G | 140 | ARG | 2.2 |
| 1 | J | 181 | GLU | 2.2 |
| 1 | J | 230 | ASN | 2.2 |
| 1 | K | 304 | ASN | 2.2 |
| 1 | L | 324 | LEU | 2.2 |
| 1 | E | 250 | PHE | 2.2 |
| 1 | A | 93 | VAL | 2.1 |
| 1 | K | 286 | ILE | 2.1 |
| 1 | J | 242 | ASN | 2.1 |
| 1 | H | 59 | GLY | 2.1 |
| 1 | L | 233 | GLU | 2.1 |
| 1 | L | 321 | ASP | 2.1 |
| 1 | J | 186 | GLY | 2.1 |
| 1 | A | 108 | ALA | 2.1 |
| 1 | L | 187 | ILE | 2.1 |
| 1 | G | 241 | THR | 2.1 |
| 1 | G | 186 | GLY | 2.1 |
| 1 | G | 225 | ILE | 2.1 |
| 1 | G | 287 | GLY | 2.1 |
| 1 | I | 340 | PHE | 2.1 |
| 1 | C | 54 | ASP | 2.1 |
| 1 | F | 274 | ALA | 2.1 |
| 1 | K | 92 | ASP | 2.1 |
| 1 | D | 108 | ALA | 2.1 |
| 1 | E | 236 | ASN | 2.1 |
| 1 | H | 220 | TYR | 2.1 |
| 1 | C | 299 | ALA | 2.1 |
| 1 | L | 217 | GLY | 2.1 |
| 1 | G | 243 | LYS | 2.0 |
| 1 | I | 157 | TYR | 2.0 |
| 1 | L | 57 | GLY | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 218 | LEU | 2.0 |
| 1 | A | 321 | ASP | 2.0 |
| 1 | L | 7 | ASP | 2.0 |
| 1 | G | 44 | GLY | 2.0 |
| 1 | G | 248 | SER | 2.0 |
| 1 | G | 282 | ASP | 2.0 |
| 1 | A | 232 | GLY | 2.0 |
| 1 | G | 29 | GLU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.